Chapter 3: Methods for Simulating Data

Statisticians (and other users of data) need to simulate data for many reasons.

For example, I simulate as a way to check whether a model is appropriate. If the observed data are similar to the data I generated, then this is one way to show my model may be a good one.

It is also sometimes useful to simulate data from a distribution when I need to estimate an expected value (approximate an integral). — Ch.5

R can already generate data from many (named) distributions:

```
set.seed(400) #reproducibility

rnorm(10) # 10 observations of a N(0,1) r.v.
```

R uses a "pseudo random" number generator
⇒ we can reproduce "random" results by setting the seed.

```
##  [1] -1.0365488  0.6152833  1.4729326 -0.6826873 -0.6018386 -1.3526097
##  [7]  0.8607387  0.7203705  0.1078532 -0.5745512
```

```
rnorm(10, 0, 5) # 10 observations of a N(0,5^2) r.v.
```

```
##  [1] -4.5092359  0.4464354 -7.9689786 -0.4342956 -5.8546081  2.7596877
##  [7] -3.2762745 -2.1184014  2.8218477 -5.0927654
```

```
rexp(10) # 10 observations from an Exp(1) r.v.
```

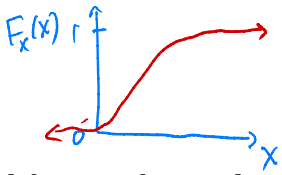
```
##  [1] 0.67720831 0.04377997 5.38745038 0.48773005 1.18690322 0.92734297
##  [7] 0.33936255 0.99803323 0.27831305 0.94257810
```

But what about when we don't have a function to do it?

↳ we need to write our own functions to simulate draws from other distributions.

1 Inverse Transform Method

Theorem 1.1 (Probability Integral Transform) If X is a continuous r.v. with cdf F_X, then $U = F_X(X) \sim \text{Uniform}[0, 1]$.



This leads to to the following method for simulating data.

Inverse Transform Method:

First, generate u from Uniform$[0, 1]$. Then, $x = F_X^{-1}(u)$ is a realization from F_X.

Note:

F^{-1} may not be available in closed form. If that's the case, use something else.

1.1 Algorithm

1. Derive the inverse function F_X^{-1}. To do this, let $F(x) = u$. Then solve for x to find $x = F^{-1}(u)$.
2. Write a function to compute $x = F_X^{-1}(u)$.
   ↳ in R
3. For each realization, → simulated value
   a. generate a random value u from Uniform$(0, 1)$
   b. Compute $x = F^{-1}(u)$.

Example 1.1 Simulate a random sample of size 1000 from the pdf $f_X(x) = 3x^2, 0 \le x \le 1$.

1. Find the cdf F

$$F(x) = \int_0^x 3y^2\,dy = y^3 \Big|_0^x = x^3 \qquad x \in [0,1]$$

2. Find F^{-1}

$$u = F(x) = x^3 \Rightarrow u^{1/3} = x$$

$$\text{so } F^{-1}(u) = u^{1/3} \qquad 0 \le u \le 1$$

↑ Range of $F(x)$

3.
```
# write code for inverse transform example
# f_X(x) = 3x^2, 0 <= x <= 1
```

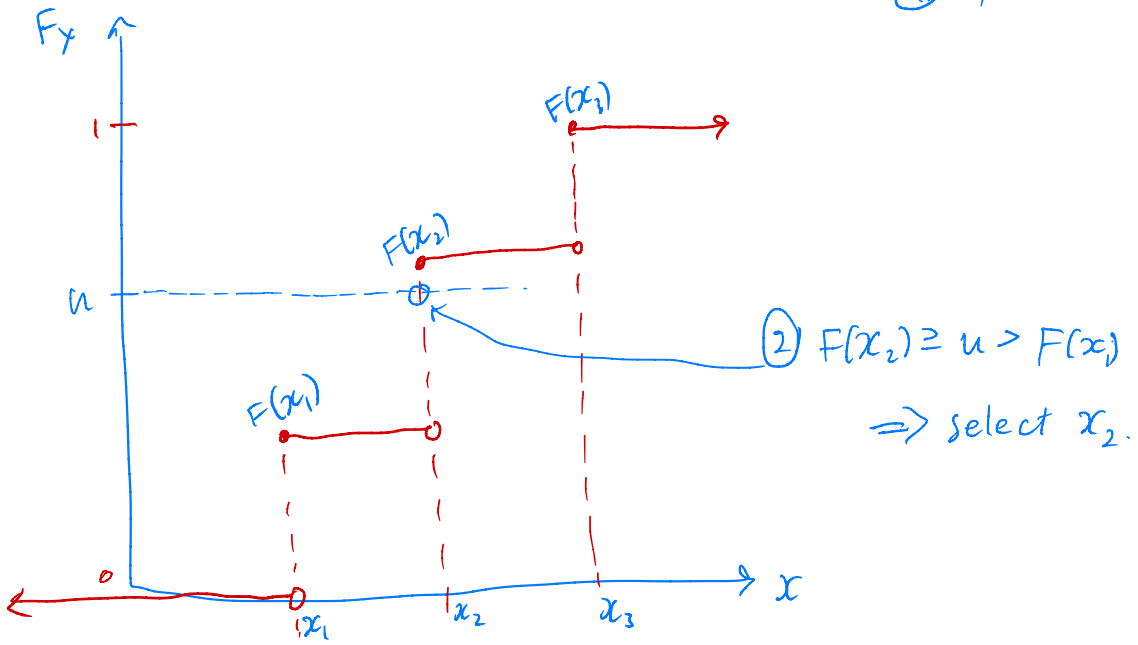
① Write function for F^{-1}
② Sample u values from Unif$(0,1)$
③ evaluate $x = F^{-1}(u)$.

