Bootstrapping and Resampling Methods

Stefan Eng

5/26/2021

Overview

- Resampling methods generally fall into one of 3 categories

1. Estimating the uncertainty of an estimator (bootstrapping, jackknife)
2. Performing significance tests by permuting data (permutation/randomization tests)
3. Validating models (bootstrapping, cross-validation)

- Resampling can be done with replacement or without replacement, depending on the purpose of the resampling method.

Bootstrapping Overview

"The population is to the sample as the sample is to the bootstrap samples." (Fox 2008)

- The basic idea is that we resample, with replacement, from our sample and use the distribution of those resamples to compute the standard error and confidence intervals.

Random Variable

- A random variable is a mapping (a function) $X : \Omega \to \mathbb{R}$ that assigns a real number $X(\omega)$ to each outcome ω.
- We almost never write $X(\Omega)$ but simply write X
- Example: Flip a coin and let X be the number of heads shown
- The sample space is $\Omega = \{\{H, H\}, \{H, T\}, \{T, H\}, \{T, T\}\}$

coin 1	coin 2	Number of heads
H	H	2
H	T	1
T	H	1
T	T	0

Random Variable - Dice Example

- The sample space is $\Omega = \{\{1,1\},\{1,2\},\{2,1\},\ldots\}$
- $X(\{3,4\}) = 7$

die 1	die 2	Sum of dice
1	1	2
1	2	3
2	1	3
1	3	4
2	2	4
3	1	4

Cumulative Distribution Function

For a random variable X, the **cumulative distribution function** (CDF), $F_X : \mathbb{R} \to [0, 1]$ is

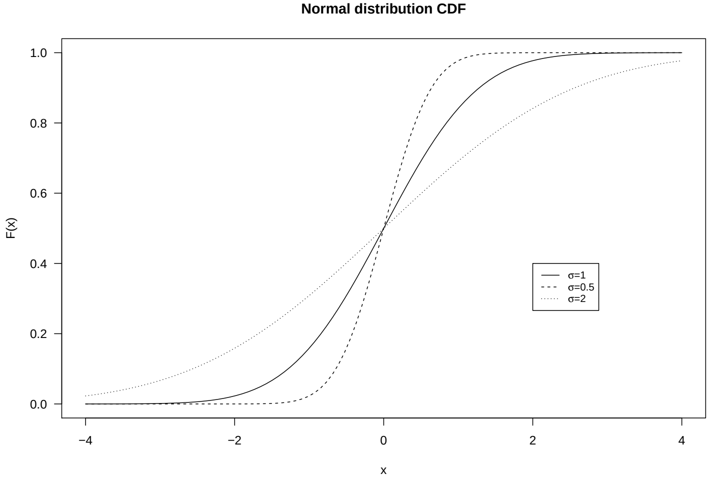
$$F_X(x) = P(X \leq x)$$

Notation

- If $X \sim F$ then we say that X has distribution F.
- For example, $X \sim \exp(\lambda)$ means that X is exponentially distributed with rate λ and

