

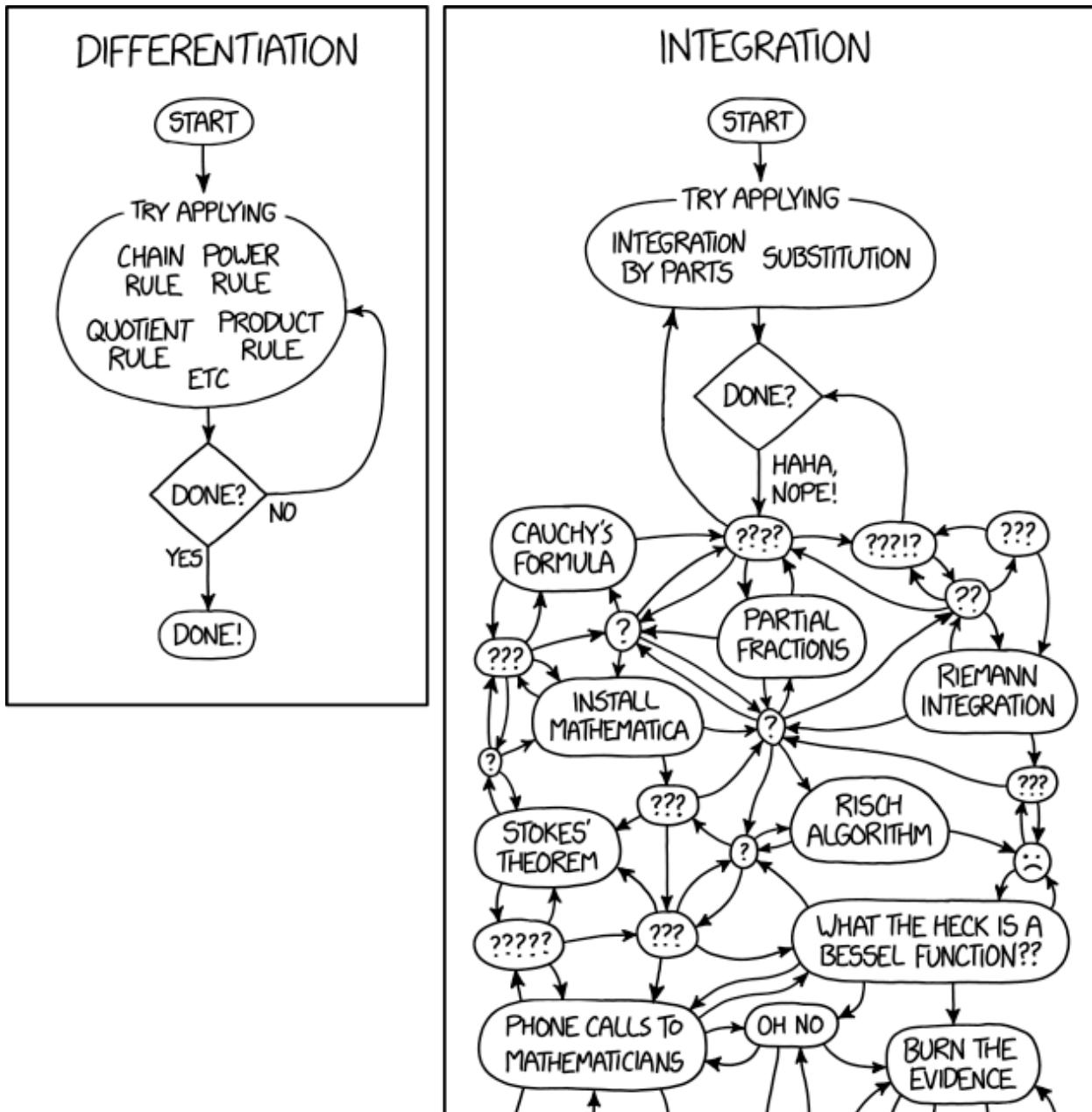
What I've  
been calling Ch. 5.

# Chapter 6: Monte Carlo Integration

Ch. 3.

Monte Carlo integration is a statistical method based on random sampling in order to approximate integrals. This section could alternatively be titled,

“Integrals are hard, how can we avoid doing them?”



# 1 A Tale of Two Approaches

Consider a one-dimensional integral.

$$\int_a^b f(x) dx$$

"integrand"

The value of the integral can be derived analytically only for a few functions,  $f$ . For the rest, numerical approximations are often useful.

Why is integration important to statistics?

