

# Direct Sampling

PUBH 8442: Bayes Decision Theory and Data Analysis

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

03/22/2021

# 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  $g(\theta)$ 
  - ▶ e.g.,  $p$  may be a posterior distribution  $p(\theta | \mathbf{y})$
- ▶ Assume we can generate samples  $\theta_1, \dots, \theta_N \stackrel{iid}{\sim} p(\theta)$ 
  - ▶ 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

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

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

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

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

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

# Direct Monte Carlo integration

- ▶ Consider  $g(\theta) = \mathbb{1}_{a < c(\theta) < b}$  for some function  $c(\theta)$

- ▶ Then,  $Eg(\theta) = P(a < c(\theta) < b) \approx \frac{1}{N} \sum_{i=1}^N g(\theta_i)$

- ▶ 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  $c(\theta)$ .

## Example: Eye exam

- ▶ 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.
  - ▶  $p(\theta | y) = \text{Beta}(16.5, 4.5)$

## Example: Eye exam

- ▶ Consider the logit transformation  $g(\theta) = \log\left(\frac{\theta}{1-\theta}\right)$ .
- ▶ Approximate distribution of  $g(\theta)$  induced by beta posterior.
- ▶ For  $j = 1, \dots, N$ :
  - ▶ Simulate  $\theta_j$  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

## Example: Eye exam

- 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

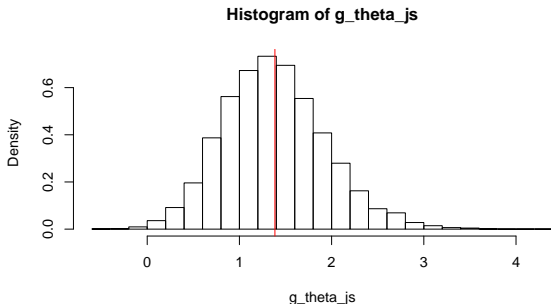
$$\sqrt{0.310/10000} = 0.006$$

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



# Example: Eye exam

- Estimated density of  $g(\theta)$ :



[http://www.ericfrazerlock.com/Direct\\_Sampling\\_Rcode1.r](http://www.ericfrazerlock.com/Direct_Sampling_Rcode1.r)

# Direct sampling: multivariate density

- ▶ Let  $\theta = (\theta_1, \dots, \theta_k)$ .  $p(\theta_1, \theta_2) = p(\theta_2 | \theta_1) p(\theta_1)$
- ▶ Note that

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

$\nearrow (\tilde{\theta}_1, \dots, \tilde{\theta}_k)$

- ▶ 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  $p(\theta_2 | \tilde{\theta}_1)$ ,
  - ▶ ..., draw  $\tilde{\theta}_k$  from  $p(\theta_k | \tilde{\theta}_{k-1}, \dots, \tilde{\theta}_1)$ .
- ▶ Useful for simulating difficult marginal densities
  - ▶  $p(\theta_1)$  and  $p(\theta_2 | \theta_1)$  may be easy to obtain, but not  $p(\theta_2)$
  - ▶ Here  $\tilde{\theta}_2$  is a draw from  $p(\theta_2)$ .

## Example: Body Fat (cont.)

- ▶ 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

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

where

- ▶  $\mathbf{y}$  is population-centered  $BF\%$
- ▶  $\mathbf{X}$  is the standardized matrix of predictor variables

## Example: Body Fat (cont.)

- ▶ 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  $\sigma^2$
- ▶ Gives the conditional posterior

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

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

and  $V_\beta = (X^T X + \frac{1}{0.62})^{-1}$

## Example: Body Fat (cont.)

- ▶ The marginal posterior for  $\sigma^2$  is

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

where  $a_n = 3 + \frac{100}{2}$  and

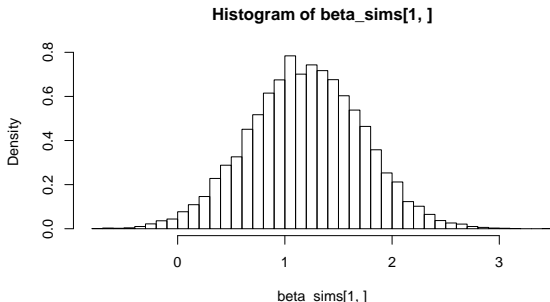
$$b_n = 20 + \frac{1}{2}[\mathbf{y}^T \mathbf{y} - \tilde{\beta}^T (X^T X + \frac{1}{0.62} I)^{-1} \tilde{\beta}]$$