1.2 Discrete RVs → inverse function won't be so straightforward.

If X is a discrete random variable and $\cdots < x_{i-1} < x_i < \cdots$ are the points of discontinuity (↑ jumps) of $F_X(x)$, then the inverse transform is $F_X^{-1}(u) = x_i$ where $F_X(x_{i-1}) < u \le F_X(x_i)$. This leads to the following algorithm:

1. Generate a r.v. U from Unif$(0,1)$.
2. Select x_i where $F_X(x_{i-1}) < U \le F_X(x_i)$.

① If $u = 0.5$ e.g.



② $F(x_2) \ge u > F(x_1)$

$\Rightarrow$ select x_2.

Example 1.2 Generate 1000 samples from the following discrete distribution.

```
x <- 1:3
p <- c(0.1, 0.2, 0.7)
```

x	1.0	2.0	3.0
f	0.1	0.2	0.7

```
# write code to sample from discrete dsn
n <- 1000
```

There is a simpler way to do this using sample() function.

* Remember to allow replacement and specify the probability vector. *

something we can try if we can't find F^{-1}

2 Acceptance-Reject Method

the distribution we want to sample from.

The goal is to generate realizations from a *target density*, f.

Most cdfs cannot be inverted in closed form. $x = F^{-1}(u)$.

The Acceptance-Reject (or "Accept-Reject") samples from a distribution that is *similar* to f and then adjusts by only accepting a certain proportion of those samples.

↑ target

and rejecting the rest.

The method is outlined below:

Let g denote another density from which we **know how to sample** (1) and we can **easily calculate** $g(x)$. (2) ← requirements for g.

Let $e(\cdot)$ denote an *envelope*, having the property $e(x) = cg(x) \geq f(x)$ for all $x \in \mathcal{X} = \{x : f(x) > 0\}$ for a given constant $c \geq 1$. ← the envelope covers all of f.

support

← support of g must include support of f.!

The Accept-Reject method then follows by sampling $Y \sim g$ and $U \sim \text{Unif}(0, 1)$.

If $U < f(Y)/e(Y)$, accept Y. Set $X = Y$ and consider X to be an element of the target random sample.

Note: $1/c$ is the expected proportion of candidates that are accepted.

We can use this to evaluate the efficiency of the algorithm.

Question: What might be hard/slow about accept/reject?

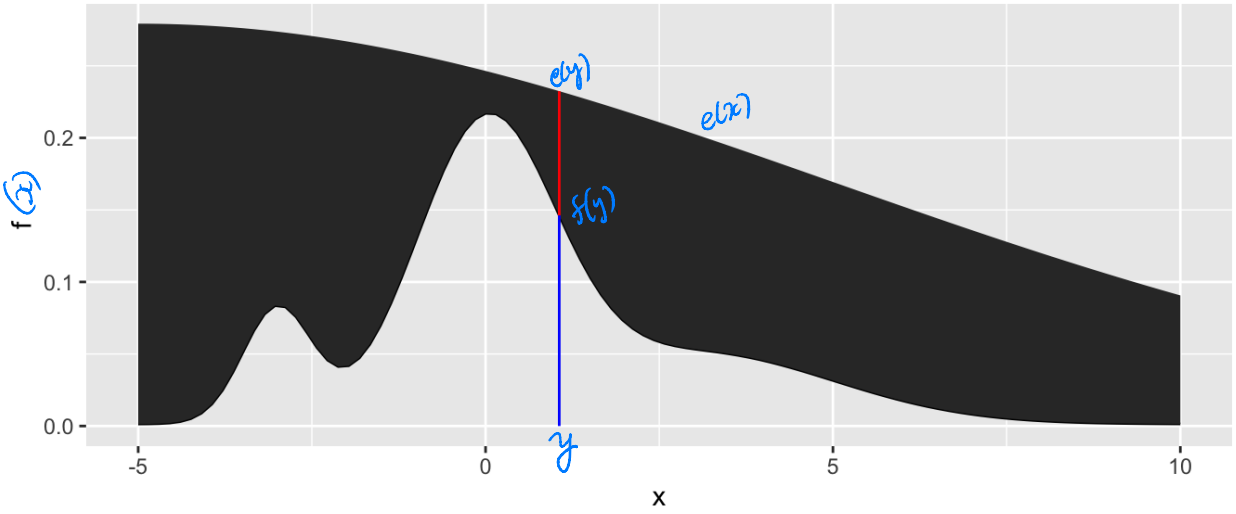
2.1 Algorithm

1. Find a suitable density g and envelope e.
2. Sample $Y \sim g$.
3. Sample $U \sim \text{Unif}(0, 1)$.
4. If $U < f(Y)/e(Y)$, accept Y.
5. Repeat from Step 2 until you have generated your desired sample size.

⚠ Requirement: The support of g must include the support of f ⚠

(BAD) Example: If $f = N(0,2)$ and $g = \text{Unif}(-10, 10)$

This would NOT be appropriate because support of f is $(-\infty, \infty)$!



2.2 Envelopes

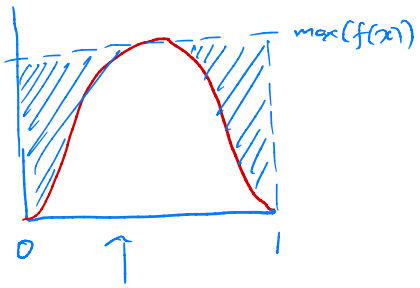
Good envelopes have the following properties:

① Envelope exceeds target everywhere ← support of g MUST include support of f!
② Easy to sample from g
③ Generate few rejected draws (save time)

A simple approach to finding the envelope: (in some cases.) Say the support of f is $0 \le x \le 1$.

Find $\max(f(x))$ and let $c = \max(f(x))$

Let $g(x) = \text{Unif}(0,1) = \begin{cases} 1 & \text{if } x \in [0,1] \\ 0 & \text{o.w.} \end{cases}$ ← support of g matches support of f!



