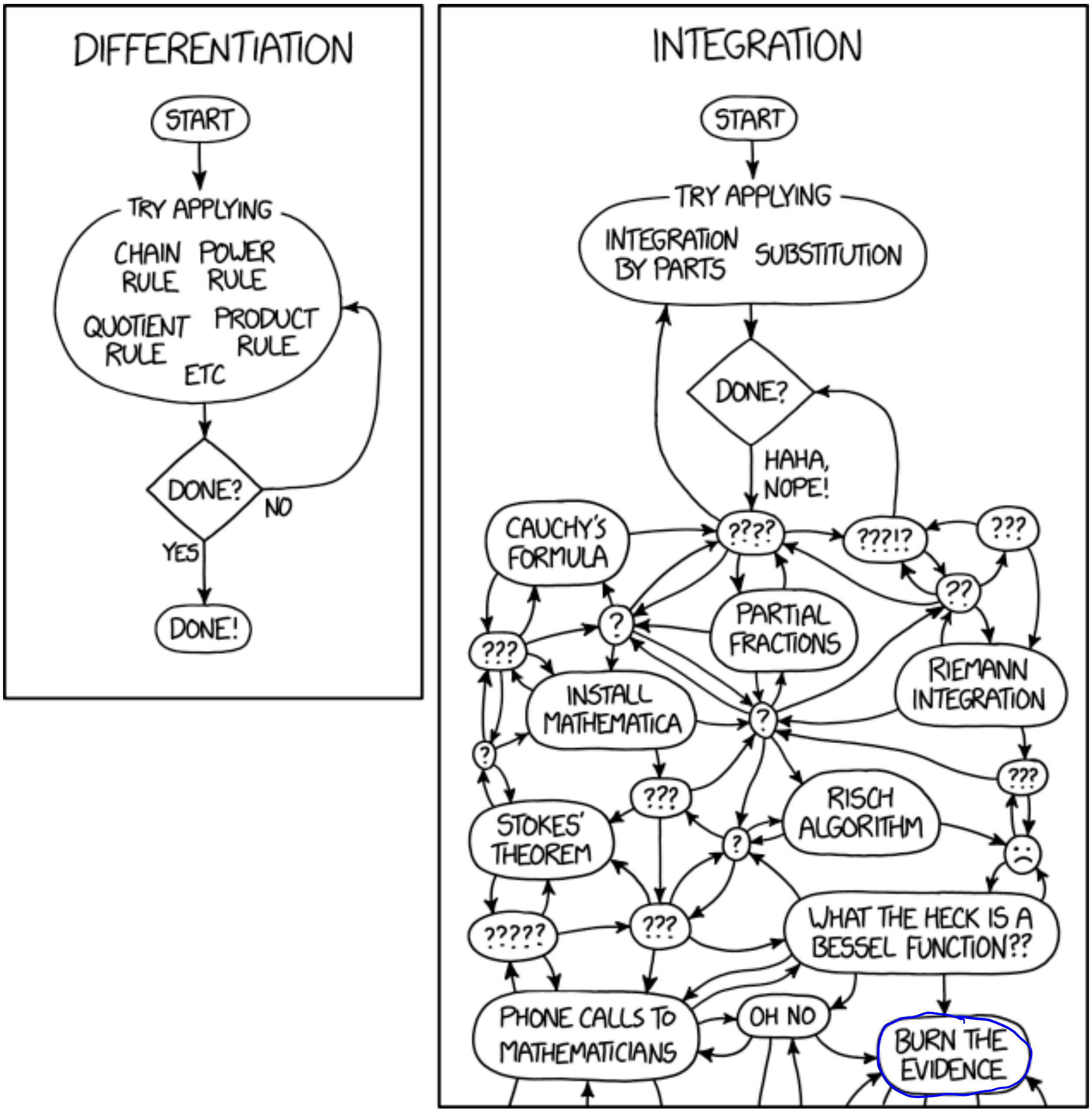
Chapter 6: Monte Carlo Integration

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?"



