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.
```

```
##  [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
```

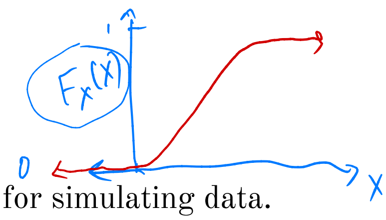
But what about when we don't have a function to do it?

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

1 Inverse Transform Method

"PIT"

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.

$$U = F_X(X)$$

$$F_X^{-1}(U) = F_X^{-1}(F_X(X)) = X$$

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 unif$(0,1)$.
   b. Compute $x = F^{-1}(u)$.

Typically repeat a-b many times.

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.

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

2. Find F^{-1}

   $$u = F(x) = x^3 \Rightarrow u^{1/3} = x = F^{-1}(u) \qquad 0 \leq u \leq 1$$

   range of $F(x)$.

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

① Write a function for F^{-1}

② Sample 1000 u values from Unif(0,1)

③ evaluate $x_i = F^{-1}(u_i)$ for $i = 1, \dots, 1000$.

1.2 Discrete RVs

If X is a discrete random variable and $\cdots < x_{i-1} < x_i < \cdots$ are the points of discontinuity (where cdf jumps) 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:

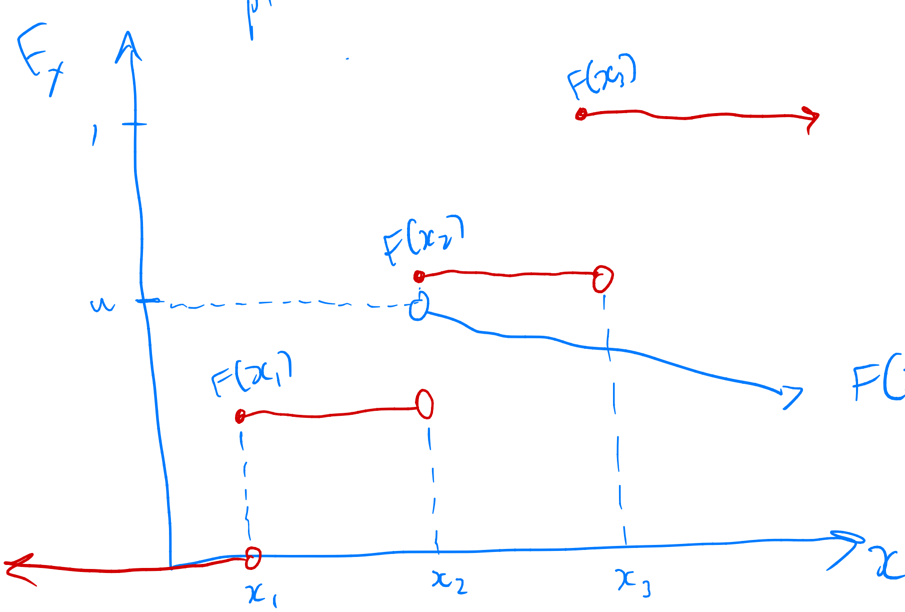
1. Generate a r.v. U from Unif$(0, 1)$.

2. Select x_i where $F_X(x_{i-1}) < U \leq F_X(x_i)$.

repeat many times.

discontinuity pt

① If $u = 0.5$ for example.



$F(x_1) < u \leq F(x_2)$.

$\Rightarrow$ ② 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 using sample() function in R.

* Remember to allow replacement and specify the probability vector if using sample() *

Something we can do if we can't find F^{-1} in closed form

2 Acceptance-Reject Method

specifies the distribution we want to sample from.

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

sample

Most cdfs cannot be inverted in closed form. ⟹ we can't use inverse transform method.

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

⟹ we reject the rest.

The method is outlined below:

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

target pdf

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