$$F(x) = \begin{cases} 1 - e^{-\lambda x} & x \geq 0 \\ 0 & x < 0 \end{cases}$$

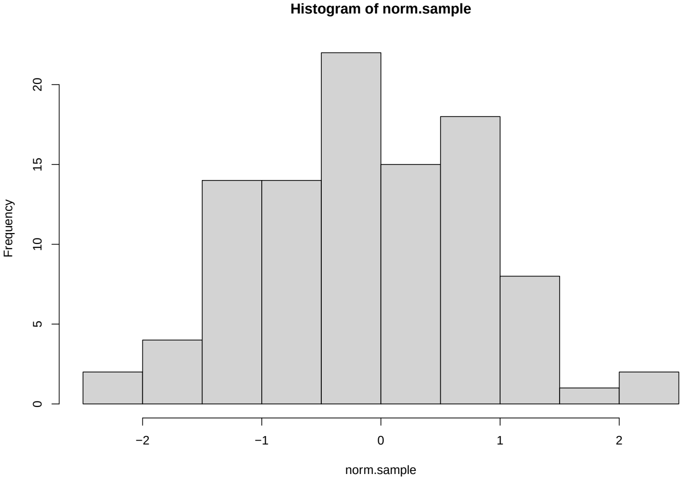
CDF - Normal



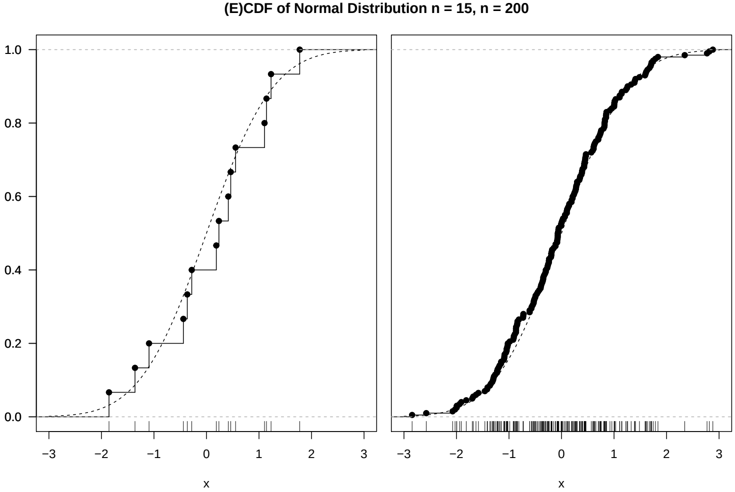
Empirical Distribution Function

- Let $X_1, \ldots, X_n \sim F$ be iid random variables
- Note that this means that X has a distribution function F.
- We can estimate F from the data by using the empirical distribution function $\hat{F}_n$.
- This distribution $\hat{F}_n$ puts probability of 1/n on each data point

Example - Normal Distribution



Example - Normal (E)CDF



Sampling Distribution

- Let $X_1, \ldots, X_n$ be iid random variables
- A function of the data is called a **statistic**
- The mean of these random variables is an example of a statistic

$$\overline{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i$$

- $\overline{X}_n$ is itself a random variable, and thus has a distribution (called the sampling distribution of the statistic).
- Example: If $X_1, \ldots, X_n \sim N(\mu, \sigma)$ then $\overline{X}_n \sim N\left(\mu, \frac{\sigma}{\sqrt{n}}\right)$

Statistical Inference

- Given a sample $X_1, \ldots, X_n \sim F$ we want to infer the distribution F.
- We approximate F using a statistical model, which is a set of distributions
  - Parametric models use a set of distributions that can be parameterized by a finite set of parameters.
  - Example: Two-parameter model for a set of Gaussians
  - Non-parametric models cannot be parameterized by a finite set of parameters

Example

- Say we have a sample of iid random variables $X_1, \ldots, X_n$.
- Computing the variance (and confidence intervals) of the mean is relatively easy.
- What about some arbitrary statistic: $T_n = g(X_1, \ldots, X_n)$?
  - Option 1: Do some possibly complicated mathematics.
  - Option 2: Bootstrap

Bootstrap

"The population is to the sample as the sample is to the bootstrap samples." (Fox 2008)

1. Compute $T_n = g(X_1, \ldots, X_n)$, our statistic of interest.
2. Draw a sample $X_1^*, \ldots, X_n^* \sim \hat{F}_n$ - All this means is to sample n times with replacement from the original data $X_1, \ldots, X_n$.
3. Compute our statistic of interest $T_n^* = g(X_1^*, \ldots, X_n^*)$
4. Repeat B times, to get $T_{n,1}^*, \ldots, T_{n,B}^*$
5. Compute the variance of $T_{n,1}^*, \ldots, T_{n,B}^*$ to get v_{boot}, and standard error $\hat{\text{se}}_{\text{boot}} = \sqrt{v_{\text{boot}}}$

