

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 (later)*

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

```
set.seed(400) #reproducibility
```

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

```
## [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.
```

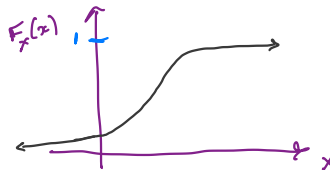
```
## [1] 0.67720831 0.04377997 5.38745038 0.48773005 1.18690322 0.92734297
## [7] 0.33936255 0.99803323 0.27831305 0.94257810
```

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 the following method for simulating data.

Inverse Transform Method:

First, generate u from $\text{Uniform}[0, 1]$. Then, $x = \underline{F_X^{-1}(u)}$ 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 $x = F_X^{-1}(u)$.
 \hookrightarrow in R.
3. For each realization, \longrightarrow simulated value.

remember
think about
realization
in R.

- a. generate a random value u from $\text{Unif}(0, 1)$.
- b. Compute $x = F^{-1}(u)$.

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

1. Find the cdf F_X :

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

2. Find F_X^{-1} :

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

$$\Rightarrow F_X^{-1}(u) = u^{1/3} \quad \underbrace{0 \leq u \leq 1}_{\text{range of } F(x)}$$

3. # write code for inverse transform example

$f_X(x) = 3x^2, 0 \leq x \leq 1$

① Write function for F^{-1} in R.

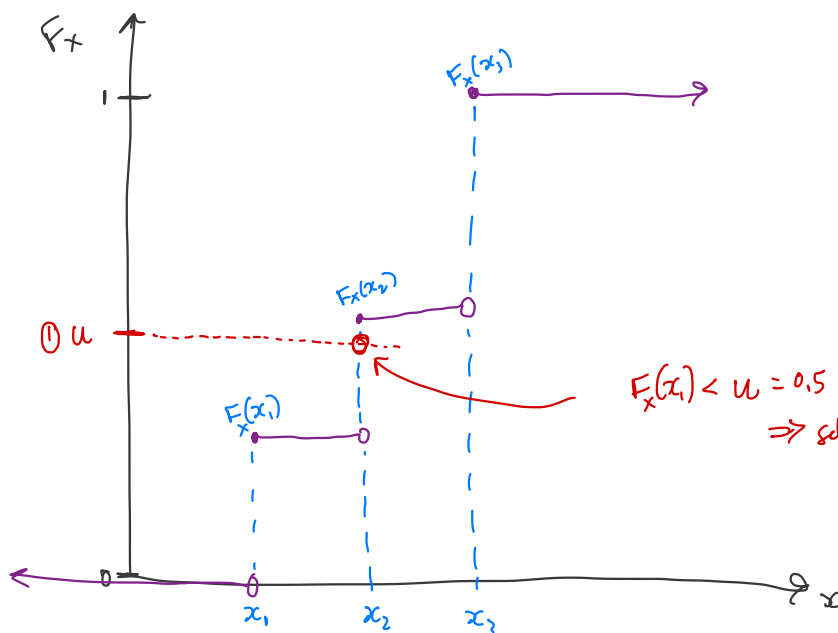
② sample values from $\text{Unif}(0, 1)$.

③ evaluate $x = F^{-1}(u)$.

1.2 Discrete RVs

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

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



① If $u = 0.5$ e.g.

$F_X(x_1) < u = 0.5 \leq F_X(x_2)$
 \Rightarrow select x_2

jumps in
 step function
 (support of
 R.V.)

*Your
Turn*

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 prob vector

2 Acceptance-Reject Method

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

Most cdfs cannot be inverted in closed form. \Rightarrow inverse transform method not possible.

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.

The method is outlined below:

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

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 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 efficiency of our algorithm.

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 .

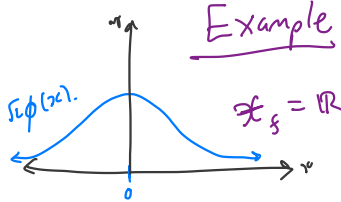
5. Repeat from Step 2 until you have generated your desired sample size.