*Many quantities of interest in inferential statistics can be expressed as the expectation of a function of a r.v.*

$$E g(x) = \int g(x) f(x) dx.$$

## 1.1 Numerical Integration

**Idea:** Approximate  $\int_a^b f(x) dx$  via the sum of many polygons under the curve  $f(x)$ .

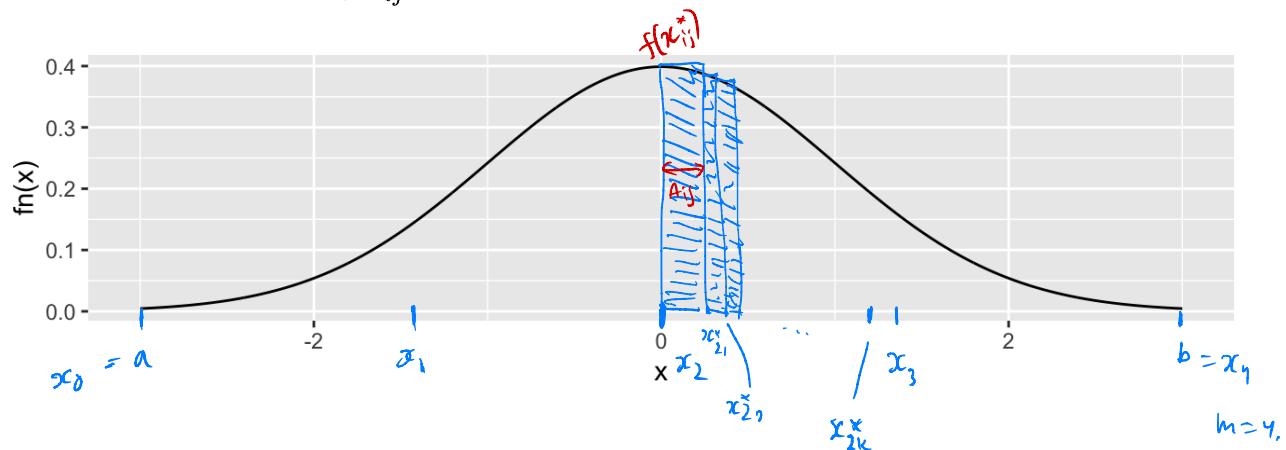
To do this, we could partition the interval  $[a, b]$  into  $m$  subintervals  $[x_i, x_{i+1}]$  for  $i = 0, \dots, m-1$  with  $x_0 = a$  and  $x_m = b$ .

Within each interval, insert  $k + 1$  nodes, so for  $[x_i, x_{i+1}]$  let  $x_{ij}^*$  for  $j = 0, \dots, k$ , then

$$\int_a^b f(x) dx = \sum_{i=0}^{m-1} \int_{x_i}^{x_{i+1}} f(x) dx \approx \sum_{i=0}^{m-1} \sum_{j=0}^k A_{ij} f(x_{ij}^*)$$

↑      ↑  
 width   height

for some set of constants,  $A_{ij}$ .



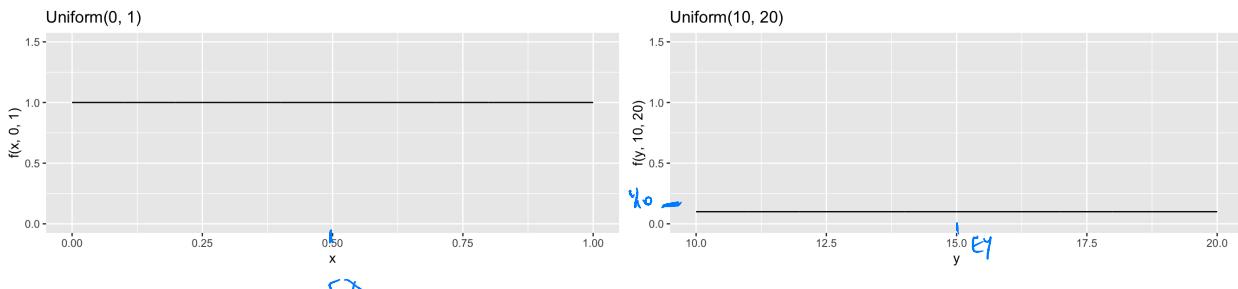
## 1.2 Monte Carlo Integration

How do we compute the mean of a distribution?