Bootstrap

- Bootstraping does not improve our original estimate in any way
- The idea is to provide a way of estimating the uncertainty in the computed statistic
- Need to have a fairly large sample to get accurate estimation, especially if the statistic depends on a small number of observations (like the median).
- Highly skewed distributions may not work well for bootstrapping without a transformation

Approximations

$$\mathrm{Var}_F(T_n) \approx \mathrm{Var}_{\hat{F}_n}(T_n) \approx v_{\mathrm{boot}}$$

- Multiple approximations are happening during bootstrapping (different sources of error)
- First we approximate F with $\hat{F}_n$. Error depends on how big the sample is.
- Approximating $\mathrm{Var}_{\hat{F}_n}(T_n)$ by v_{boot} depends on the size of the bootstrap samples B.

Bias

The bias of an estimator $\hat{\theta}$ is

$$\mathsf{B} = E(\hat{\theta}) - \theta$$

We can estimate the bias with

$$\hat{\mathsf{B}} = E_{\hat{F}}(\hat{\theta}^*) - \hat{\theta}$$

That is, the difference between the mean of the bootstrap distribution and the observed statistic.

Bootstrap Confidence Intervals

- Once we have $\hat{\text{se}}_{\text{boot}}$ how do we compute a confidence interval?
- **Normal** Interval: Don't use unless distribution of T_n is close to normal. Can also replace $z_{\alpha/2}$ with $t_{\alpha/2,n-1}$ for more accurate intervals.

$$T_n \pm z_{\alpha/2}\hat{\text{se}}_{\text{boot}}$$

- **Percentile** Interval: Simply use the $\alpha/2$ and $1-\alpha/2$ quantiles of the bootstrap sample.
  - For small samples, may not be accurate
  - Benefit is that they are transformation invariant, you can apply a monotone transformation to the data and get the same CI after inverse transformation.
  - In general the following methods are more accurate though

Bootstrap Confidence Intervals

- **Basic** (Pivotal) Interval: Incorporate the bias into the confidence interval.
- **Studentized** Interval: Need to compute the standard error of each of the bootstrap samples
- **Bias Corrected, Accelerated (Bca)**: estimate a bias and acceleration term.
  - Corrects for skew in sampling distribution.
  - Requires a large number of bootstrap samples
  - Translation invariant

Bootstrap Example

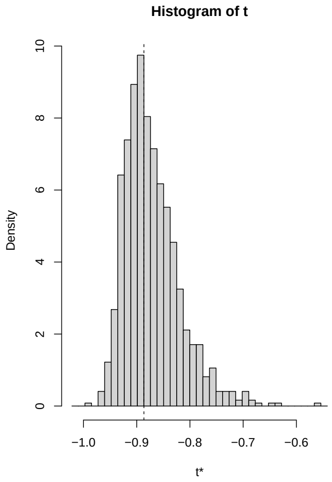
- `mtcars` built-in data set in R.
- Correlation of car weight and miles per gallon (mpg)

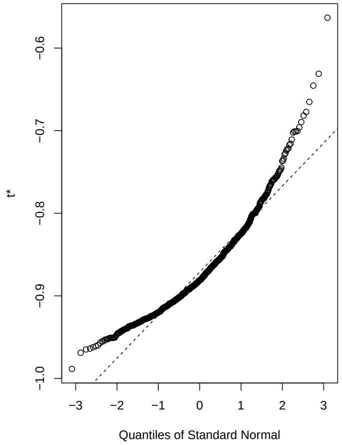
```
library(boot)
boot.cor <- function(data, indices) {
  d <- data[indices,]
  cor(d$wt, d$mpg, method = "spearman")
}

results <- boot(data=mtcars, statistic=boot.cor, R=1000)
results
```

