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
```

set the seed so that we can reproduce our results later...

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

```
##  [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.
```

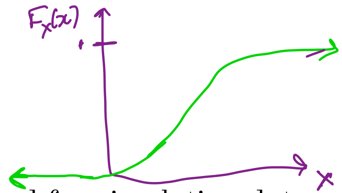
```
##  [1] 0.67720831 0.04377997 5.38745038 0.48773005 1.18690322 0.92734297
##  [7] 0.33936255 0.99803323 0.27831305 0.94257810
```

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

↳ we need to write our own functions to simulate data 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

on paper 1. Derive the inverse function F_X^{-1}. To do this, let $F(x) = u$, solve for x to find $x = F^{-1}(u)$.

in R 2. Write a function to compute $x = F_X^{-1}(u)$.

3. For each realization, simulated value

   a. generate a random value u from Unif(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

$$F(x) = \int_0^x 3y^2\,dy = y^3\Big|_0^x = \begin{cases} 0 & \text{for } x < 0 \\ x^3 & \text{for } x \in [0,1] \\ 1 & \text{for } x > 1 \end{cases}$$

2. Find F^{-1}

for $x \in [0,1]$ $\quad u = F(x) = x^3 \Rightarrow u^{1/3} = x = F^{-1}(u)$.

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

3.
```
# write code for inverse transform example
# f_X(x) = 3x^2, 0 <= x \<= 1
```
   1. Write function for F^{-1}
   2. Sample u from Unif(0,1)
   3. evaluate $x = F^{-1}(u)$.

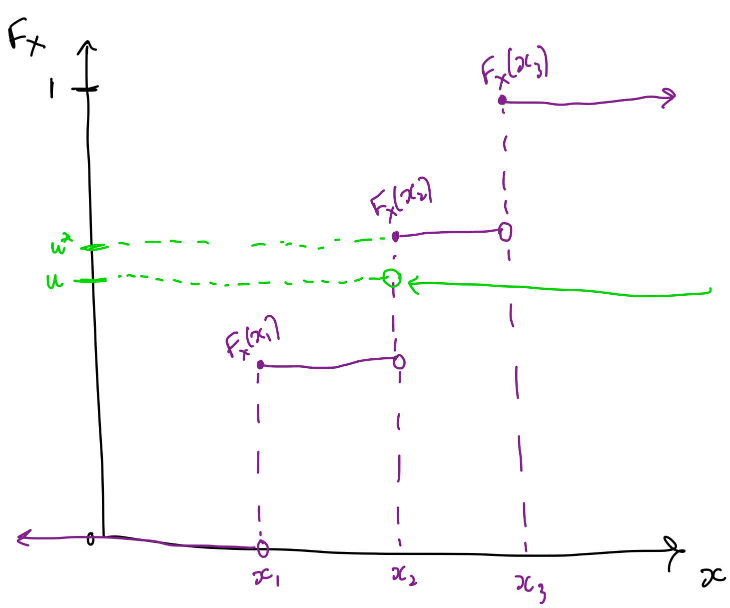
1.2 Discrete RVs

→ inverse function won't be so straightforward.

jumps in cdf ⟺ support of X

If X is a discrete random variable and $\cdots < x_{i-1} < x_i < \cdots$ are the points of discontinuity 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 $F_X(x_{i-1}) < U \le F_X(x_i)$.



$F(x_1) < u^* \le F(x_2)$
$\Rightarrow$ pick x_2 still!

$F(x_1) < u \le F(x_2)$
$\Rightarrow x_2$

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

pmf

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

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

* Remember to allow replacement and specify the probability vector *

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

2 Acceptance-Reject Method

density 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.

requirements for g.