https://xkcd.com/2117/

1 A Tale of Two Approaches

Consider a one-dimensional integral.

$$\int_a^b \underbrace{f(x)}_{\text{integrand.}} dx$$

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 statistics can be written as the expectation of a function of a random variable

$$E[g(X)] = \int_{\mathcal{X}} \underbrace{g(x)f(x)}_{\text{integrand}} dx$$

1.1 Numerical Integration

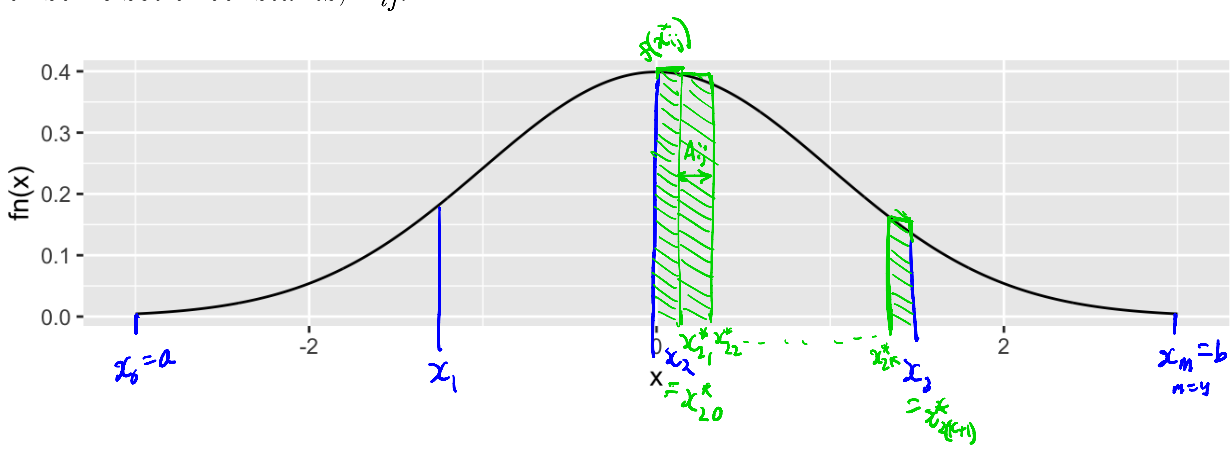
Idea: Approximate $\int_a^b f(x)dx$ via the sum of many polygons under the curve $f(x)$.

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

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

for some set of constants, A_{ij}.



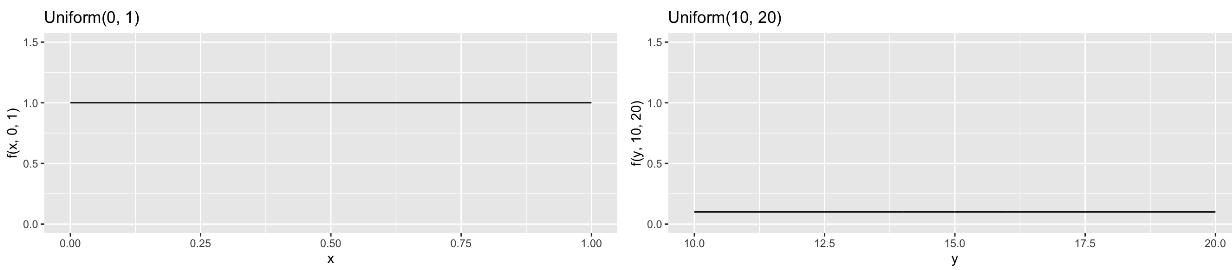
1.2 Monte Carlo Integration

How do we compute the mean of a distribution?