support of g must include the 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 efficency of the algorithm.

What might be hard/slow?

2.1 Algorithm

1. Find a suitable density g and envelope e. finding constant $c \geq 1$.

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.

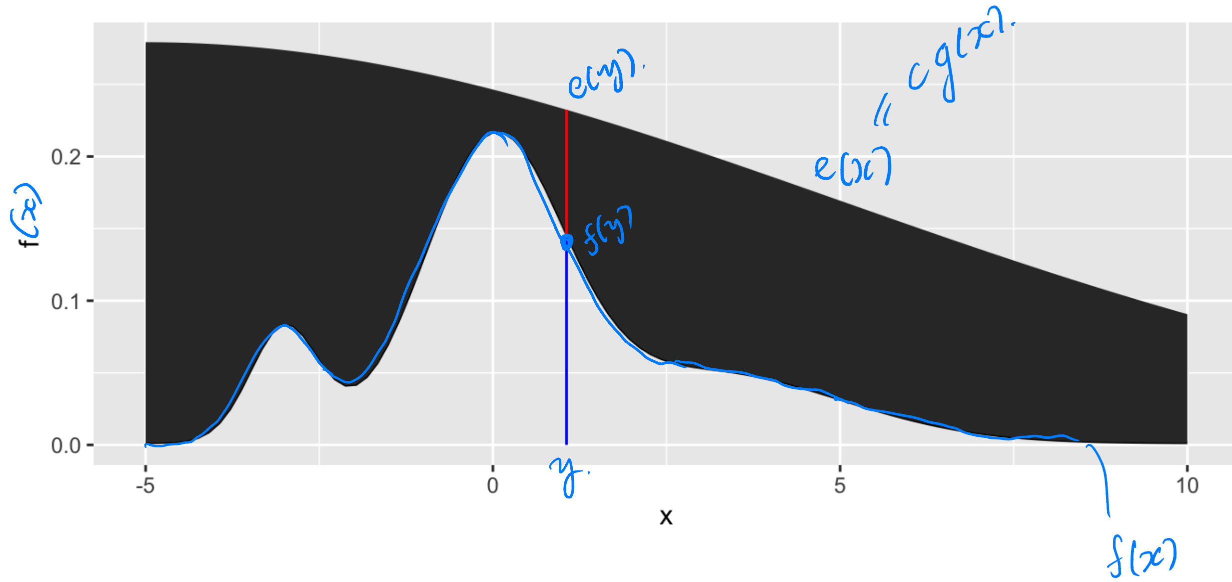
slow: we may throw away a lot of draws - depending on efficiency.

hard: finding $e(\,)$.

☆ 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 would NOT be appropriate because the support of f $\mathcal{X}_f = (-\infty, \infty)$, $\mathcal{X}_g = [-10, 10]$.



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 and easy to evaluate.
3. Generate few rejected draws (save time).

In some cases

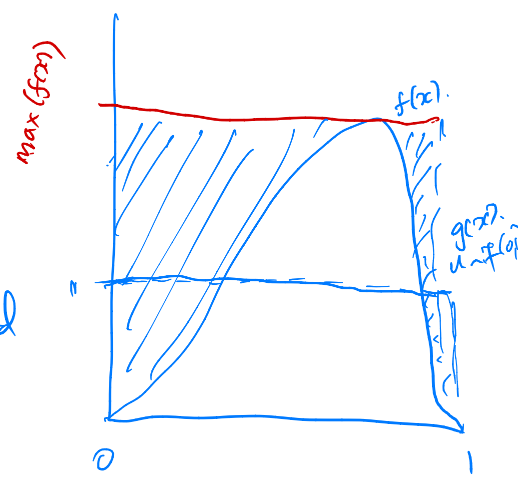
A simple approach to finding the envelope: Say the support of $X_f = [0,1]$.

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

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

This is ONLY USEFUL if support is $[0,1]$.

plotting is your friend here!



This may not be efficient if you know more about the shape, use it!

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.

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

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

could be $\boxed{x=0, x=1}$ ✗ $\boxed{x = \frac{3}{5}}$

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

$$c = f\left(\frac{3}{5}\right) = 2.0736$$

target pdf

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

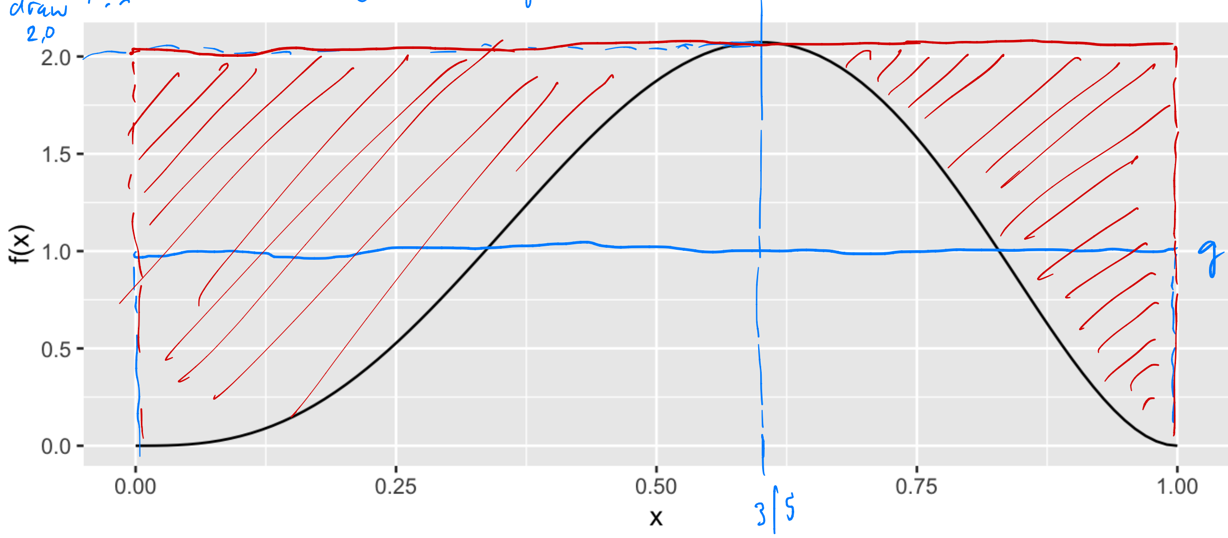
in base R.

make x values to evaluate f at.

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

draw line evaluate target pdf at x values.

$e(x) = c \cdot g(x)$



$g(x)$

FILL IN

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

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

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

empty vector of length n.

while we don't have enough accepted samples, keep going.

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

unif(0,1).

FILL IN

y <- runif(1).