The method is outlined below:

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

envelope covers all of f.

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 $c \geq 1$. (3) $\Rightarrow$ support of g must include the support of f!

support of $X \sim f$

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 our algorithm.

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

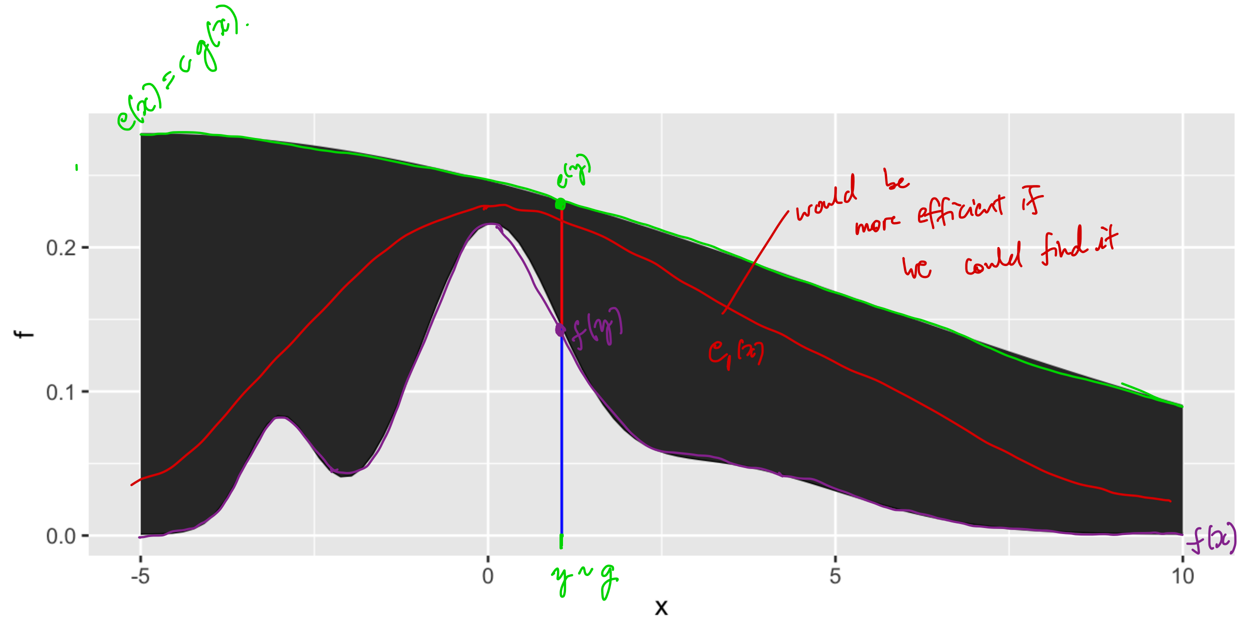
- If c is big $\Rightarrow$ low efficiency $\Rightarrow$ rejecting a lot. Sample a lot more from g.
- Need to pick g and find c.

2.1 Algorithm

1. Find a suitable density g and envelope e. find constant c s.t. $cg(x) \geq f(x)$ $\forall x \in \mathcal{X}$.
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 $f \equiv N(0,2)$ and $g \equiv \text{Unif}(-10,10)$.
This is NOT an appropriate choice of g because support of f is $\mathbb{R}$.



2.2 Envelopes

Good envelopes have the following properties:

requirement ① Envelope must exceed target everywhere ← support of g must include support of f.

nice ② Easy to sample from g.

nicer ③ Generate few rejected draws (save time).

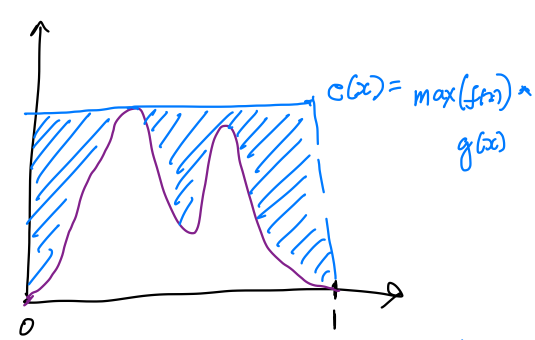
A simple approach to finding the envelope: in some cases

Say support of f is $0 \le x \le 1$

Find $\max_{x \in [0,1]} (f(x))$ and $c = \max_{x \in [0,1]} (f(x))$

support matches support of f!

Let $g(x) \equiv \text{Unif}(0,1) = \begin{cases} 1 & \text{if } x \in [0,1] \\ 0 & \text{o.w.} \end{cases}$



This is often not efficient if we know more about shape of f we can maybe select a better envelope

Plotting is our friend here.

★ This is only relevant if $\mathcal{X} = [0,1]$.

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.

could just use rbeta() in R.

Can we invert $F(x)$ analytically?

NO.

let $g \equiv$ Unif(0,1), find c

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

$$f'(x) = 60[3x^2(1-x)^2 + 2x^3(1-x)\cdot -1]$$
$$= 60x^2(1-x)[3(1-x) - 2x]$$
$$= 60x^2(1-x)(3-5x) = 0$$

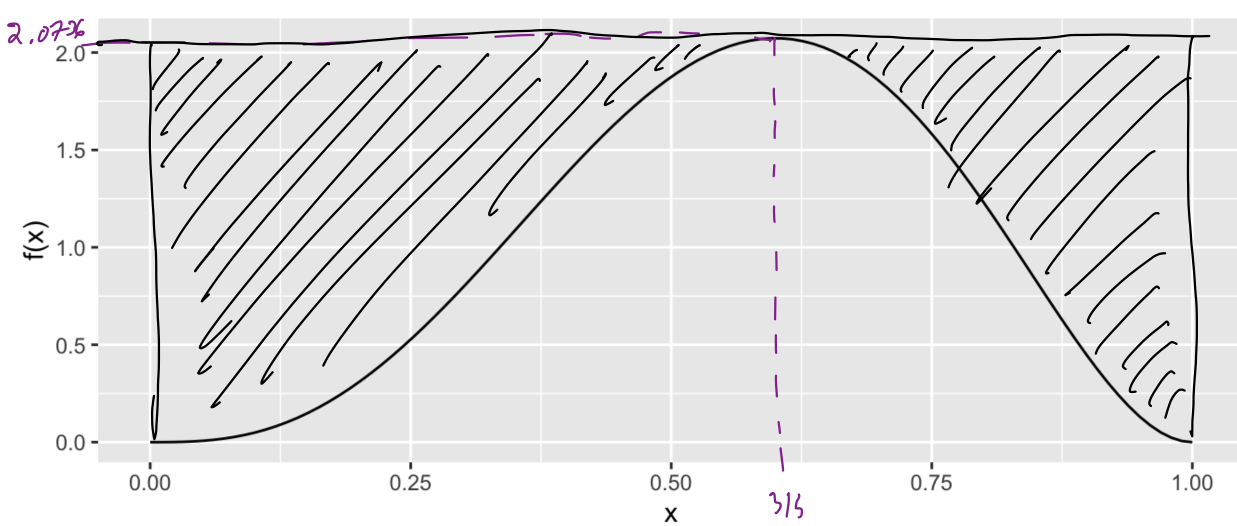
solve ... at $x=0$, $x=1$, $\boxed{x = \frac{3}{5}}$

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

$$\Rightarrow c = \max_{x\in[0,1]} f(x) = f\left(\tfrac{3}{5}\right) = 2.0736.$$