** This is ONLY relevant if $0 \le x \le 1$.

This is often not efficient. If you know more about the shape of f you can select a better envelope.

Plotting is your friend here!

Example 2.1 We want to generate a random variable with pdf $f(x) = 60x^3(1-x^2)$, $0 \le x \le 1$. This is a Beta$(4,3)$ distribution.

$(1-x)^2$

could just use rbeta() in R.

Can we invert $F(x)$ analytically? NO.

If not, find the maximum of $f(x)$.

$f(x) = 60x^3(1-x)^2$

$f'(x) = 60\left(3x^2(1-x)^2 - 2x^3(1-x)\right)$

$= 60x^2(1-x)\left[3(1-x) - 2x\right]$

$= 60x^2(1-x)(3-5x) = 0$ at $x=0, x=1,$ or $x = \frac{3}{5}$

$f(0) = f(1) = 0.$

$x = 3/5$ is a max and $c = f(\frac{3}{5}) = 2.0736$

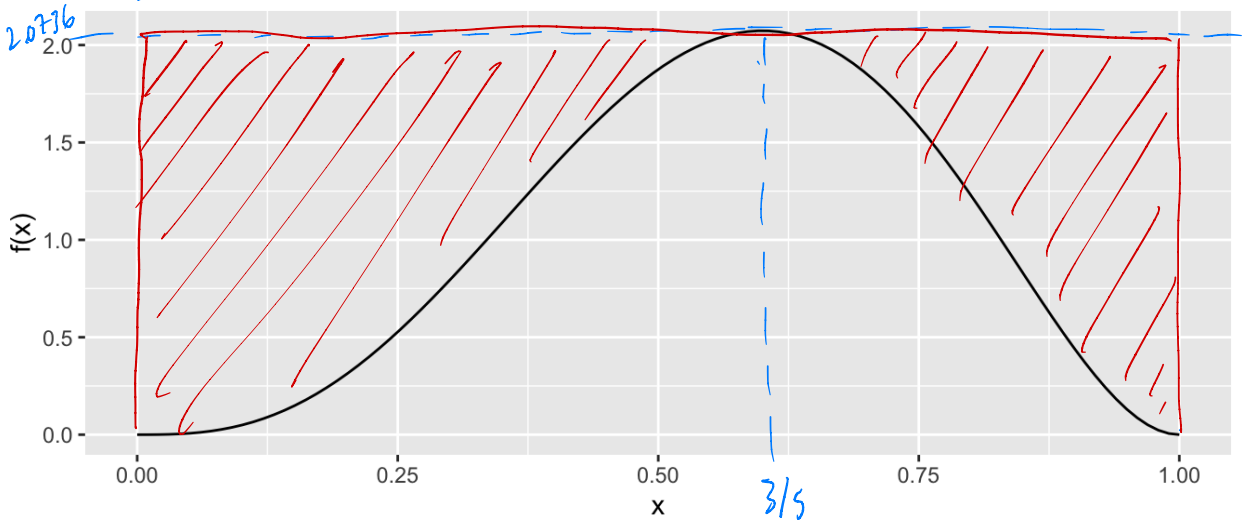
```
# pdf function, could use dbeta() instead
f <- function(x) {
    60*x^3*(1-x)^2
}

# plot pdf
x <- seq(0, 1, length.out = 100)
ggplot() +
  geom_line(aes(x, f(x)))
```

in base R.

make x values

draw line.

evaluate f at x values



```
envelope <- function(x) {
  ## create the envelope function
}

# Accept reject algorithm
n <- 1000 # number of samples wanted
accepted <- 0 # number of accepted samples
samples <- rep(NA, n) # store the samples here

while(accepted < n) {
  # sample y from g
  y <- runif(1)
  # sample u from uniform(0,1)
  u <- runif(1)

  if(u < f(y)/envelope(y)) {
    # accept
    accepted <- accepted + 1
    samples[accepted] <- y
  }
}
```

envelope <- function(x) { ## create the envelope function } ← c · unif(0,1) pdf. = c · 1 = f(3/5).

while we don't have enough accepted samples, keep running the loop.

g ← unif(0,1).

y <- runif(1)

increment accepted so loop ends eventually.

store samples

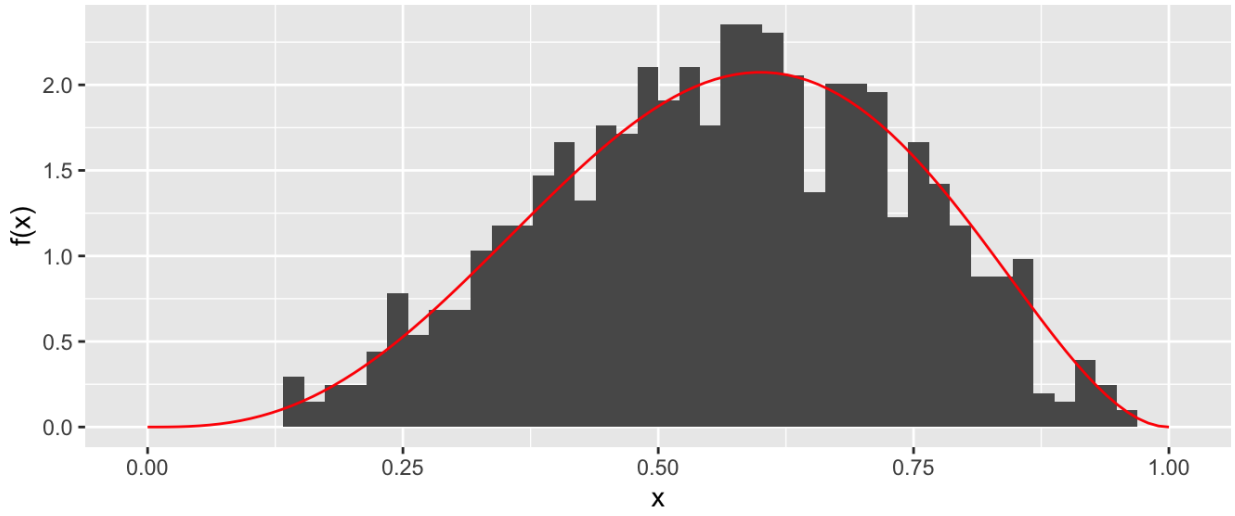
```
ggplot() +
  geom_histogram(aes(sample, y = ..density..), bins = 50, ) +
  geom_line(aes(x, f(x)), colour = "red") +
  xlab("x") + ylab("f(x)")
```

samples from f

necessary so that histogram is on the same scale as the density instead of raw counts.

