Direct Sampling

PUBH 8442: Bayes Decision Theory and Data Analysis

Eric F. Lock
UMN Division of Biostatistics, SPH
elock@umn.edu

03/20/2024

Simulating from pdf or pmf

- ▶ In statistics it is common to encounter integrals that are difficult to solve analytically.
 - Computing expected values or variances
 - ▶ Computing the normalizing constant for marginal distributions
 - Finding probabilities when the cdf is unknown

- ▶ Encounter these issues often in Bayesian statistics....
- ▶ Monte Carlo simulation, in which observations are randomly generated from the model, is helpful to overcome this.

Direct Monte Carlo integration: expected value

- ▶ Assume $\theta \sim p(\theta)$, and consider the functional form $g(\theta)$
 - ightharpoonup e.g., p may be a posterior distribution $p(\theta \mid \mathbf{y})$
- ▶ Assume we can generate samples $\theta_1, \ldots, \theta_N \stackrel{\textit{iid}}{\sim} p(\theta)$
 - ▶ Using R (and other software) it is easy to generate from known distributions such as the Beta, Binomial, Poisson, Normal, or Gamma.
- Then, by the Law of Large Numbers,

$$\int g(\theta)p(\theta)\,d\theta = Eg(\theta) \approx \frac{1}{N}\sum_{j=1}^{N}g(\theta_{j})$$

for large N

Direct Monte Carlo integration: standard error

- $\blacktriangleright \text{ Let } \hat{\gamma} = \frac{1}{N} \sum_{j=1}^{N} g(\theta_j).$
- ▶ The variance of $g(\theta)$ under p can be approximated similarly:

$$\mathsf{Var}(g(heta)) pprox rac{1}{\mathsf{N}-1} \sum_{j=1}^{\mathsf{N}} [g(heta_j) - \hat{\gamma}]^2$$

• We can derive the standard error for $\hat{\gamma}$ using $Var(\hat{\gamma}) = Var(g(\theta))/N$:

$$\hat{se}(\hat{\gamma}) = \sqrt{rac{1}{N(N-1)}\sum_{j=1}^{N}[g(heta_j)-\hat{\gamma}]^2}.$$

- ▶ This does NOT represent uncertainty of $g(\theta)$ implied by p
- ▶ It represents simulation uncertainty in our estimate for $Eg(\theta)$
- \triangleright Converges to 0 as we increase number of simulations N
- ▶ By Central Limit Theorem, $\hat{\gamma} \sim N(E(g(\theta)), \hat{se}(\hat{\gamma})^2)$ for large N

Direct Monte Carlo integration

- ▶ Consider $g(\theta) = \mathbb{1}_{a < c(\theta) < b}$ for some function $c(\theta)$
- ▶ Then, $Eg(\theta) = P(a < c(\theta) < b)$
- ▶ We can estimate this probability under simulation:

$$\hat{p} = \frac{\text{number of } c(\theta_j)s \in (a, b)}{N}$$

and our standard error for this estimate is $\sqrt{\hat{p}(1-\hat{p})/N}$.

▶ Implication: a histogram of the $c(\theta_j)s$ approximates the density for $c(\theta)$.

- ➤ An eye patient is asked to identify shapes from a given distance
- ▶ She is shown n = 20 shapes
- Jeffreys beta-binomial model for number of shapes she identifies correctly:

$$y \sim \text{Binomial}(20, \theta),$$

 $\theta \sim \text{Beta}(0.5, 0.5).$

- Assume she identifies 16 shapes correctly.
 - $\rho(\theta \mid y) = \text{Beta}(16.5, 4.5)$

- ▶ Consider the logit transformation $g(\theta) = \log\left(\frac{\theta}{1-\theta}\right)$.
- ▶ Approximate distribution of $g(\theta)$ induced by beta posterior.
- ▶ For j = 1, ..., N:
 - ▶ Simulate θ_j from Beta(16.5, 4.5)
 - ▶ Compute $g(\theta_j) = \log\left(\frac{\theta_j}{1-\theta_j}\right)$
- ▶ Consider distribution of $g(\theta_j)s$ for N=10000 sims

The estimated posterior expected value is

$$\frac{1}{10000} \sum_{j=1}^{N} g(\theta_j) = 1.386$$

• The estimated posterior variance is

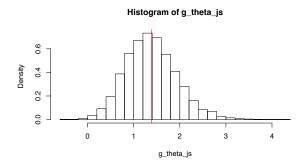
$$\frac{1}{N-1} \sum_{j=1}^{N} [g(\theta_j) - \hat{\gamma}]^2 = 0.310$$

• The standard error for our estimate of $Eg(\theta)$ is

$$\sqrt{0.310/10000} = 0.006$$

• Approximate 95% confidence interval: $1.386 \pm 2 \cdot 0.006$

• Estimated density of $g(\theta)$:



http://www.ericfrazerlock.com/Direct_Sampling_Rcode1.r

Direct sampling: multivariate density

- $\blacktriangleright \text{ Let } \theta = (\theta_1, \dots, \theta_k).$
- Note that

$$p(\theta_1,\ldots,\theta_k)=\prod_{i=1}^k p(\theta_i\mid\theta_{i-1},\ldots,\theta_1)$$