```
  # sample u from uniform(0,1)
  u <- runif(1)
```

calculating the proportion.

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

increment accepted so my loop ends eventually.

store accepted sample.

plot histogram of samples w/ theoretical pdf on top.

samples from f obtained from accept-reject.

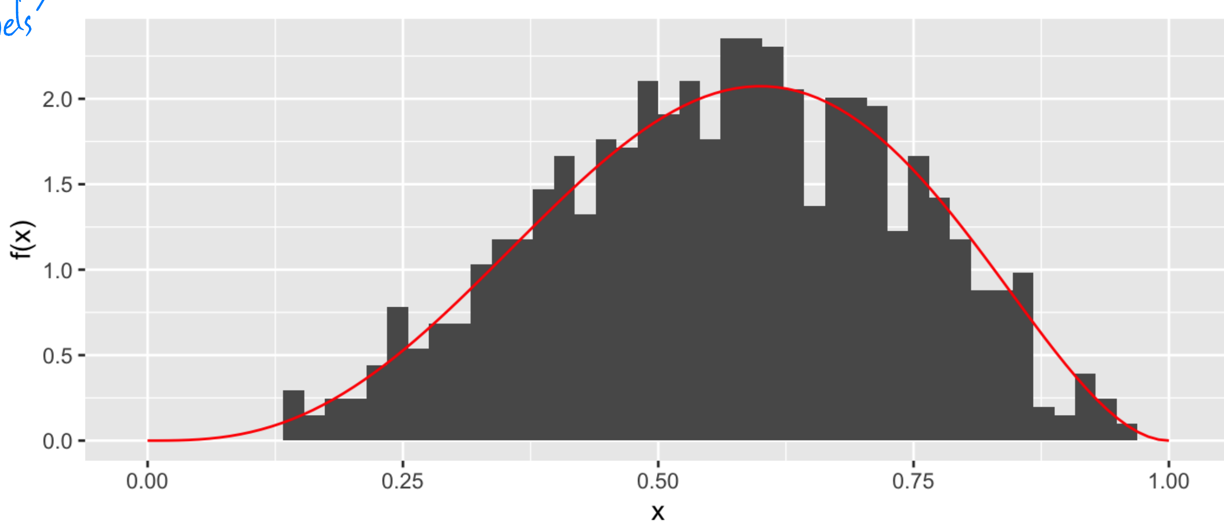
necessary so that histogram is on the same scale as the density instead of raw counts.

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

theoretical pdf

x & y labels

important for your hw!



2.3 Why does this work?

Recall that we require

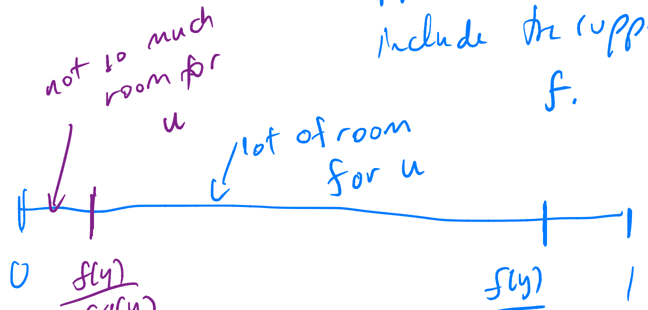
$e(y)$

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

and require support of g to include the support f.

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.

come read in OH or in library on reserve.

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 $V = Z^2 \sim$ χ^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 $X = \frac{U}{U+V} \sim$ 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. *

indep. & identically distributed, i.e. "random sample."

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 $\sum X_i \sim$ 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 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 function

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

– 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 $X_1, \dots, X_p$ 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 $X_1 \sim f_{X_1}, \dots, X_p \sim \boxed{f_{X_p}}$ / either be straight forward (named) could use inverse method, 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.

parameter of χ^2 dsn
- degrees of freedom
- controls shape of dsn.

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?

1. Sample p draws from the $N(0,1)$.
2. square all X's, sum them up. $\sum X_i^2$
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
}
```