~~Requirement:~~ The support of g must include the support of f .

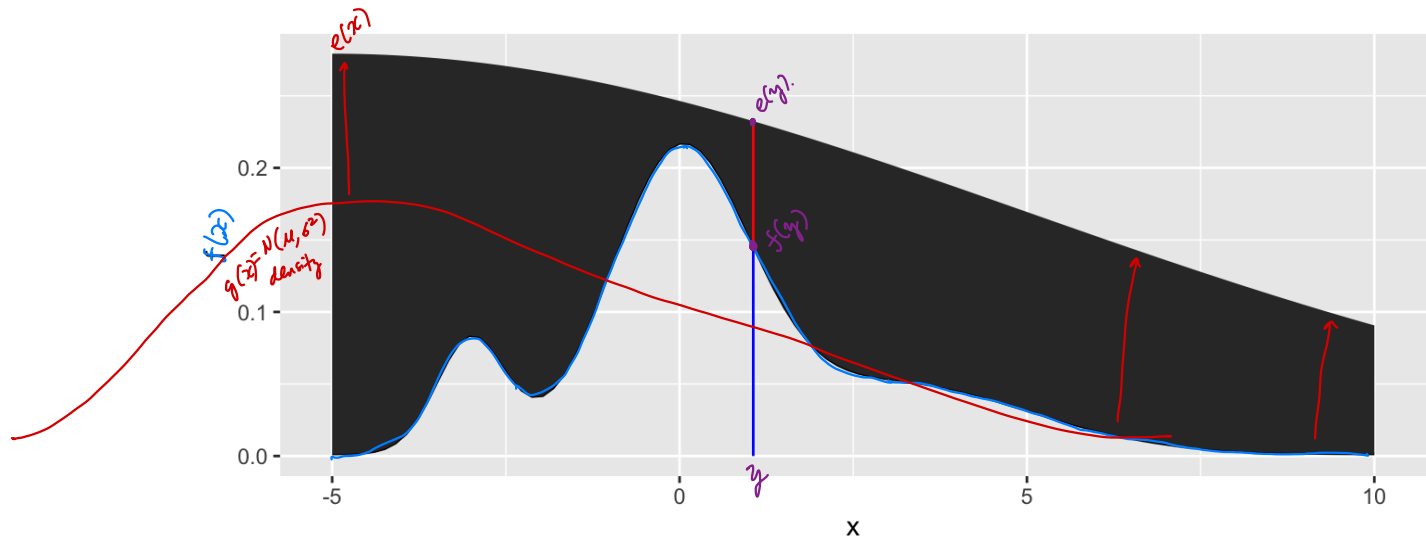
Example: If $f \equiv N(0, 2)$ and $g \equiv \text{Unif}(-10, 10)$.

$\mathcal{X}_g = [-10, 10]$.

BAD idea.



is it true that $[-10, 10] \supseteq \mathbb{R}$? No.



2.2 Envelopes

Good envelopes have the following properties:

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

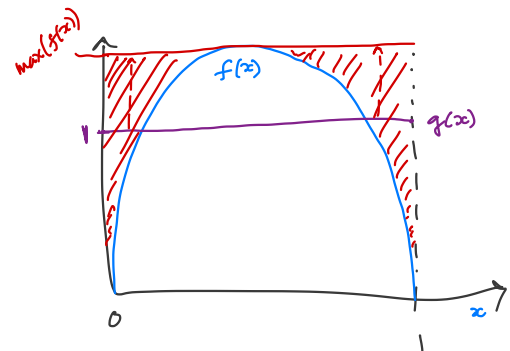
A simple approach to finding the envelope: ^{in some cases.} Say the support of f is $0 \leq x \leq 1$.

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

Find $\max_{0 \leq x \leq 1} (f(x))$ and let $C = \max_{0 \leq x \leq 1} (f(x))$

* This is ONLY relevant if $\mathcal{X}_f = [0,1]$ *

plotting is your friend for other supports.
to help find C .