This is important for your hw!

theoretical pdf



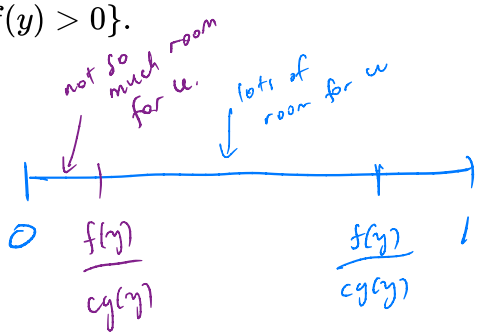
2.3 Why does this work?

Recall that we require

$$cg(y) \geq f(y) \qquad \forall y \in \{y : f(y) > 0\}.$$

Thus,

$$0 \leq \frac{f(y)}{cg(y)} \leq 1$$



The larger the ratio $\frac{f(y)}{cg(y)}$, the more the random variable Y looks like a random variable distributed with pdf f_X and the more likely Y is to be accepted.

2.4 Additional Resources

See p.g. 69-70 of Rizzo for a proof of the validity of the method.

↑ can come read in OH or in library on reserve.

3 Transformation Methods

Inverse transform method

We have already used one transformation method – ~~Probability Inverse Transforms~~ – but there are many other transformations we can apply to random variables.

1. If $Z \sim N(0,1)$, then $V = Z^2 \sim \chi^2_1$
2. If $U \sim \chi^2_m$ and $V \sim \chi^2_n$ are independent, then $F = \frac{U/m}{V/n} \sim F_{m,n}$
3. If $Z \sim N(0,1)$ and $V \sim \chi^2_n$ are independendent, then $T = \frac{Z}{\sqrt{V/n}} \sim t_n$
4. If $U \sim \text{Gamma}(r,\lambda)$ and $V \sim \text{Gamma}(s,\lambda)$ are independent, then $X = \frac{U}{U+V} \sim \text{Beta}(r,s)$

$X \to g(X)$

Definition 3.1 A *transformation* is any function of one or more random variables.

Sometimes we want to transform random variables if observed data don't fit a model that might otherwise be appropriate. Sometimes we want to perform inference about a new statistic.

Example 3.1 If $X_1, \ldots, X_n \overset{iid}{\sim} \text{Bernoulli}(p)$. What is the distribution of $\sum_{i=1}^n X_i$?

$X_i = 0$ or 1 w.p. p

Can derive $\sum X_i \sim \text{Binomial}(n,p)$

Example 3.2 If $X \sim N(0,1)$, what is the distribution of $X + 5$?

Can derive $X+5 \sim N(5,1)$.

Example 3.3 For $X_1, \ldots, X_n$ iid random variables, what is the distribution of the median of $X_1, \ldots, X_n$? What is the distribution of the order statistics? $X_{[i]}$?

This is more complex...

There are many approaches to deriving the pdf of a transformed variable.

- change of variable

if g monotone, then for cts X and $Y = g(X)$,

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) \left| \frac{d}{dy} g^{-1}(y) \right|, & y \in \mathcal{Y} \\ 0 & \text{o.w.} \end{cases}$$

- Moment generating functions

$M_X(t) = E(e^{tX})$

- Convolution Theorem

$Z = X + Y$

etc.

Use computational statistical methods to simulate from the transformed distribution.

But the theory isn't always available. What can we do?

3.1 Algorithm

Let $X_1, \ldots, X_p$ be a set of independent random variables with pdfs $f_{X_1}, \ldots, f_{X_p}$, respectively, and let $g(X_1, \ldots, X_p)$ be some transformation we are interested in simulating from.

1. Simulate $X_1 \sim f_{X_1}, \ldots, X_p \sim f_{X_p}$. ← either straight forward (named) inverse, accept-reject, etc.
2. Compute $G = g(X_1, \ldots, X_p)$. This is one draw from $g(X_1, \ldots, X_p)$.
3. Repeat Steps 1-2 many times to simulate from the target distribution.

Example 3.4 It is possible to show for $X_1, \ldots, X_p \overset{iid}{\sim} N(0,1)$, $Z = \sum_{i=1}^{p} X_i^2 \sim \chi^2_p$. Imagine that we cannot use the `rchisq` function. How would you simulate Z?