we can change p - p = # r.v.'s, df of χ^2_p.

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

this will add up the p squared X's, n times.

```
# 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),
```

```
                    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")
```

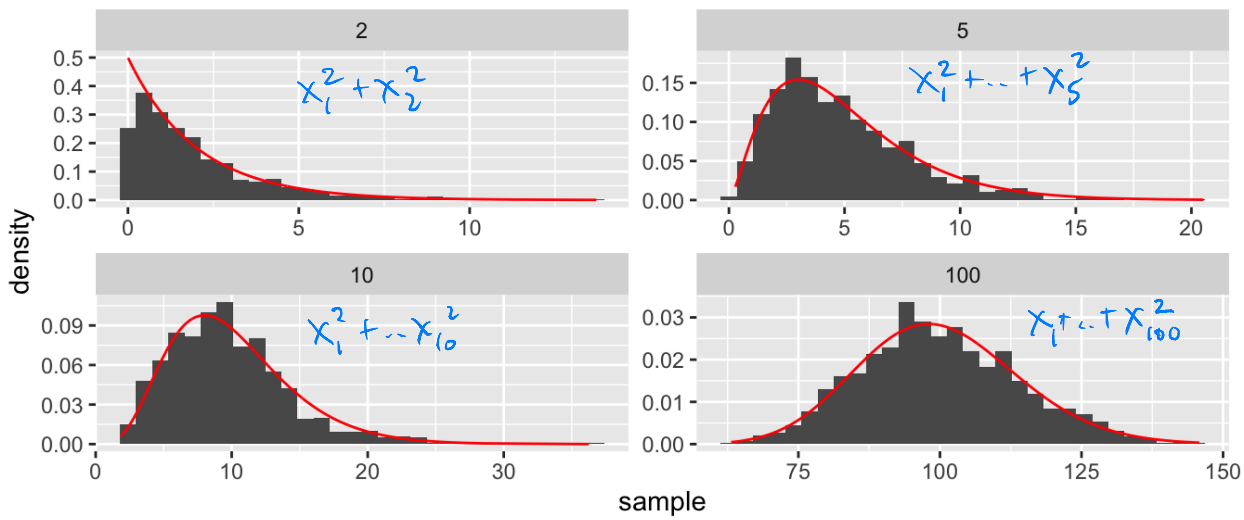
wide data → tall data

degrees of freedom

adds true density values

remember to plot on the same scale.