↑
this isn't always the most efficient way
but it will always work when $\mathcal{X}_f = [0,1]$.

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

Can we invert $F(x)$ analytically? *→ could just use `rbeta()` in R.*

No.

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

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

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

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

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

f(0)=f(1)=0

$$\text{max } f(x) \text{ occurs at } x = \frac{3}{5} \Rightarrow C = \max_{x \in [0,1]} f(x) = f\left(\frac{3}{5}\right) = 60\left(\frac{3}{5}\right)^3\left(1-\frac{3}{5}\right)^2 = 2.0736.$$

pdf function, could use `dbeta()` instead

```
f <- function(x) {  
  60*x^3*(1-x)^2  
}
```

in base R.

plot pdf

```
x <- seq(0, 1, length.out = 100)
```

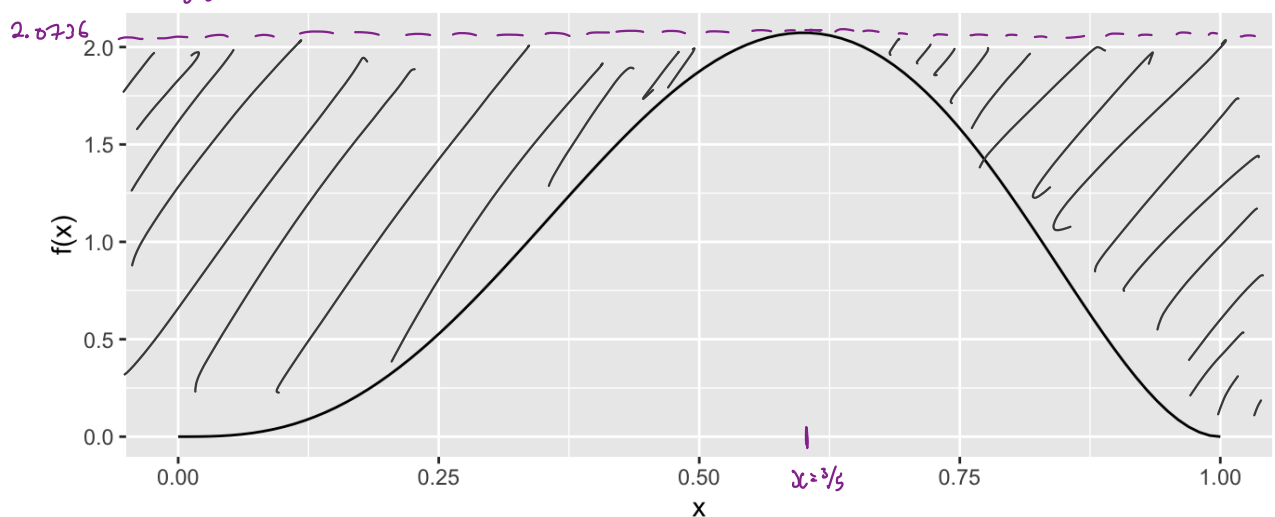
made sequence of x values.

```
ggplot() +
```

```
  geom_line(aes(x, f(x)))
```

↑ draw black line

↑ evaluate f at each x.