- ▶ We can draw direct samples $\tilde{\theta}$ from $p(\theta_1, \dots, \theta_k)$ as follows:
 - ▶ Draw $\tilde{\theta}_1$ from $p(\theta_1)$,
 - ▶ Draw $\tilde{\theta}_2$ from $p(\theta_2 \mid \tilde{\theta}_1)$,
 - \blacktriangleright ..., draw $\tilde{\theta_k}$ from $p(\theta_k \mid \tilde{\theta}_{k-1}, \dots, \tilde{\theta}_1)$.
- Useful for simulating difficult marginal densities
 - ▶ $p(\theta_1)$ and $p(\theta_2 \mid \theta_1)$ may be easy to obtain, but not $p(\theta_2)$
 - ▶ Here $\tilde{\theta}_2$ is a draw from $p(\theta_2)$.

- ▶ Recall: % body fat (*BF*%) measured for 100 adult males.
- ► Also measured 9 predictor variables
 - ▶ Age, Weight, Height; circumference of neck, chest, abdomen, ankle, bicep, and wrist.
- Consider the model

$$\mathbf{y} = \boldsymbol{\beta} X + \boldsymbol{\epsilon}$$

where

- ▶ **y** is population-centered *BF*%
- ▶ X is the standardized matrix of predictor variables

▶ Used iid normal prior for $\beta_i's$:

$$\beta \sim \text{Normal}(0, 0.62\sigma^2 I)$$

with $\hat{\tau}^2 = 0.62$ estimated empirically.

- ▶ IG(3,20) prior for σ^2
- Gives the conditional posterior

$$p(\beta \mid \mathbf{y}, \sigma^2) = \text{Normal}\left(\tilde{\beta}, \sigma^2 V_{\beta}\right)$$

where
$$\tilde{\beta} = (X^TX + \frac{1}{0.62})^{-1}(X^T\mathbf{y})$$
 and $V_{\beta} = (X^TX + \frac{1}{0.62})^{-1}$

▶ The marginal posterior for σ^2 is

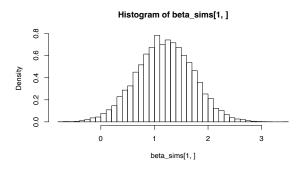
$$p(\sigma^2 \mid \mathbf{y}) = IG(a_n, b_n)$$

where
$$a_n = 3 + \frac{100}{2}$$
 and $b_n = 20 + \frac{1}{2} [\mathbf{y}^T \mathbf{y} - \tilde{\beta}^T (X^T X + \frac{1}{0.62} I)^{-1} \tilde{\beta}]$

- ▶ Direct sampling scheme:
 - ▶ For samples j = 1, ..., N = 10000:
 - ▶ Draw σ_j from $p(\sigma^2 \mid \mathbf{y})$
 - ▶ Draw β_j from $p(\beta \mid \mathbf{y}, \sigma_j^2)$

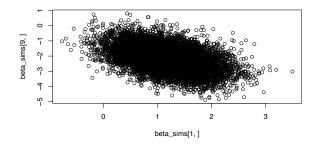
http://www.ericfrazerlock.com/More_on_Direct_ Sampling_Rcode1.r

• Simulated marginal posterior of *Age* coefficient β_1 :



- 95% credible interval from simulations: (0.152, 2.220)
- 95% credible interval from t-dist: (0.157, 2.229)

• Scatterplot of simulated coefficients for $Age \beta_1$ and $Wrist \beta_2$:



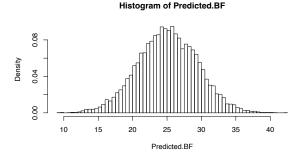
http:

//www.ericfrazerlock.com/More_on_Direct_Sampling_Rcode1.r

- Assume an individual has the following standardized measurements:
 - ▶ Age: 1.20, Weight:0.5, Height:-0.4; circumference of neck:2.2, chest:0.3, abdomen:0.8, ankle:0.2, bicep:0.3, and wrist:0.6.

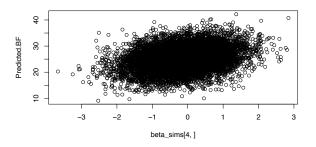
- Denote his vector of predictors as x₁₀₁
- ▶ Simulate from the posterior predictive for y_{101} :
 - ▶ Draw σ_j , β_j as before
 - ▶ Draw $y_{101,j}$ from Normal($\mathbf{x}_{101}\beta_j, \sigma_j$)

• Histogram of predicted body fat % for individual 101:



http: //www.ericfrazerlock.com/More_on_Direct_Sampling_Rcode1.r

• Scatterplot of simulated predicted body fat for individual 101, and *Neck* coefficient β_4 :



http:

//www.ericfrazerlock.com/More_on_Direct_Sampling_Rcode1.r