**Example 1.1** Let  $X \sim \text{Unif}(0, 1)$  and  $Y \sim \text{Unif}(10, 20)$ .

```
x <- seq(0, 1, length.out = 1000)
f <- function(x, a, b) 1/(b - a)
ggplot() +
  geom_line(aes(x, f(x, 0, 1))) +
  ylim(c(0, 1.5)) +
  ggtitle("Uniform(0, 1)")

y <- seq(10, 20, length.out = 1000)
ggplot() +
  geom_line(aes(y, f(y, 10, 20))) +
  ylim(c(0, 1.5)) +
  ggtitle("Uniform(10, 20)")
```



Theory

$$\begin{aligned} E(X) &= \int_0^1 x f(x) dx \\ &= \int_0^1 x \cdot 1 dx \\ &= \left[ \frac{x^2}{2} \right]_0^1 = \frac{1}{2} \end{aligned}$$

$$\begin{aligned} E(Y) &= \int_{10}^{20} y f(y) dy \\ &= \int_{10}^{20} y \cdot \frac{1}{10} dy \\ &= \frac{1}{10} \left[ \frac{y^2}{2} \right]_{10}^{20} = 15. \end{aligned}$$

How about a func that looks like  
??

Probably can't do this in closed form.  
need to approximate.

### 1.2.1 Notation

$\theta$  = parameter (unknown).

$\hat{\theta}$  = estimator of  $\theta$ , statistic (sometimes we write  $\bar{X}$ ,  $S^2$ , etc. instead of  $\hat{\theta}$ ).

Distribution of  $\hat{\theta}$  = sampling distribution

$E[\hat{\theta}]$  = on average, what's the value of  $\hat{\theta}$ ?  
theoretical mean of the distribution of  $\hat{\theta}$  (sampling dsn).

$Var(\hat{\theta})$  = theoretical variance of  $\hat{\theta}$   
variance of the sampling dsn of  $\hat{\theta}$ .

- $\hat{E}[\hat{\theta}]$  = estimated mean of dsn of  $\hat{\theta}$
  - $\hat{Var}(\hat{\theta})$  = estimated variance of dsn of  $\hat{\theta}$ .
  - $se(\hat{\theta}) = \sqrt{Var(\hat{\theta})}$  = theoretical se. of  $\hat{\theta}$  = sd of sampling dsn of  $\hat{\theta}$ .
  - $\hat{se}(\hat{\theta}) = \sqrt{\hat{Var}(\hat{\theta})}$  = estimated se of  $\hat{\theta}$  = estimated sd of sampling dsn of  $\hat{\theta}$ .
- estimated versions of theoretical quantities

### 1.2.2 Monte Carlo Simulation

What is Monte Carlo simulation?

Computer simulation that generates a large number of samples from a distribution. The distribution characterizes the population from which the sample is drawn.

(Sounds a lot like Ch. 3).

### 1.2.3 Monte Carlo Integration

parameter  
characterizes  
a population.  
thing we care  
about  $\theta$  want  
to estimate.

To approximate  $\theta = E[X] = \int xf(x)dx$ , we can obtain an iid random sample  $X_1, \dots, X_n$  from  $f$  and then approximate  $\theta$  via the sample average  $\hat{\theta}$

$$\hat{\theta} = \frac{1}{m} \sum_{i=1}^m X_i \approx EX$$

**Example 1.2** Again, let  $X \sim Unif(0, 1)$  and  $Y \sim Unif(10, 20)$ . To estimate  $E[X]$  and  $E[Y]$  using a Monte Carlo approach,

① draw  $X_1, \dots, X_m \sim Unif(0, 1)$ .

② Compute  $\hat{\theta} = \frac{1}{m} \sum_{i=1}^m X_i$

① draw  $Y_1, \dots, Y_m \sim Unif(10, 20)$

② Compute  $\hat{\theta} = \frac{1}{m} \sum_{i=1}^m Y_i$

This is useful when we can't compute the  $EX$  in closed form. Also useful for approximating other integrals.

Now consider  $E[g(X)]$ .

$$\theta = E[g(X)] = \int_{-\infty}^{\infty} g(x)f(x)dx.$$

The Monte Carlo approximation of  $\theta$  could then be obtained by

1. Draw  $X_1, \dots, X_m \sim f$

2. Compute  $\hat{\theta} = \frac{1}{m} \sum_{i=1}^m g(X_i)$

**Definition 1.1** Monte Carlo integration is the statistical estimation of the value of an integral using evaluations of an integrand at a set of points drawn randomly from a distribution with support over the range of integration.

### Example 1.3

(A) Parameter estimation! Linear models vs. generalized linear models.  
 $y = x\beta + \varepsilon$ ,  $\varepsilon \sim N(0, \sigma^2)$ ,  $\hat{\beta} = (X^T X)^{-1} X^T Y$  closed form solution.