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

$c = \text{unif}(0,1)$ pdf
 $c = f(\frac{3}{5})$.

```
# 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  $g \leftarrow \text{unif}(0,1)$ .
  y <- runif(1).
  # sample u from uniform(0,1)
  u <- runif(1) ← always from  $\text{unif}(0,1)$ .

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

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

sample from proposal.

increment accepted counter so loop eventually ends.

accept y as a sample from f ⇒ store it

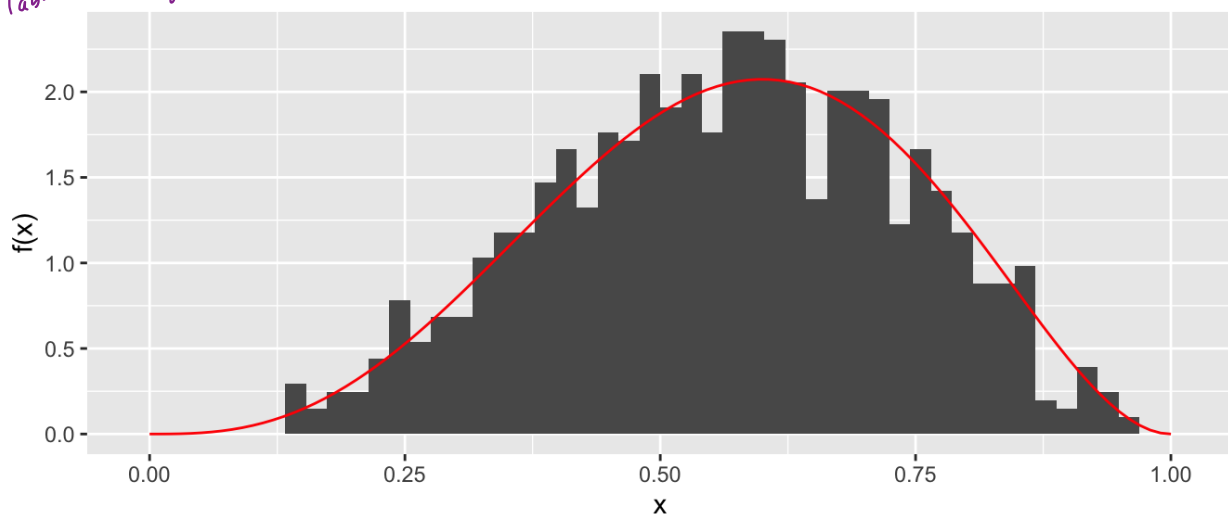
```
ggplot() +
  geom_histogram(aes(samples, y = ..density..), bins = 50, ) +
  geom_line(aes(x, f(x)), colour = "red") +
  xlab("x") + ylab("f(x)")
```

theoretical pdf.

labels for x, y axes.

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

important for your homework.



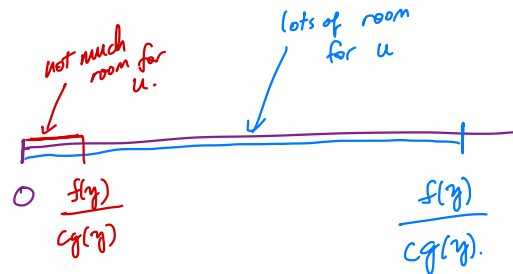
2.3 Why does this work?

Recall that we require

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

Thus,

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



The larger the ratio $\frac{f(y)}{cg(y)}$, the more the random variable $Y \sim g$ 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.
recommended text.
Come read in OIT or in library.

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 independent, 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 $X = \frac{U}{U+V} \sim \text{Beta}(r, s)$.