```
# 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)))
```



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

$c \cdot g(x)$
$= c \cdot 1 \cdot 1_{[0,1]}(x).$
$= f(3/5) \cdot 1_{[0,1]}(x).$

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

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

```
while(accepted < n) {
  # sample y from g
```

← Unif (0,1).

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
  }
}
```

increment accepted so loop ends eventually

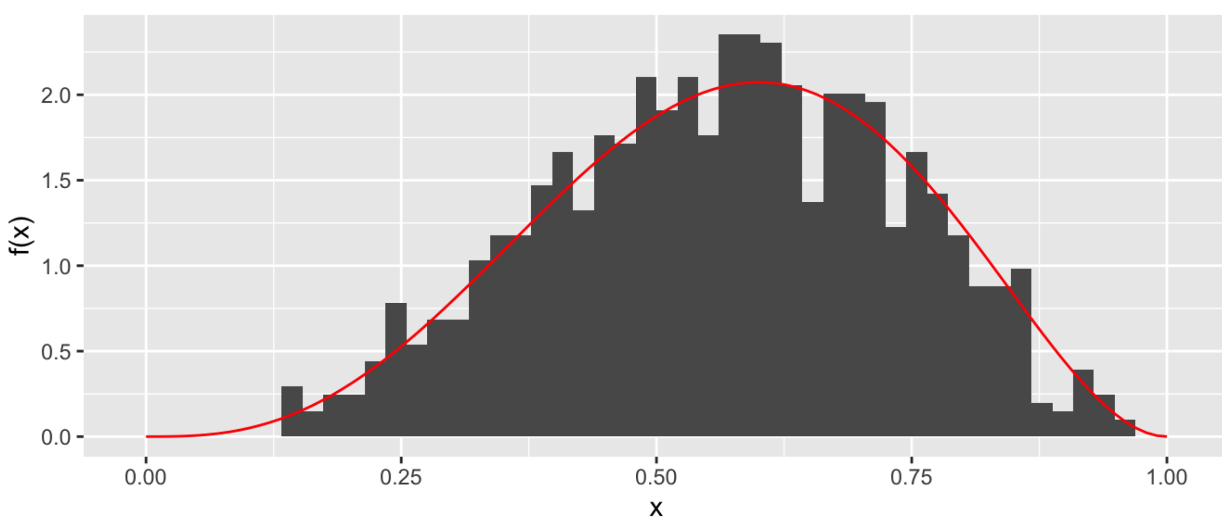
store sample ("accept" it).