different scales for each df   scales = "free_y"   scales = "free_x"



4 Mixture Distributions

A special transformation.

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

```
head(faithful)
```

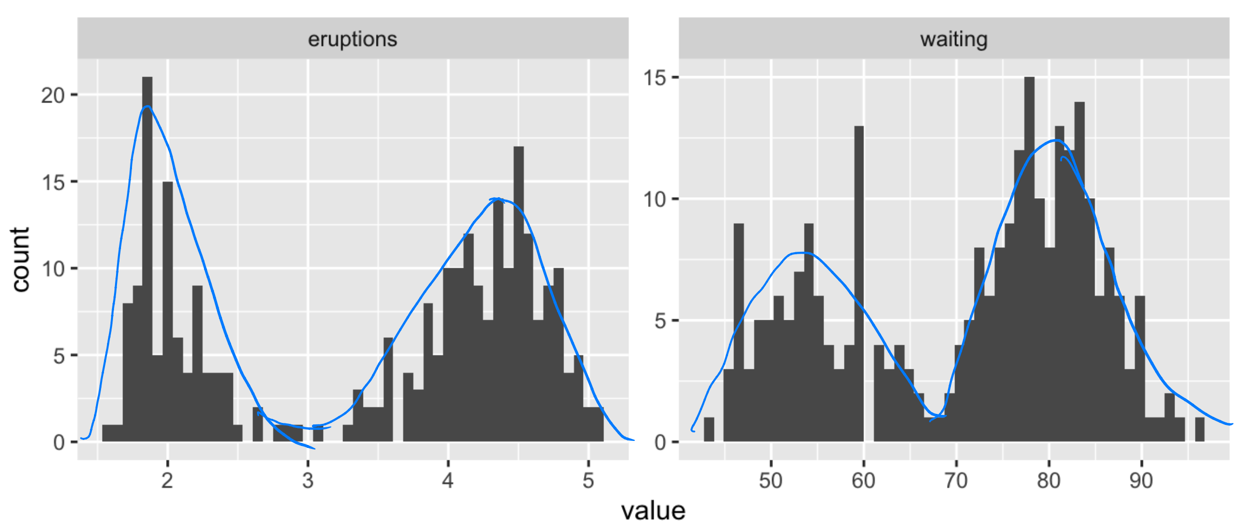
length of eruptions

waiting time until next eruption

```
##   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")
```

bimodal.



What is the shape of these distributions?

Bimodal

i.e. two modes.

does not mean discrete dsn.

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

summing countable # of distributions.

weights

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 two sources of variability.

with probability θ.