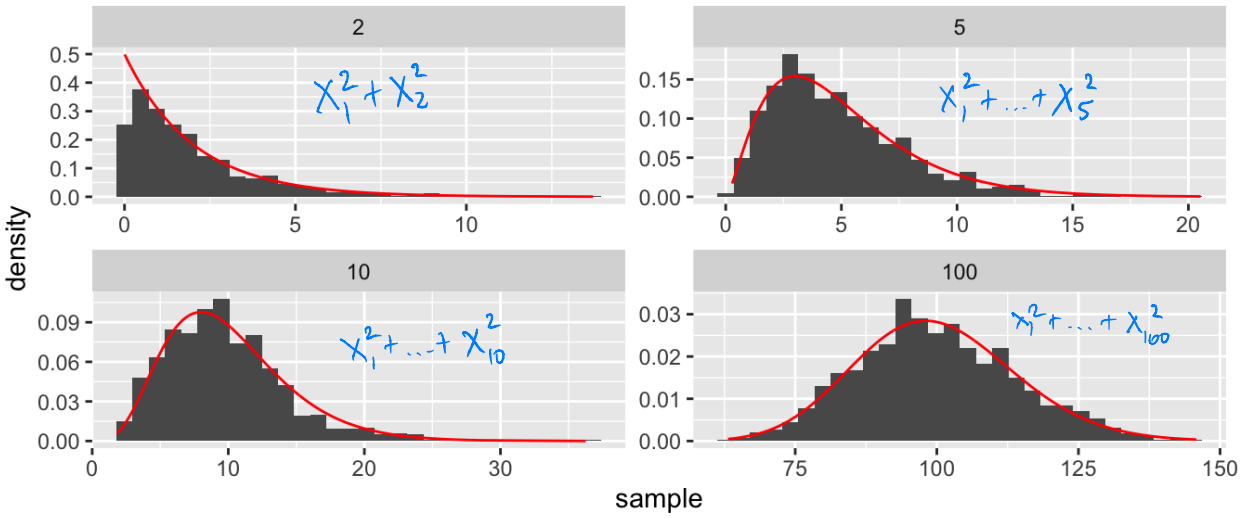
degrees of freedom, controls shape of dsn.

1. Simulate from $N(0,1)$
2. Compute $\sum X_i^2$
3. Repeat 1-2.

```
library(tidyverse)

# function for squared r.v.s
squares <- function(x) x^2

sample_z <- function(n, p) {   # of r.v.'s   df of χ²_p
  # store the samples
  samples <- data.frame(matrix(rnorm(n*p), nrow = n))

  samples %>%
    mutate_all("squares") %>% # square the rvs
    rowSums() # sum over rows
}

# get samples
n <- 1000 # number of samples

# apply our function over different degrees of freedom
```

this is n samples of p N(0,1) indep. random variables.

```
samples <- data.frame(chisq_2 = sample_z(n, 2),
                      chisq_5 = sample_z(n, 5),
                      chisq_10 = sample_z(n, 10),
                      chisq_100 = sample_z(n, 100))

# plot results
samples %>%
  gather(distribution, sample, everything()) %>% # make easier to
  plot w/ facets
  separate(distribution, into = c("dsn_name", "df")) %>% # get the df
  mutate(df = as.numeric(df)) %>% # make numeric
  mutate(pdf = dchisq(sample, df)) %>% # add density function values
  ggplot() + # plot
  geom_histogram(aes(sample, y = ..density..)) + # samples
  geom_line(aes(sample, pdf), colour = "red") + # true pdf in red
  facet_wrap(~df, scales = "free")
```



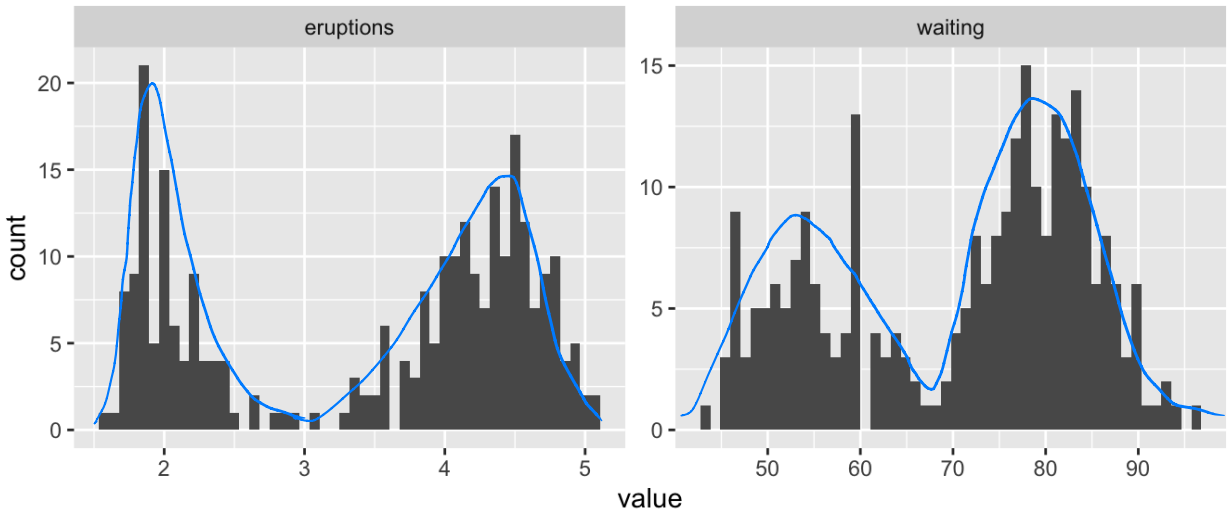
4 Mixture Distributions

The `faithful` dataset in `R` contains data on eruptions of Old Faithful (Geyser in Yellowstone National Park).

```
head(faithful)
```

```
##   eruptions waiting
## 1     3.600      79
## 2     1.800      54
## 3     3.333      74
## 4     2.283      62
## 5     4.533      85
## 6     2.883      55
```

```
faithful %>%
  gather(variable, value) %>%
  ggplot() +
  geom_histogram(aes(value), bins = 50) +
  facet_wrap(~variable, scales = "free")
```



What is the shape of these distributions?

Bimodal.

i.e. Two modes.

Definition 4.1 A random variable Y is a discrete mixture if the distribution of Y is a weighted sum $F_Y(y) = \sum \theta_i F_{X_i}(y)$ for some sequence of random variables $X_1, X_2, \ldots$ and $\theta_i > 0$ such that $\sum \theta_i = 1$.

For 2 r.v.s,

$$f(x) = \theta f_{X_1}(x) + (1-\theta) f_{X_2}(x)$$

two different distributions.