samples from f

* scale histogram to be same scale as density.

theoretical pdf.

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



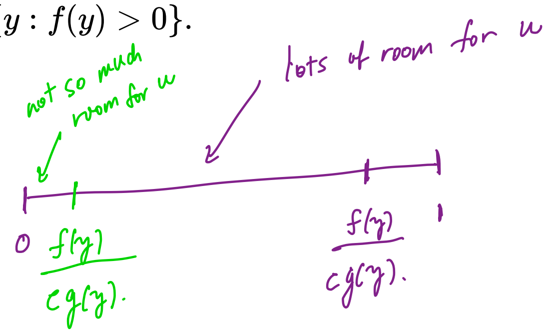
2.3 Why does this work?

Recall that we require

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

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 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.

3 Transformation Methods

We have already used one transformation method – **Inverse transform method** – 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 $U \sim \text{Gamma}(r, \underline{\lambda})$ and $V \sim \text{Gamma}(s, \underline{\lambda})$ are independent, then $X = \frac{U}{U+V} \sim \text{Beta}(r, s).$

X transformation $g(X)$.

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.

$X_i = \begin{cases} 1 & \text{w.p. } p \\ 0 & \text{o.w.} \end{cases}$

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

Can derive $\sum_{i=1}^n X_i \sim \text{Binom}(n, p).$

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 one is more complex... but we can derive.

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

- Change of variable

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

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

delta method.

- Moment generating functions

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

- Convolution theorem

$Z = X + Y.$

etc.

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

Use computational statistical methods to simulate from transformed dsns.

3.1 Algorithm

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

1. Simulate $X_1 \sim f_{X_1}, \dots, X_p \sim \boxed{f_{X_p}}$. could be named dsns (straightforward), inverse cdf, accept-reject.
2. Compute $G = g(X_1, \dots, X_p)$. This is one draw from $g(X_1, \dots, X_p)$.
3. Repeat Steps 1-2 many times to simulate from the target distribution.

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

degrees of freedom controls shape.