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

```
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
(exact)

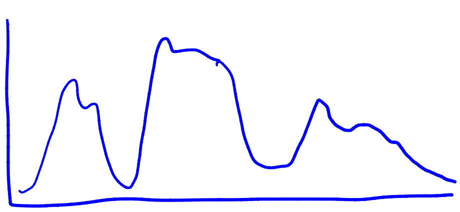
$$EX = \int_0^1 x f(x)\,dx = \int_0^1 x \cdot 1\,dx = \left[\frac{x^2}{2}\right]_0^1 = \frac{1}{2}$$

$$EY = \int_{10}^{20} y f(y)\,dy \quad \text{where } f(y) = \begin{cases} \frac{1}{10} & 10 \le y \le 20 \\ 0 & \text{o.w.} \end{cases}$$

$$= \int_{10}^{20} y \cdot \frac{1}{10}\,dy = \frac{1}{10}\left[\frac{y^2}{2}\right]_{10}^{20} = 15.$$

How about some other dsn?

$x \sim$



want to find

EX

Probably can't do this in closed form

$\Rightarrow$ need an approximation.

1.2.1 Notation

θ = parameter (unknown)

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

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

$\hat{\theta}$ is a function of random variables $\Rightarrow$ a random variable.

$E[\hat{\theta}]$ = on average, what is the value of $\hat{\theta}$?
theoretic mean of the sampling distribution of $\hat{\theta}$.

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

estimated versions.

$\hat{E}[\hat{\theta}]$ = estimated mean of distribution 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 $\hat{\theta}$

1.2.2 Monte Carlo Simulation

What is Monte Carlo simulation?

Computer simulation that generates a large quantity 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 the population. Thing we care about!

To approximate $\theta = E[X] = \int x f(x) dx$, we can (1) obtain an iid random sample $X_1, \ldots, X_n$ from f and then (2) approximate θ via the sample average

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

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 $X_1, \ldots, X_m \sim Unif(0,1)$

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

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

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

This is useful when we can't compute EX in closed form. Also useful to approximate other integrals.

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

parameter of interest

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

The Monte Carlo approximation of θ could then be obtained by

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

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

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

$Y = X\beta + \varepsilon \quad \varepsilon \sim N(0, \sigma^2), \quad \hat{\beta} = (X^T X)^{-1} X^T Y$ closed form solution

GLM: $Y \sim Binom(p)$

$logit(p) = \beta_0 + \beta_1 X$ no estimate for β_0, β_1 in closed form.

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

Why the mean?

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

$$E(\hat{\theta}) = E\left[\frac{1}{m}\sum_{i=1}^{m} g(X_i)\right] = \frac{1}{m}\sum_{i=1}^{m} E(g(X_i)) = \frac{1}{m}[\underbrace{\theta + \cdots + \theta}_{m \text{ times}}] = \theta$$

so $\hat{\theta}$ obtained from MC integration approach is unbiased

and, by the strong law of large numbers,

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

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

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

We can estimate this using a Monte Carlo approach.

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

(1) Sample $X_1, \ldots, X_m$ from f

(2) Compute $\frac{1}{m}\sum_{i=1}^{m}[g(X_i) - \theta]^2$ don't know this! can replace with $\hat{\theta} = \frac{1}{m}\sum_{i=1}^{m} g(X_i)$

Use to estimate sampling variance. $\Rightarrow$ $Var\,\hat{\theta} = Var\left[\frac{1}{m}\sum_{i=1}^{m} g(X_i)\right]$

$= \frac{1}{m^2}\sum Var\, g(X_i) = \frac{1}{m} Var\, g(X)$ can estimate using $\hat{Var}\, g(x)$.

estimate $se(\hat{\theta})$ by $\sqrt{\frac{1}{m}\hat{Var}\, g(x)}$

When $\mathrm{Var}\, g(X)$ exists and is finite, the CLT states

$$\frac{\hat{\theta} - \overbrace{E\hat{\theta}}^{=\theta}}{\sqrt{\mathrm{Var}\,\hat{\theta} = \frac{\mathrm{Var}\, g(X)}{m}}} \xrightarrow{d} N(0,1) \quad \text{as } m \to \infty.$$

Hence if m is large,

$$\hat{\theta} \stackrel{\cdot}{\sim} N\left(\theta, \frac{\boxed{\mathrm{Var}\, g(X)}}{m}\right)$$

can plug in estimate $\widehat{\mathrm{Var}}\, g(X)$ from above.

We can use this knowledge to create confidence limits or error bounds on the MC estimate of the integral $\hat{\theta}$.

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.

numeric integration cannot say the same.

- MC integration does not attempt a systematic exploration of the p-dimensional support region of f. (curse of dimensionality).
- MC doesn't require integrand to be smooth, does not require finite support!

1.2.4 Algorithm

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

before R

1. Select f, g to define θ $= E[g(X)],\ X\sim f$ as an expected value.
2. derive estimator s.t. $\hat{\theta}$ approximates $\theta = E[g(X)] = \int_{-\infty}^{\infty} g(x)f(x)dx = \int_{-\infty}^{\infty} h(x)dx.$

in R.

3. Sample $X_1, \dots, X_m$ from f ← Many ways to do this.
4. Compute $\hat{\theta} = \frac{1}{m}\sum_{i=1}^{m} g(X_i).$

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

(1) Let f be the Unif(0,1) density $\Rightarrow g(x) = h(x)$.

(2) Then $\theta = \int_0^1 h(x)dx = \int_0^1 g(x)\cdot \underset{\text{unif}(0,1)\text{ density}}{1}\, dx = E[g(X)]$ ✓

(3) Sample $X_1, \dots, X_m$ from f