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

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

This is more complex...

but possible.

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

– change of variable

If g is monotone, then for cts X and

$Y = g(X)$,

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

– Moment generating functions

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

– Convolution theorem

$$Z = X + Y$$

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

Use computational statistical methods. we can simulate from transformed distribution.

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 $X_1 \sim f_{X_1}, \dots, X_p \sim f_{X_p}$. *either straightforward (named) or 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 $X_1, \dots, X_p \stackrel{iid}{\sim} N(0, 1)$, $Z = \sum_{i=1}^p X_i^2 \sim \chi_p^2$. Imagine that we cannot use the `rchisq` function. How would you simulate Z ?

① Simulate $X_1, \dots, X_p \sim N(0, 1)$.

② Compute $Z = \sum X_i^2$

③ repeat ①-②.

`library(tidyverse)`

`# function for squared r.v.s`

`squares <- function(x) x^2`

`sample_z <- function(n, p) {`

`# 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),`

of r.v.'s
df χ_p^2

this is n samples of
p $N(0, 1)$ indep.
r.v.'s.

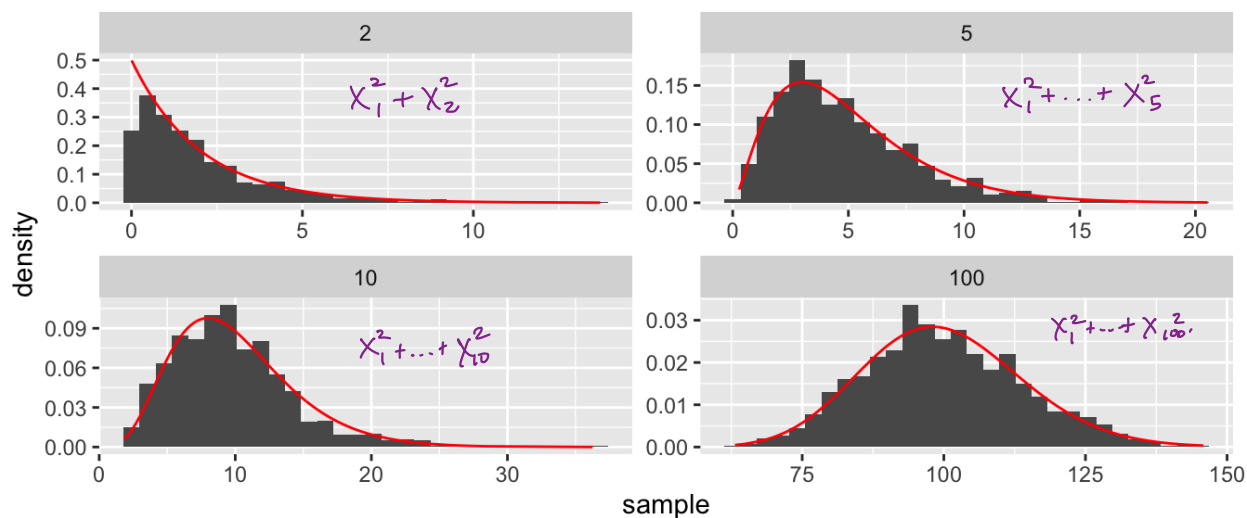
```