1. Simulate $X_1, \dots, X_p \overset{iid}{\sim} N(0,1)$.
2. Compute $\sum X_i^2$
3. repeat 1-2.

alternatively; $X_1, \dots, X_p \overset{iid}{\sim} N(0, \sigma_i^2)$ interested in $\sum_{i=1}^p X_i^2 \sim$?

```
library(tidyverse)

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

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

sample size

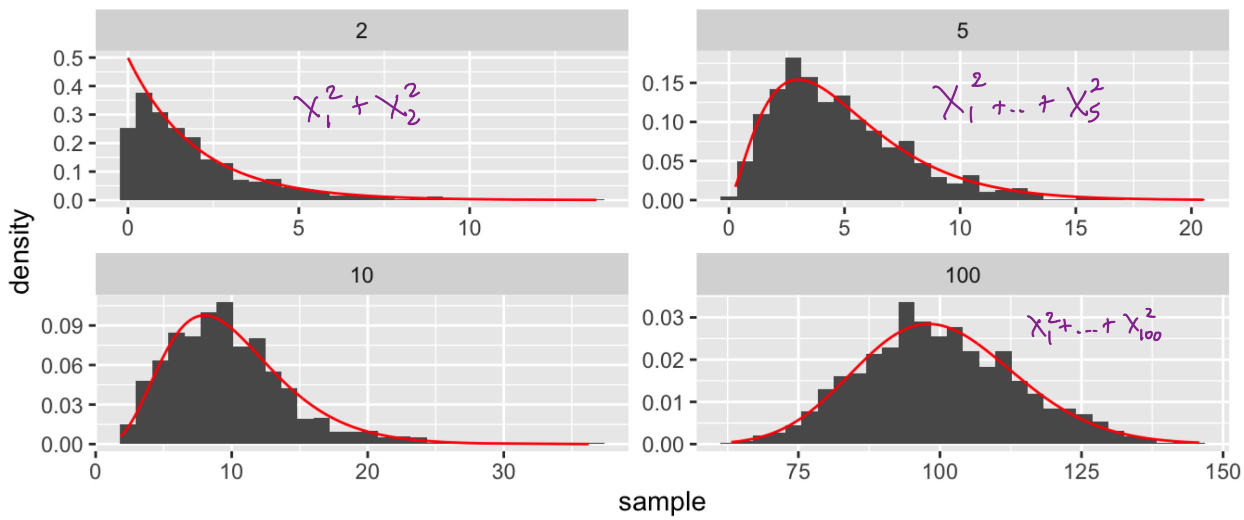
r.v.'s

get sample of size n for p r.v.'s ~~at a time.~~

df.

```
                    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
  facet_wrap(~df, scales = "free")
```



$n \overset{\shortparallel}{}$ 1000 samples

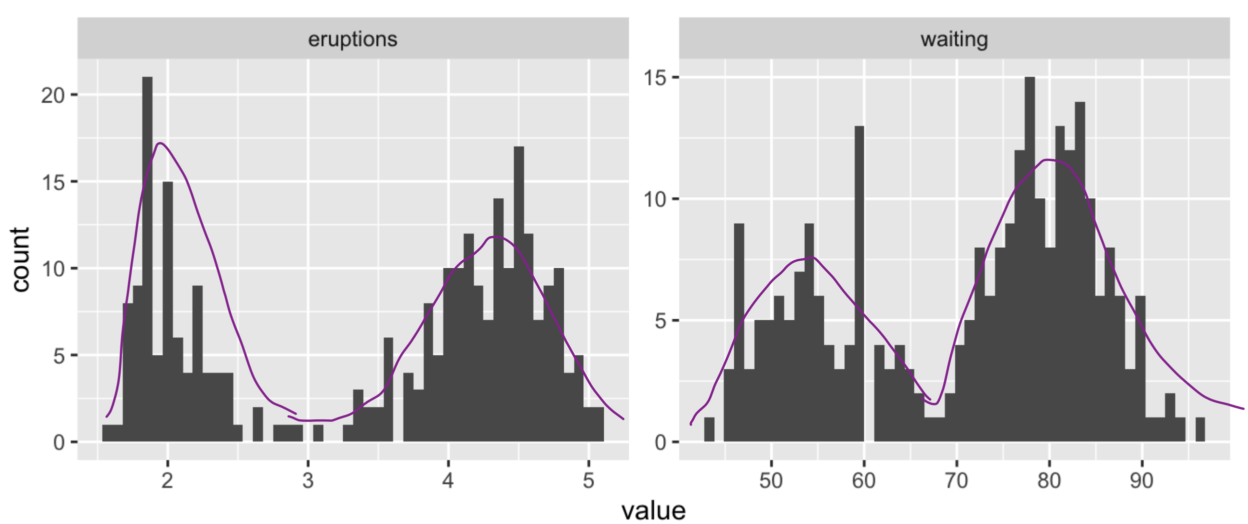
4 Mixture Distributions

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. 2 modes

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

→ same holds for pdfs.

For 2 r.v.s,

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

two different densities!

How can we simulate from this distribution?

There are two sources of variability.

with prob θ

$Y \sim \text{Bernoulli}(\theta) \rightarrow$ if $Y=1$, then $X \sim f_{X_1}(x)$

if $Y=0$, then $X \sim f_{X_2}(x)$.

with prob $(1-\theta)$.

Example 4.1

vector of means

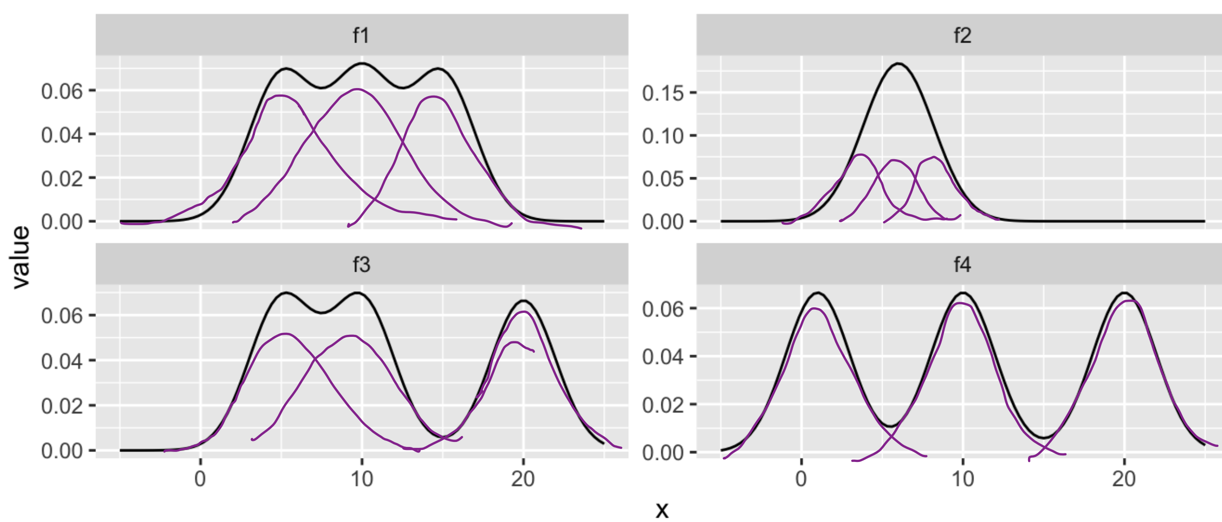
```
x <- seq(-5, 25, length.out = 100)