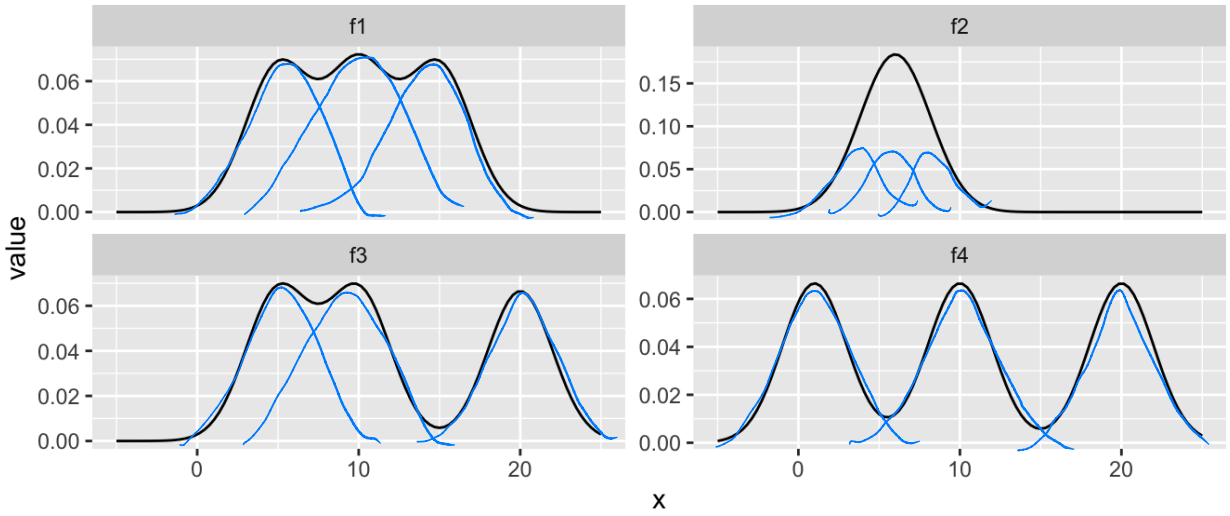
How do we simulate from this distribution?

There are 2 sources of variability.

$Y \sim \text{Bernoulli}(\theta) \longrightarrow$ if $\begin{cases} y=1 & X \sim f_{X_1} \\ y=0 & X \sim f_{X_2} \end{cases}$

Example 4.1

```
x <- seq(-5, 25, length.out = 100)

mixture <- function(x, means, sd) {
  # x is the vector of points to evaluate the function at
  # means is a vector, sd is a single number
  f <- rep(0, length(x))
  for(mean in means) {
    f <- f + dnorm(x, mean, sd)/length(means) # why do I divide?
  }
  f
}

# look at mixtures of N(mu, 4) for different values of mu
data.frame(x,
           f1 = mixture(x, c(5, 10, 15), 2),
           f2 = mixture(x, c(5, 6, 7), 2),
           f3 = mixture(x, c(5, 10, 20), 2),
           f4 = mixture(x, c(1, 10, 20), 2)) %>%
  gather(mixture, value, -x) %>%
  ggplot() +
  geom_line(aes(x, value)) +
  facet_wrap(.~mixture, scales = "free_y")
```



4.1 Mixtures vs. Sums

Note that mixture distributions are *not* the same as the distribution of a sum of r.v.s.

Example 4.2 Let $X_1 \sim N(0,1)$ and $X_2 \sim N(4,1)$, independent.

$S = \frac{1}{2}(X_1 + X_2)$

also called a convolution

$E(S) = E\left(\frac{1}{2}(X_1+X_2)\right)$

$= \frac{1}{2}(EX_1 + EX_2) = \frac{1}{2}(0+4) = 2$

$Var(S) = Var\left(\frac{1}{2}(X_1+X_2)\right) \overset{\text{indep.}}{=} \frac{1}{4}(Var X_1 + Var X_2) = \frac{1}{4}(1+1) = \frac{1}{2}$

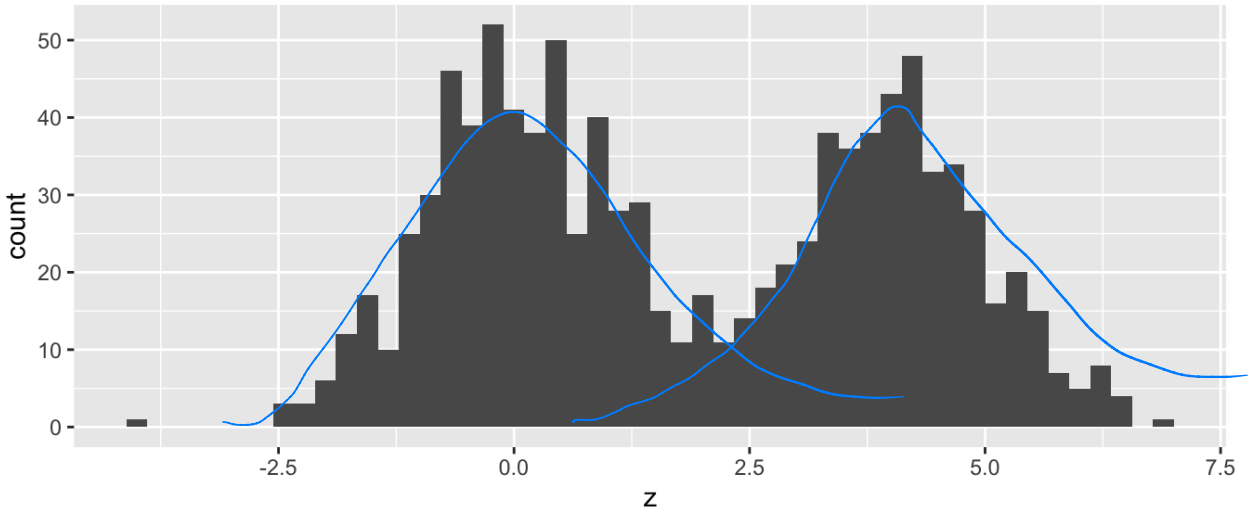
Can show in fact $S = \frac{1}{2}(X_1+X_2) \sim N(2, \frac{1}{2})$ a unimodal dsn.