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

Example 4.1

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

vector of means

```
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))
```

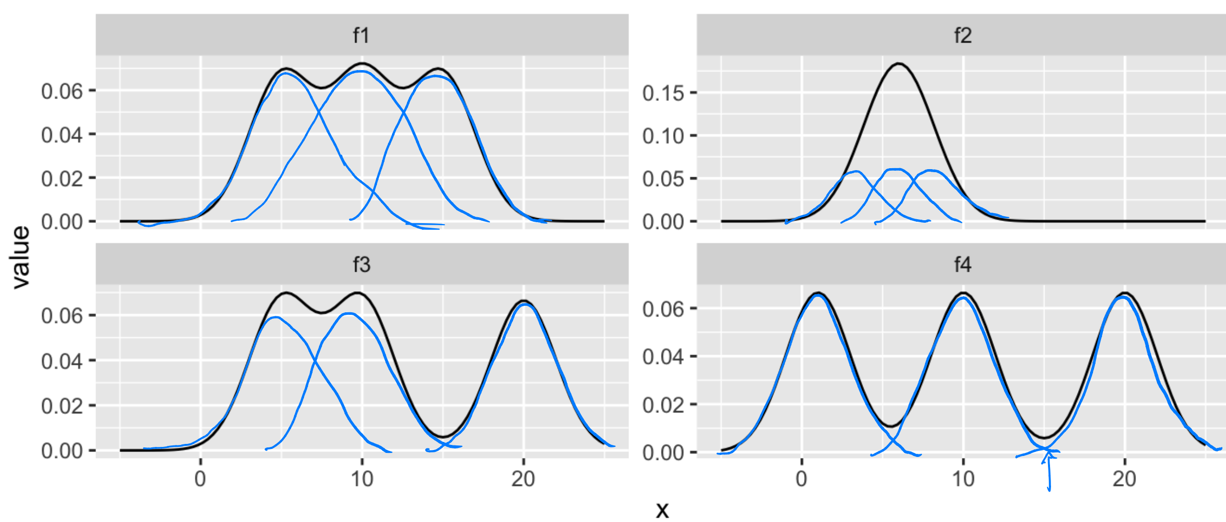
storage container to store pdf values.

```
  for(mean in means) {
    f <- f + dnorm(x, mean, sd)/length(means) # why do I divide?
  }
  f
}
```

I am equally weighting each dsn.