```
> X <- runif(m, 0, 1).
```

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

write this function in R.

```
> mean(g(x))
```

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

① Choose $f \equiv \text{Unif}(a,b) \Rightarrow f(x) = \begin{cases} \frac{1}{b-a} & a \le x \le b \\ 0 & \text{o.w.} \end{cases}$

Then $g(x) = (b-a)\cdot h(x)$.

② So that $\theta = \int_a^b h(x)dx = \int_a^b (b-a)h(x)\cdot \frac{1}{b-a}\,dx = \int_a^b g(x)f(x)\,dx = Eg(X)$, $X \sim \text{Unif}(a,b)$

③ Sample $X_1, \dots, X_m$ from $\text{Unif}(a,b)$. > x <- runif(m, a, b).

④ Compute $\hat{\theta} = \frac{1}{m}\sum_{i=1}^{m}(b-a)\cdot h(x_i)$ > (b-a) mean(h(x)).

Another approach:

(a,b) maps $(0,1)$.

What if I chose $Y \sim \text{Unif}(0,1)$ instead?

Then $f(y) = \begin{cases} 1 & 0 \le y \le 1 \\ 0 & \text{o.w.} \end{cases}$

But we care about $E[g(Y)] = \int_{\mathcal{Y}} g(y) f(y)\,dy$

$\mathcal{Y}$: support of f.

We want to integrate from (a,b), but support of dsn is $(0,1)$. So we need a change of variable to use MC integration.

Need a function to map $x \in (a,b)$ to $y \in (0,1)$. We will use linear transformation.

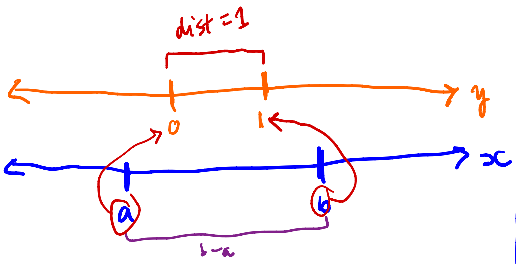
$(y \to x)$ $\quad \frac{x-a}{b-a} = \frac{y-0}{1-0} \Rightarrow \frac{x-a}{b-a} = y.$

$\downarrow$ solve for x

$x = a + (b-a)y.$

$dx = (b-a)dy.$

$$\theta = \int_a^b g(x)\,dx = \int_0^1 \underbrace{g(a+(b-a)y)\cdot(b-a)}_{g}\,dy. \quad f(y) = 1.$$



To get $\hat{\theta}$,

① Simulate $Y_1, \dots, Y_m$ from $\text{Unif}(0,1)$.

② $\hat{\theta} = \frac{1}{m}\sum_{i=1}^{m}\{g(a+y_i(b-a))(b-a)\}$

We can use this if the limits of integration don't match any density!

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

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

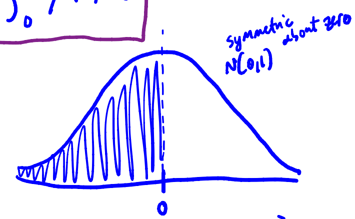
and the cdf of X is

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

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

Now we have an integral with finite limits of integration

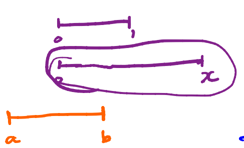
Method 1 Note for $x>0$, $\Phi(x) = \underbrace{\int_{-\infty}^{0} \phi(x)\,dx}_{P(X \le 0),\ X\sim N(0,1) = \frac{1}{2}} + \boxed{\int_0^x \phi(t)\,dt}$