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")
```

equally weighting each componet density.

$f(x) = \frac{1}{3} N(\mu_1, 4) + \frac{1}{3} N(\mu_2, 4) + \frac{1}{3} N(\mu_3, 4)$



4.1 Mixtures vs. Sums

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

mixtures are weighted sums of distributions

NOT distributions of weighted sums!!

$\nearrow f_{X_1}$ $\quad f_{X_2}$

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

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

$$E(S) = E\left[\tfrac{1}{2}(X_1+X_2)\right]$$
$$= \tfrac{1}{2}\left[EX_1 + EX_2\right] = \tfrac{1}{2}(0+4) = 2$$
$$Var(S) = Var\left[\tfrac{1}{2}(X_1+X_2)\right] \overset{\text{indep.}}{=} \tfrac{1}{4}\left(Var X_1 + Var X_2\right) = \tfrac{1}{4}(1+1) = \tfrac{1}{2}.$$

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

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

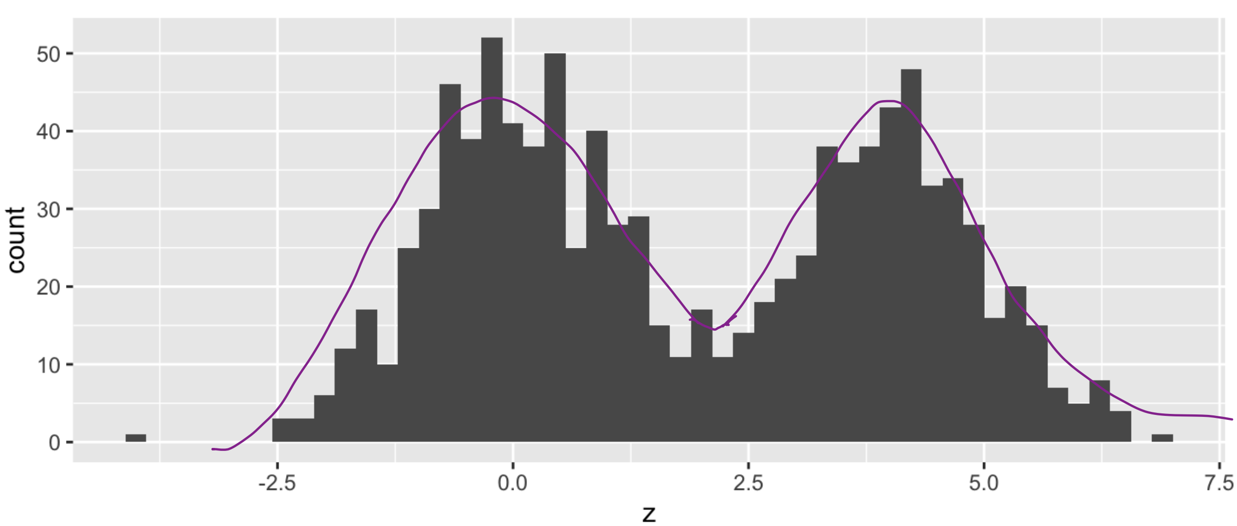
```
n <- 1000
u <- rbinom(n, 1, 0.5)