(we don't have to equally weight, we just need $\sum \theta_i = 1$).

```
# 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.

mixtures are weighted sums of distributions.

NOT distributions of weighted sums!

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.

$$E(S) = E\left(\tfrac{1}{2}(X_1+X_2)\right) = \tfrac{1}{2}(EX_1 + EX_2) = \tfrac{1}{2}(0+4) = 2.$$

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

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

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

$\overset{\shortparallel}{\theta}$

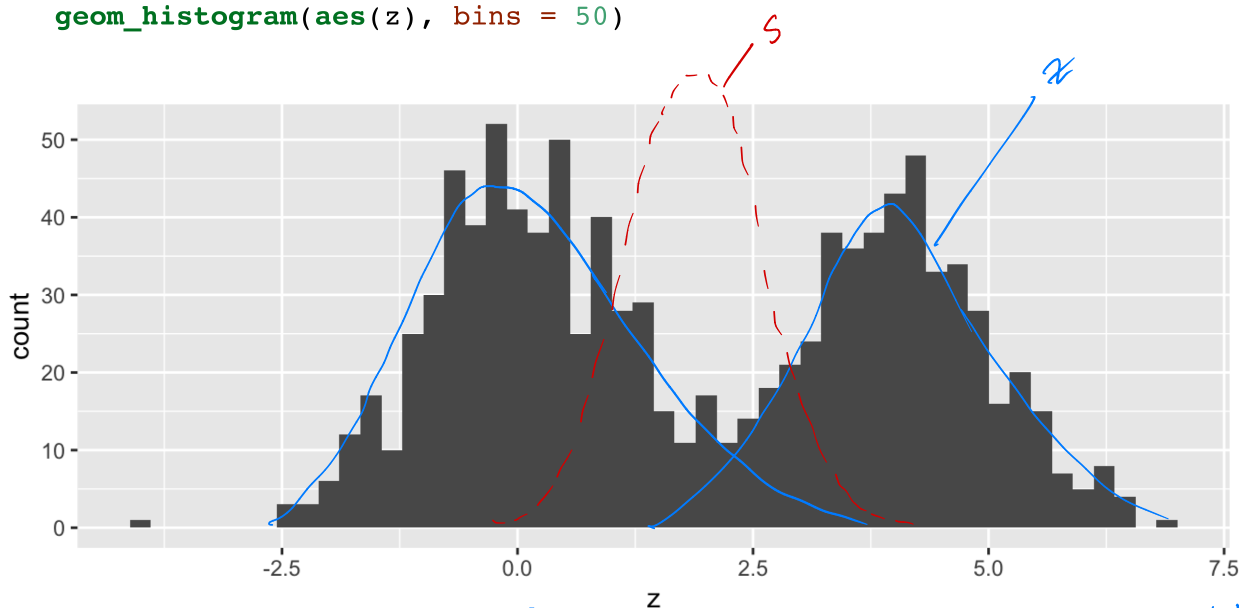
```
n <- 1000
u <- rbinom(n, 1, 0.5)
```

θ ← choose which dsn we sample from w/ $\theta = 0.5$.

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

$N(0,1)$ $N(4,1)$

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



$\theta = 0.7$ $1-\theta = 0.3$

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

"with probability"

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

4.2 Models for Count Data (refresher)

λ low

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 (λ) increases, the skewness goes away and the distribution becomes approximately normal.

high λ.

With the Poisson distribution,

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

restricts the shape of the dsn!

Example 4.3

- # of meows in a 2 minute cat video on youtube.
- # of baskets made in a minute.
- # of cars that drive by during class.

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.

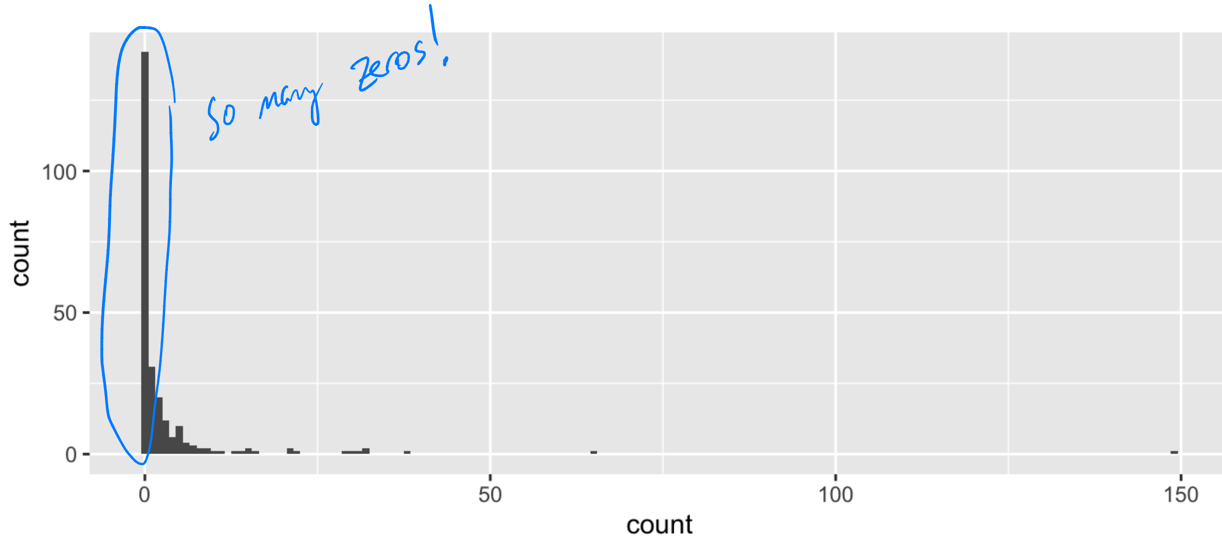
Note, this is modified from https://stats.idre.ucla.edu/r/dae/zip/.

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

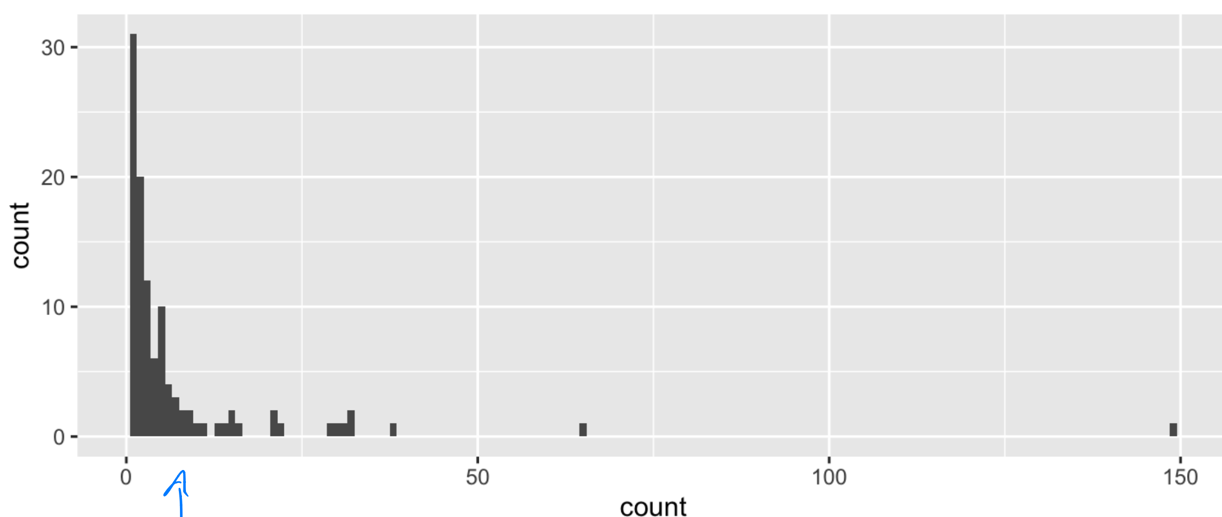
# of fish caught by each party.

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

so many zeros!