Z such that $f_Z(z) = 0.5 f_{X_1}(z) + 0.5 f_{X_2}(z)$.

```
n <- 1000
u <- rbinom(n, 1, 0.5)

z <- u*rnorm(n) + (1 - u)*rnorm(n, 4, 1)

ggplot() +
  geom_histogram(aes(z), bins = 50)
```

choose which dsn

N(0,1) N(4,1).



What about $f_Z(z) = 0.7 f_{X_1}(z) + 0.3 f_{X_2}(z)$?

change u ← rbinom(n, 1, 0.7) to choose f_{X_1} w.p. 0.7.

4.2 Models for Count Data (refresher)

Recall that the Poisson(λ) distribution is useful for modeling count data.

$$f(x) = \frac{\lambda^x \exp\{-\lambda\}}{x!}, \quad x = 0, 1, 2, \ldots$$

Where X = number of events occuring in a fixed period of time or space.

When the mean λ is low, then the data consists of mostly low values (i.e. $0, 1, 2$, etc.) and less frequently higher values.

As the mean count increases, the skewness goes away and the distribution becomes approximately normal.

With the Poisson distribution,

$$E[X] = VarX = \lambda$$

restricts the shape of the dsn!

Example 4.3

- # homes sold per day by a real estate company
- # of calls coming per minute into a hotel reservation call center
- # of meows in a 2 minute cat video on youtube.

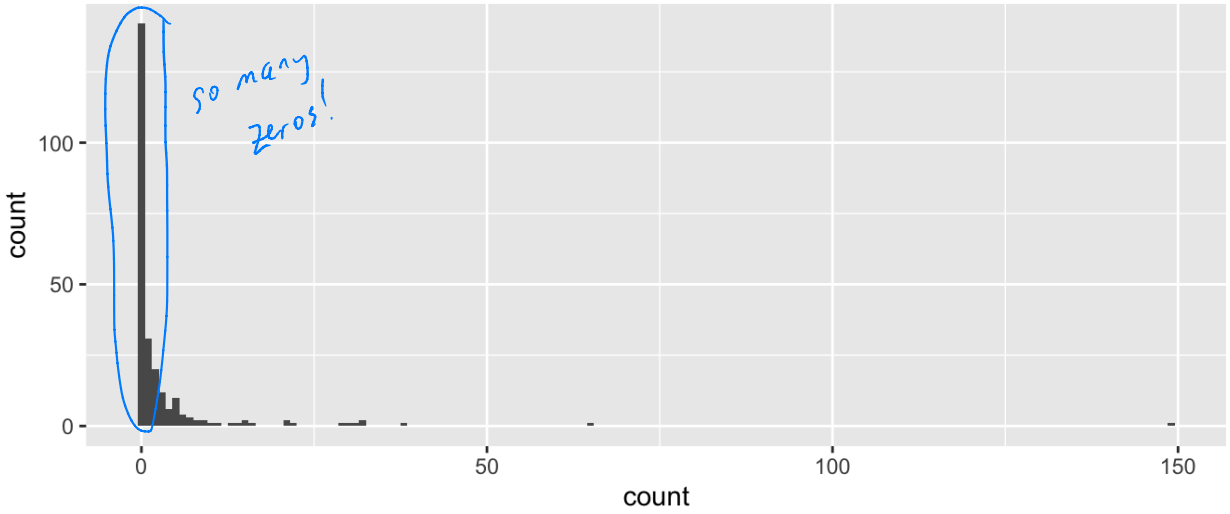
Example 4.4 The Colorado division of Parks and Wildlife has hired you to analyze their data on the number of fish caught in Horsetooth resevoir by visitors. Each visitor was asked - How long did you stay? - How many fish did you catch? - Other questions: How many people in your group, were children in your group, etc.

Some visiters do not fish, but there is not data on if a visitor fished or not. Some visitors who did fish did not catch any fish.