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

[http://www.ericfrazerlock.com/More\\_on\\_Direct\\_Sampling\\_Rcode1.r](http://www.ericfrazerlock.com/More_on_Direct_Sampling_Rcode1.r)

## Example: Body Fat (cont.)

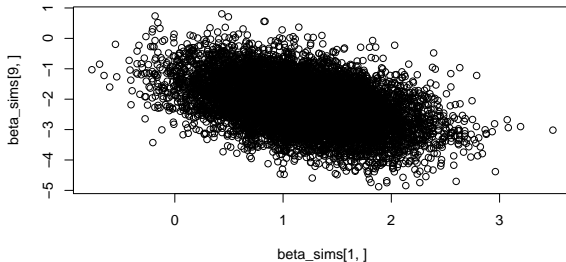
- Simulated marginal posterior of Age coefficient  $\beta_1$ :



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

## Example: Body Fat (cont.)

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



[http:](http://www.ericfrazierlock.com/More_on_Direct_Sampling_Rcode1.r)

[//www.ericfrazierlock.com/More\\_on\\_Direct\\_Sampling\\_Rcode1.r](http://www.ericfrazierlock.com/More_on_Direct_Sampling_Rcode1.r)

## Example: Body Fat (cont.)

- ▶ 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  $\mathbf{x}_{101}$
- ▶ Simulate from the posterior predictive for  $y_{101}$ :

- ▶ Draw  $\sigma_j, \beta_j$  as before

$$P(y_{101} | \vec{y}, X_{101})$$

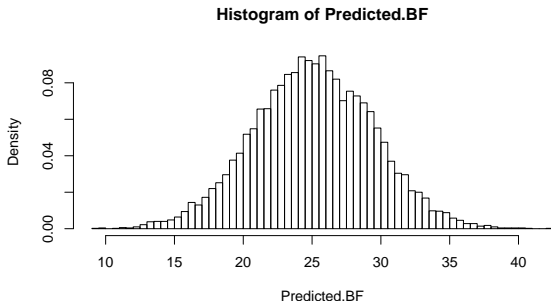
- ▶ Draw  $y_{101,j}$  from  $\text{Normal}(\mathbf{x}_{101}\beta_j, \sigma_j)$

$$P(y_{101}, \sigma^2, \beta | \vec{y}) = P(\sigma^2 | \vec{y}) \cdot P(\beta | \sigma^2, \vec{y}) \cdot P(y_{101} | \sigma^2, \beta)$$



# Example: Body Fat (cont.)

- Histogram of predicted body fat % for individual 101:

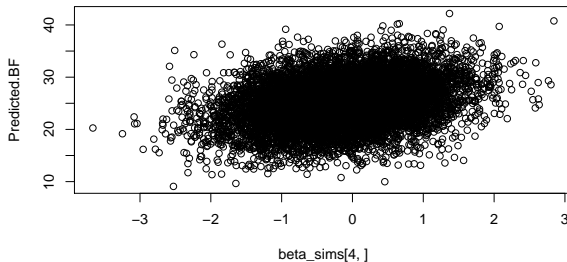


[http:](http://www.ericfrazierlock.com/More_on_Direct_Sampling_Rcode1.r)

[//www.ericfrazierlock.com/More\\_on\\_Direct\\_Sampling\\_Rcode1.r](http://www.ericfrazierlock.com/More_on_Direct_Sampling_Rcode1.r)

## Example: Body Fat (cont.)

- Scatterplot of simulated predicted body fat for individual 101, and *Neck* coefficient  $\beta_4$ :



[http:](http://www.ericfrazierlock.com/More_on_Direct_Sampling_Rcode1.r)

[//www.ericfrazierlock.com/More\\_on\\_Direct\\_Sampling\\_Rcode1.r](http://www.ericfrazierlock.com/More_on_Direct_Sampling_Rcode1.r)