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, red.
  facet_wrap(~df, scales = "free")

```

density y scale (not count scale).



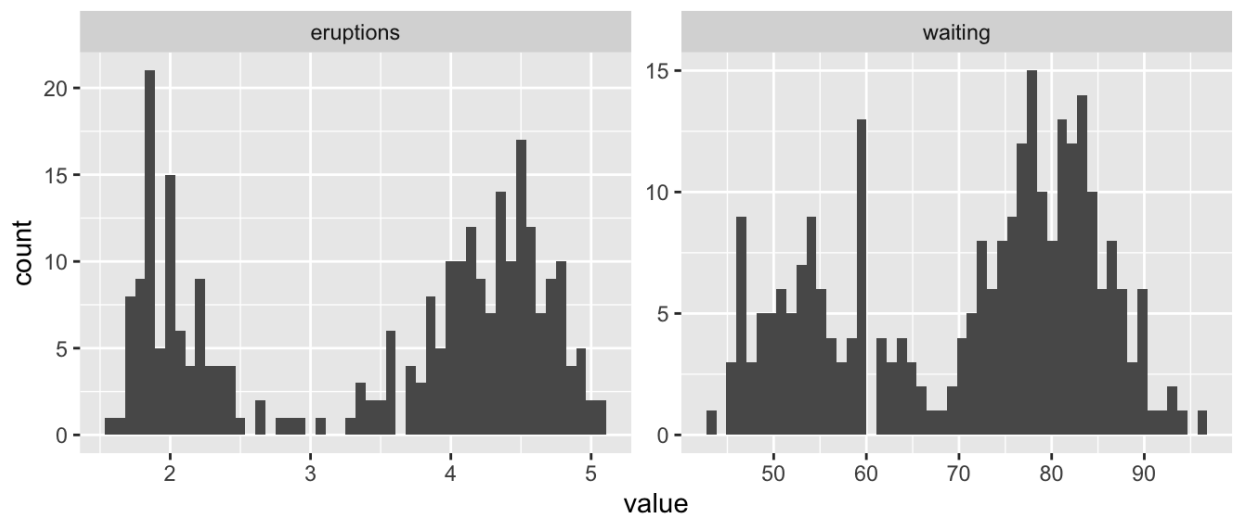
4 Mixture Distributions

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?

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, \dots and $\theta_i > 0$ such that $\sum \theta_i = 1$.

For 2 r.v.s,

Example 4.1

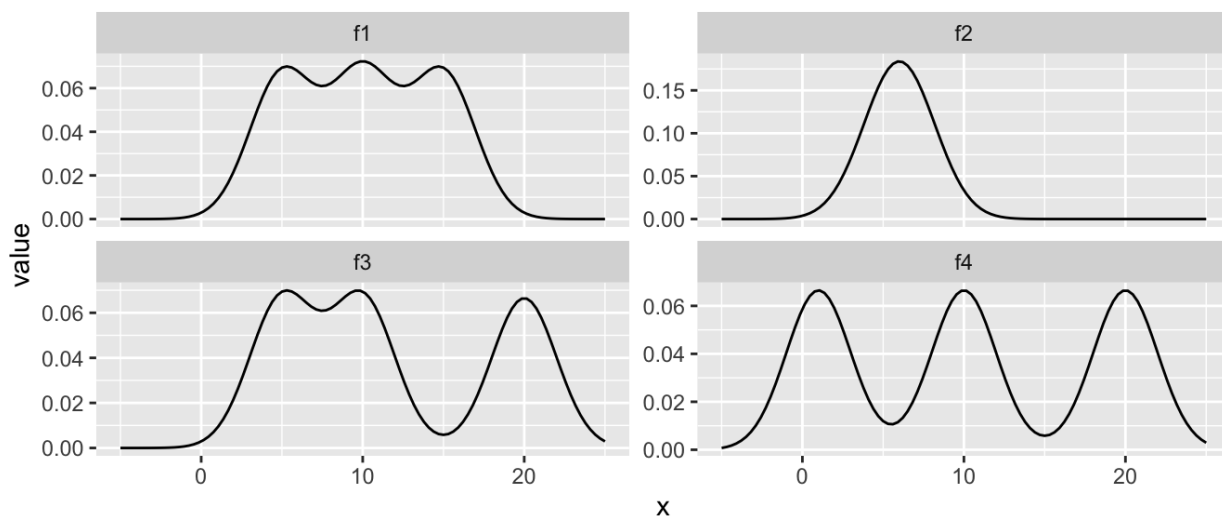
```