GLM:  $Y \sim \text{Binom}(p)$   
 $\text{logit}(p) = \beta_0 + \beta_1 x \rightarrow$  no estimates for  $\beta_0$  and  $\beta_1$  in closed form.

(B) estimate quantities of a distn. Find  $y$  s.t.  $0.9 = \int_{-\infty}^y f(x) dx$ .

Why the mean?

Let  $E[g(X)] = \theta$ , then

$$E(\hat{\theta}) = E\left(\frac{1}{m} \sum_{i=1}^m g(X_i)\right) = \frac{1}{m} \sum_{i=1}^m E[g(X_i)] \stackrel{\substack{\text{drew } X_i \text{ iid from } f \\ m \text{ times}}}{=} \frac{1}{m} \sum_{i=1}^m \underbrace{E[g(X)]}_{\theta} = \frac{1}{m} [\theta + \theta + \dots + \theta] = \theta.$$

So  $\hat{\theta}$  is unbiased.

and, by the strong law of large numbers,

$$\hat{\theta} = \frac{1}{m} \sum_{i=1}^m g(X_i) \xrightarrow{P} E(g(X)) = \theta$$

So  $\hat{\theta}$  is consistent.

**Example 1.4** Let  $v(x) = (g(x) - \theta)^2$ , where  $\theta = E[g(X)]$ , and assume  $g(X)^2$  has finite expectation under  $f$ . Then

$$Var(g(X)) = E[(g(X) - \theta)^2]$$

$$Var(g(X)) = E[(g(X) - \theta)^2] = E[v(X)].$$

We can estimate this using a Monte Carlo approach.

$$\hat{Var}(g(X)) = \hat{E}[v(X)]$$

(1) Sample  $X_1, \dots, X_m$  from  $f$ .

(2) Compute  $\frac{1}{m} \sum_{i=1}^m (g(X_i) - \theta)^2$

Approximate! We don't know this.

we can replace it with  $\hat{\theta} = \frac{1}{m} \sum_{i=1}^m g(X_i)$ .

To estimate,

$$\hat{Var}(\hat{\theta}) = \frac{1}{m} \cdot \hat{Var} g(X).$$

When  $\text{Var } g(x)$  exists and is finite, the CLT states.

$$\frac{\hat{\theta} - E\hat{\theta}}{\sqrt{\text{Var } \hat{\theta}}} \xrightarrow{d} N(0, 1) \text{ as } m \rightarrow \infty.$$

$\sqrt{\text{Var } \hat{\theta}} = \frac{\sqrt{\text{Var } g(x)}}{\sqrt{m}}$

Hence, if  $m$  is large,

$$\hat{\theta} \stackrel{\text{"approximately distributed"}}{\sim} N(\theta, \frac{\text{Var } g(x)}{m})$$

can use  
 $\hat{\theta}$   
as a plugin.

We can use this to put confidence limits or error bounds on the MC estimate of the integral  $\theta_0$ .

We can do inference on the integral  $\theta$ !

Monte Carlo integration provides slow convergence, i.e. even though by the SLLN we know we have convergence, it may take us a while to get there.

But, Monte Carlo integration is a **very** powerful tool. While numerical integration methods are difficult to extend to multiple dimensions and work best with a smooth integrand, Monte Carlo does not suffer these weaknesses.

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#### 1.2.4 Algorithm

The approach to finding a Monte Carlo estimator for  $\int g(x)f(x)dx$  is as follows.

- 1.
- 2.
- 3.
- 4.

**Example 1.5** Estimate  $\theta = \int_0^1 h(x)dx$ .

**Example 1.6** Estimate  $\theta = \int_a^b h(x)dx$ .

Another approach:

**Example 1.7** Monte Carlo integration for the standard Normal cdf. Let  $X \sim N(0, 1)$ , then the pdf of  $X$  is

$$\phi(x) = f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right), \quad -\infty < x < \infty$$

and the cdf of  $X$  is

$$\Phi(x) = F(x) = \int_{-\infty}^x \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) dt.$$

We will look at 3 methods to estimate  $\Phi(x)$  for  $x > 0$ .



### 1.2.5 Inference for MC Estimators

The Central Limit Theorem implies

So, we can construct confidence intervals for our estimator

1.

2.

But we need to estimate  $Var(\hat{\theta})$ .

So, if  $m \uparrow$  then  $Var(\hat{\theta}) \downarrow$ . How much does changing  $m$  matter?

**Example 1.8** If the current  $se(\hat{\theta}) = 0.01$  based on  $m$  samples, how many more samples do we need to get  $se(\hat{\theta}) = 0.0001$ ?

Is there a better way to decrease the variance? **Yes!**