Support of $Y \sim Unif(0,1)$ is $0 \le y \le 1$. So we want a function that maps $t \in [0, x]$ to $y \in [0,1]$.

linear transformation $\rightarrow$ $\dfrac{t-0}{x-0} = \dfrac{y-0}{1-0} \Rightarrow y = \dfrac{t}{x}$ if $t=0$, $y=0$ ✓ if $t=x$, $y=1$ ✓

$\Rightarrow t = xy \Rightarrow dt = x\,dy.$

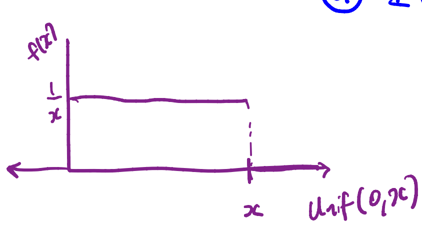


Then $\int_0^x \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{t^2}{2}\right) dt \overset{\text{change of variable}}{=} \int_0^1 \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\cdot(xy)^2\right) x\,dy.$ $\frac{1}{b-a}$, $b-a$ $f(x)$

$\Rightarrow$ We want to estimate $\theta = E_Y\Big[\underbrace{\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(xY)^2\right)\cdot x}_{g(Y)}\Big]$ where $Y \sim Unif(0,1)$.

So a MC estimate of $\Phi(x)$ could be obtained by:

1. Sample $Y_1, \ldots, Y_m \sim Unif(0,1)$
2. $\hat{\Phi}(x) = \frac{1}{2} + \frac{1}{m}\sum_{i=1}^{m}\left\{\frac{1}{\sqrt{2\pi}}\, x \exp\left(-\frac{1}{2}(xY_i)^2\right)\right\}$ for $x>0$.



Method 2 Sample from $Unif(0,x)$.

Homework.

Method 3

Let $\mathbb{I}$ be an indicator function:

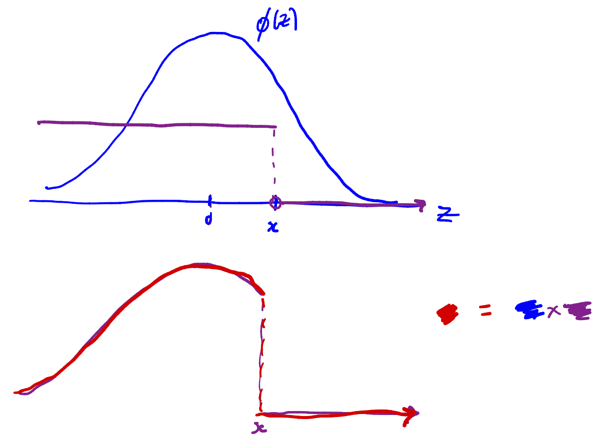
$$\mathbb{I}(Z \le z) = \begin{cases} 1 & \text{if } Z \le z \\ 0 & \text{o.w.} \end{cases}$$

Let $Z \sim N(0,1)$. Then

$$E_Z[\underbrace{\mathbb{I}(Z \le x)}_{g}] = \int_{-\infty}^{\infty} \mathbb{I}(z \le x) \cdot \phi(z)\, dz$$

$$= \int_{-\infty}^{x} \phi(z)\, dz$$

$$= \Phi(x) \text{ by definition.}$$



So a MC estimator of $\Phi(x)$:

1. Generate $Z_1, \ldots, Z_m \sim N(0,1)$. f
2. $\hat{\Phi}(x) = \frac{1}{m} \underbrace{\sum_{i=1}^{m} \mathbb{I}(Z_i \le x)}_{\text{counting}}$ # of Z_i's $\le x$.

Notes:

① Can show Method 3 has less bias in the tails and Method 2 has less bias in the center.

② Method 3 works for any dsn to approximate cdf (change f accordingly).

1.2.5 Inference for MC Estimators

The Central Limit Theorem implies

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

$se(\hat\theta) \rightarrow \sqrt{Var(\hat\theta)}$

So, we can construct confidence intervals for our estimator

ex