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

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

← choose which dsn

* simulating from mixture.*



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

change u <- rbinom(n, 1, 0.7).

4.2 Models for Count Data (refresher)

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

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

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 in Fort Collins.
- # of calls coming per minute into a hotel reservation call center.
- # of meows in a 2 minute cat video on youtube.

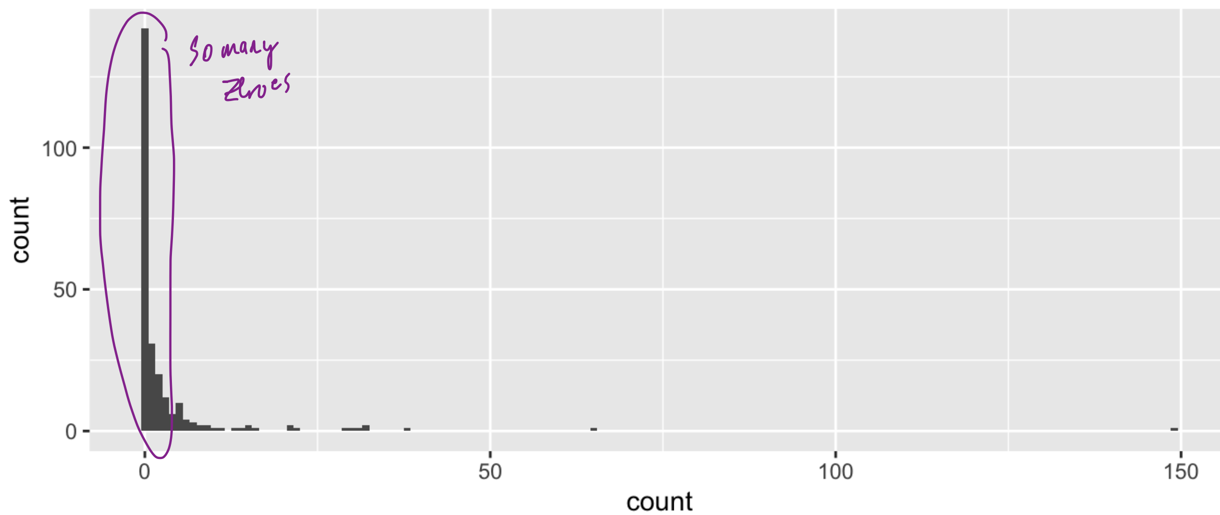
Example 4.4 The Colorado division of Parks and Wildlife has hired you to analyze their data on the number of fish caught in Horsetooth resevoir by visitors. Each visitor was asked - How long did you stay? - How many fish did you catch? - Other questions: How many people in your group, were children in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