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.

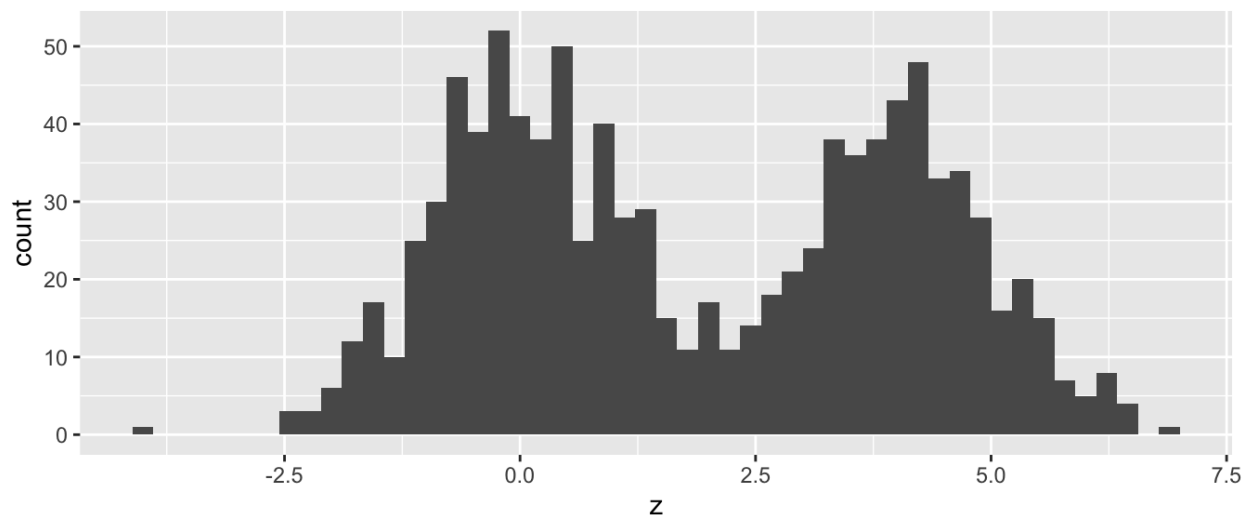
$$S = \frac{1}{2}(X_1 + X_2)$$

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

```
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)
```



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

4.2 Models for Count Data (refresher)

Recall that the $\text{Poisson}(\lambda)$ 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 occurring 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,

$$E[X] = \text{Var}X = \lambda.$$

Example 4.3

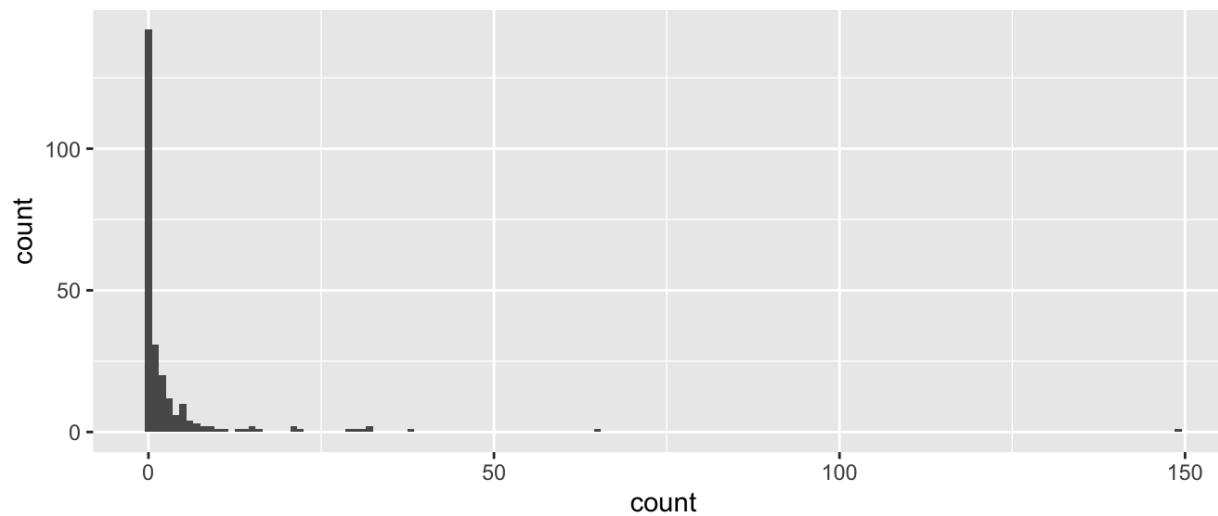
Example 4.4 The Colorado division of Parks and Wildlife has hired you to analyze their data on the number of fish caught in Horsetooth reservoir by visitors. Each visitor was asked - How long did you stay? - How many fish did you catch? - Other questions: How many people in your group, were children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

Some visitors 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.