```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 zero is possible and occurs by random chance.

↳ a non-zero value is impossible.

Example 4.5

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

↳ structural zeroes - there are no cows in a region.

↳ sampling zeroes - cows in 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 zeroes

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,

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

To simulate from this distribution,

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

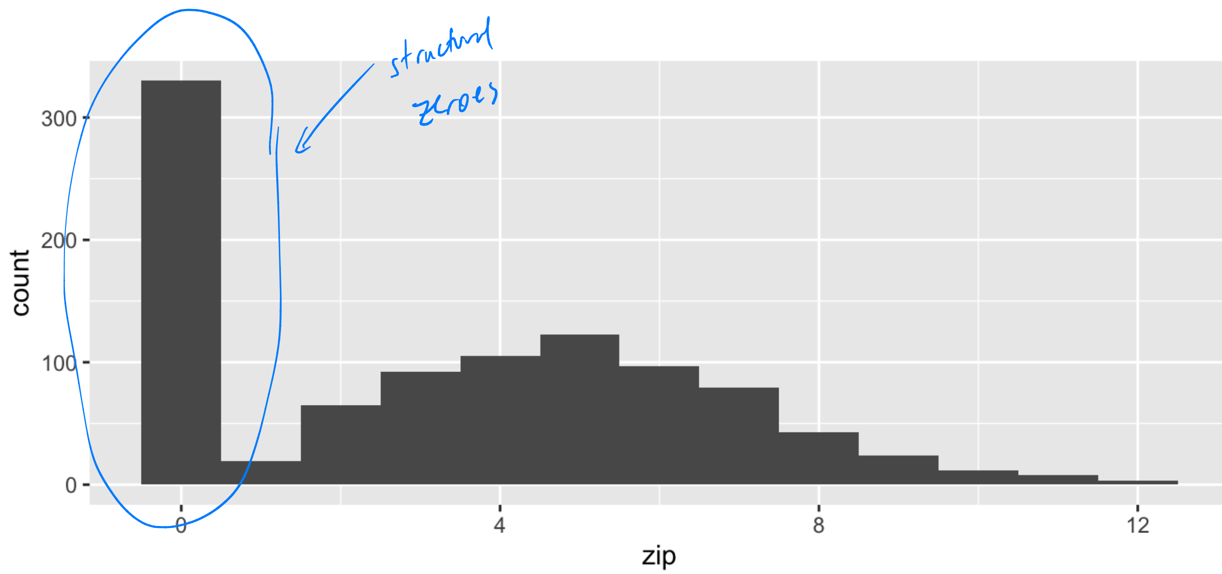
if $Z = 0$, $Y \sim \text{Poisson}(\lambda)$

if $Z = 1$, $Y = 0$

```
n <- 1000 ← how many samples
lambda <- 5 ← fix λ
pi <- 0.3   ← fix π

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

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




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