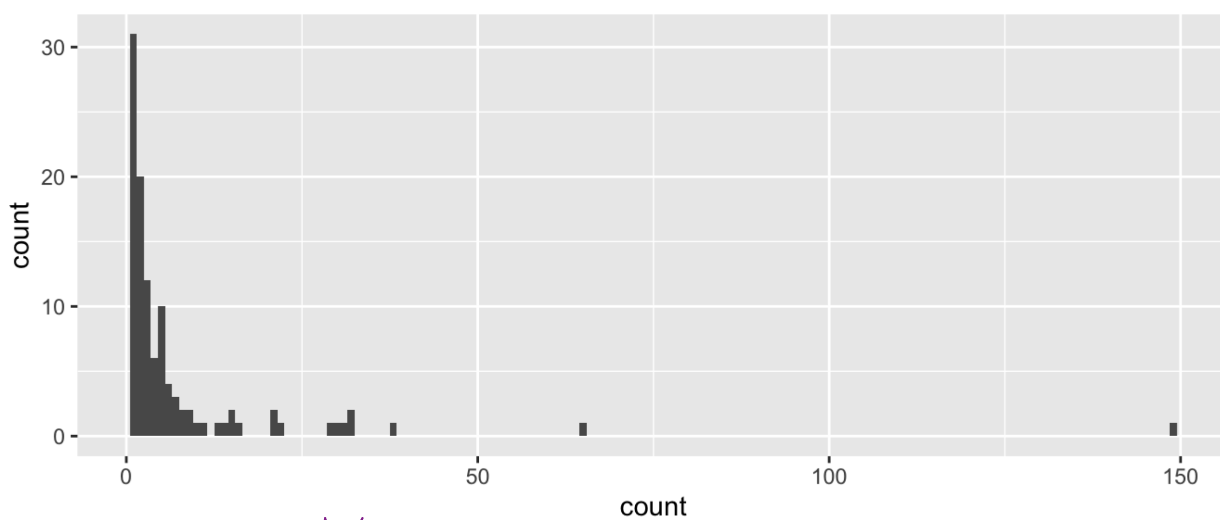
Note, this is modified from https://stats.idre.ucla.edu/r/dae/zip/.

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

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




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



This may look
more like a poisson
(with some outliers)

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

↳ a non-zero value 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 regions but no FMD.

Key point: you don't know whether a region has cows or not.

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.

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

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

So that,

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

To simulate from this distribution,

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

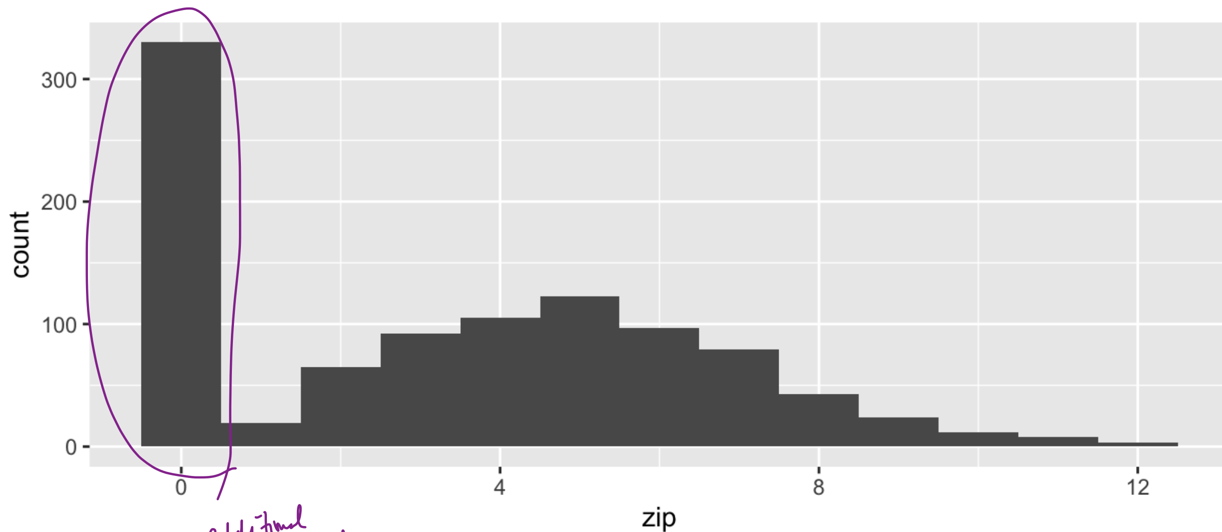
If $Z = 1$, $Y = 0$

If $Z = 0$, $Y \sim \text{Poisson}(\lambda)$.

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

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

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



additional structural zeros,

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