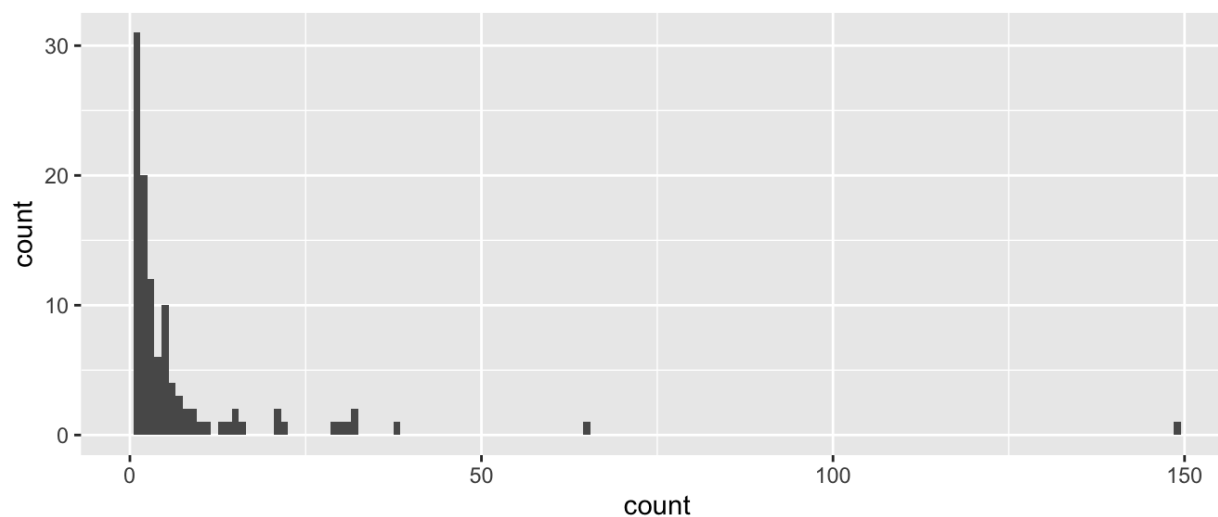
Note, this is modified from <https://stats.idre.ucla.edu/r/dae/zip/>.

```
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.

Example 4.5

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 $Y \sim ZIP(\lambda)$,

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

So that,

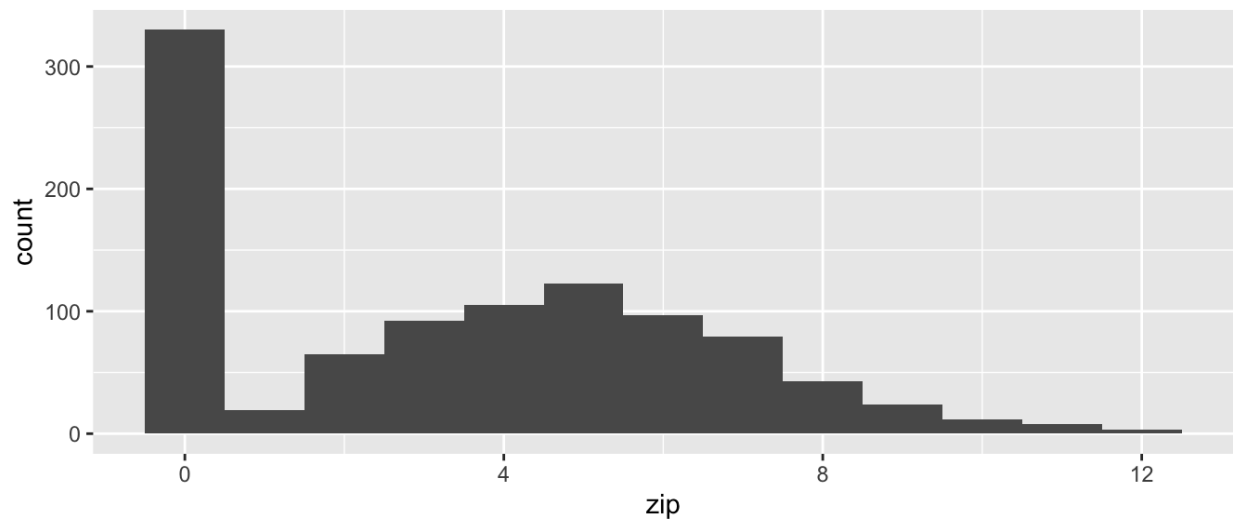
$$Y =$$

To simulate from this distribution,

```
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)
```