1. 95% CI for $E(\hat\theta)$: $\hat\theta \pm \underbrace{1.96}_{\alpha/2 \text{ quantile of Normal}(0,1).}\sqrt{\hat{Var}(\hat\theta)}$ qnorm(.975).

(HW) 2. 95% CI for $\Phi(2)$: $\hat\Phi(2) \pm 1.96\sqrt{\hat{Var}(\hat\Phi(2))}$

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

recall

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

$\sigma^2 = Var[g(X)] = E[(g(X) - Eg(X))^2]$ this is just an expected value $\Rightarrow$ we can estimate it!

Then $Var\,\hat\theta = Var\left[\frac{1}{m}\sum_{i=1}^{m} g(X_i)\right] \overset{\text{independence}}{=} \frac{1}{m^2}\sum_{i=1}^{m} Var\,g(X_i) \overset{iid}{=} \frac{\sigma^2}{m}$

So $\hat{Var}(\hat\theta) = \frac{\hat\sigma^2}{m} = \frac{1}{m}\underbrace{\left[\frac{1}{m}\sum_{i=1}^{m}\left[g(X_i) - \hat\theta\right]^2\right]}_{\hat\sigma^2 \text{ (estimated by MC integration)}} = \frac{1}{m^2}\sum_{i=1}^{m}(g(X_i) - \hat\theta)^2$

$\hat\theta$: $Eg(X)$

estimated variance of the sampling distribution of $\hat\theta$ (MC estimate).

Recall that we usually use $s^2 = \frac{1}{m-1}\sum_{i=1}^{m}(g(X_i) - \overline{g(X)})^2$ to estimate σ^2.

Why not use s^2 w/ $\frac{1}{m-1}$ instead of $\hat\sigma^2$ with $\frac{1}{m}$?

For MC integration, m is large. So $\frac{1}{m-1} \approx \frac{1}{m}$.

Ex: $m = 1000$ $\frac{1}{m-1} - \frac{1}{m} = 1\times 10^{-6}$

Some books use $\frac{1}{m-1}$ so $\hat{Var}(\hat\theta) = \frac{1}{m(m-1)}\sum_{i=1}^{m}\left[(g(X_i) - \hat\theta)^2\right]$.

$Var(\hat{\theta}) = \frac{\sigma^2}{m}$ more efficient estimation of θ

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

Good thing! $se(\hat{\theta}) = \sqrt{Var(\hat{\theta})}$

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

Current $se(\hat{\theta}) = \sqrt{Var(\hat{\theta})} = \sqrt{\frac{\sigma^2}{m}} = .01$

Want $\sqrt{\frac{\sigma^2}{a \cdot m}} = .0001$

$$\frac{\sigma^2}{m} \cdot \frac{1}{a} = (.0001)^2$$

$$(.01)^2 \cdot \frac{1}{a} = (.0001)^2$$

$$\left(\frac{.01}{.0001}\right)^2 = a \quad \rightarrow \quad a = 10{,}000$$

So we need to run $10{,}000 \times m$ to acheive $se(\hat{\theta}) = .0001$!

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

Importance sampling