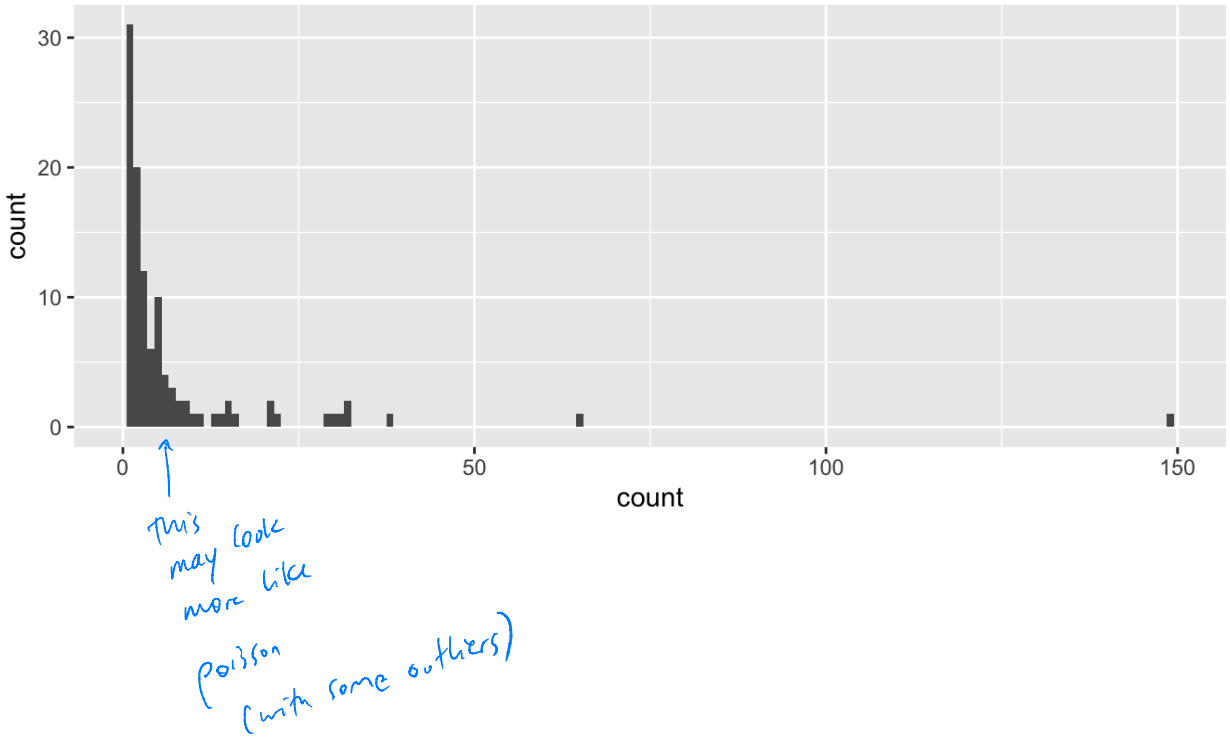
Note, this is modified from https://stats.idre.ucla.edu/r/dae/zip/.

```
fish <- read_csv("https://stats.idre.ucla.edu/stat/data/fish.csv")
```

```
# with zeroes
ggplot(fish) + geom_histogram(aes(count), binwidth = 1)
```




```
# without zeroes
fish %>%
  filter(count > 0) %>%
  ggplot() +
  geom_histogram(aes(count), binwidth = 1)
```



A *zero-inflated* model assumes that the zero observations have two different origins – structural and sampling zeroes.

→ a non-zero is impossible. → a zero is possible and occurs by random chance.

Example 4.5

Outcome of a study = # cows with foot and mouth disease (FMD) per region in Turkey

↳ structural zeroes – there are no cows in the region

↳ sampling zeroes – cows in the region, but no FMD.

Key point: you don't know whether region has no cows or no disease.

A zero-inflated model is a **mixture model** because the distribution is a weighted average of the sampling model (i.e. Poisson) and a point-mass at 0.

↑ structural zeros.

For $Y \sim ZIP(\lambda)$,

$$Y \sim \begin{cases} 0 & \text{with probability } \pi \\ \text{Poisson}(\lambda) & \text{with probability } 1-\pi \end{cases}$$

So that,

$$Y = \begin{cases} 0 & \text{w.p. } \pi + (1-\pi)\exp(-\lambda) \\ k & \text{w.p. } (1-\pi)\frac{\lambda^k \exp(-\lambda)}{k!} \quad k = 1, 2, \ldots \end{cases}$$

To simulate from this distribution,

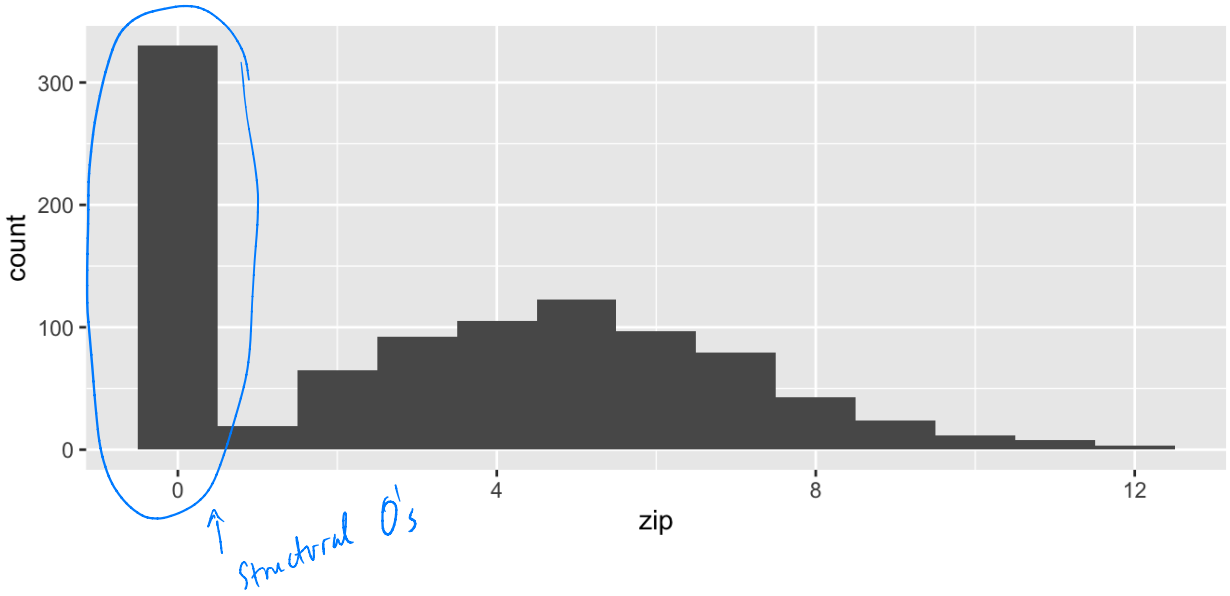
$Z \sim \text{Bern}(\pi)$

if $Z=1$, $Y \sim \text{Poisson}(\lambda)$

if $Z=0$, $Y = 0$.

```
n <- 1000
lambda <- 5
pi <- 0.3

u <- rbinom(n, 1, pi)
zip <- u*0 + (1-u)*rpois(n, lambda)
```

```
# zero inflated model
ggplot() + geom_histogram(aes(zip), binwidth = 1)
```




```
# Poisson(5)
ggplot() + geom_histogram(aes(rpois(n, lambda)), binwidth = 1)
```