Bootstrap Example

```
##
## ORDINARY NONPARAMETRIC BOOTSTRAP
##
##
## Call:
## boot(data = mtcars, statistic = boot.cor, R = 1000)
##
##
## Bootstrap Statistics :
##       original     bias    std. error
## t1* -0.886422 0.01517646  0.05213204
```

Bootstrap Example



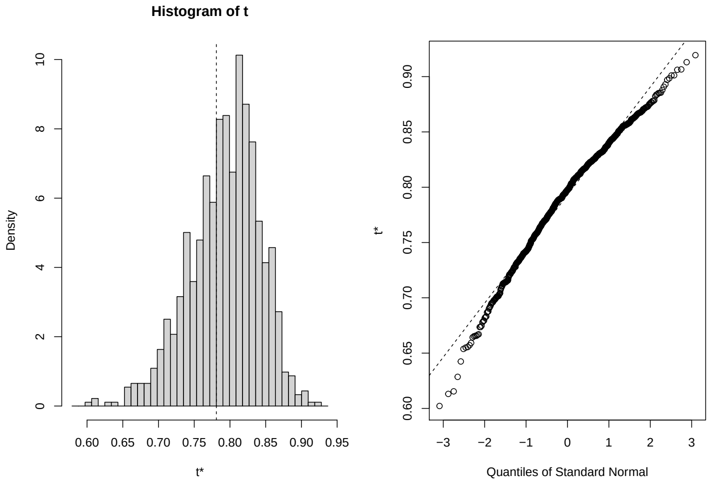


Bootstrap Confidence Intervals

```r
boot.ci(results, type = c("norm", "perc", "basic", "bca"))
```

```
## BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
## Based on 1000 bootstrap replicates
##
## CALL :
## boot.ci(boot.out = results, type = c("norm", "perc", "basic",
##     "bca"))
##
## Intervals :
## Level      Normal              Basic
## 95%   (-1.0038, -0.7994 )   (-1.0261, -0.8278 )
##
## Level     Percentile            BCa
## 95%   (-0.9450, -0.7468 )   (-0.9507, -0.7571 )
## Calculations and Intervals on Original Scale
```

Bootstrap Confidence Intervals



Bootstrap Confidence Interval

```
## BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
## Based on 1000 bootstrap replicates
##
## CALL :
## boot.ci(boot.out = results.R2, type = c("norm", "perc",
##     "bca"))
##
## Intervals :
## Level      Normal              Basic
## 95%   ( 0.6732,  0.8647 )   ( 0.6878,  0.8786 )
##
## Level     Percentile            BCa
## 95%   ( 0.6833,  0.8741 )   ( 0.6313,  0.8514 )
## Calculations and Intervals on Original Scale
## Some BCa intervals may be unstable
```

Bootstrap Linear Models

First we look at the estimates for `mpg ~ wt + disp`

```
mpg.mod <- lm(mpg ~ wt + disp, data = mtcars)
confint(mpg.mod)
```

```
##                   2.5 %       97.5 %
## (Intercept) 30.53357368 39.387534392
## wt          -5.73173459 -0.969916079
## disp        -0.03652128  0.001071794
```

Bootstrap Linear Models

```r
boot.lm <- function(formula, data, indices) {
  d <- data[indices,]
  coef(lm(formula, data = d))
}
results.lm <- boot(data=mtcars, statistic=boot.lm, R=1000,
                   formula = mpg ~ wt + disp)

# Confidence interval for wt coefficient
boot.ci(results.lm, type = c("basic", "bca"), index = 2)
```

Bootstrap Linear Models

```
## BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
## Based on 1000 bootstrap replicates
##
## CALL :
## boot.ci(boot.out = results.lm, type = c("basic", "bca"),
##
## Intervals :
## Level      Basic                    BCa
## 95%   (-5.391, -0.980 )   (-5.461, -0.852 )
## Calculations and Intervals on Original Scale
```

Other version of the bootstrap

What we have been doing is the nonparameteric bootstrap. Other options include

- **Semiparametric bootstrap**: Add noise to the resamples to produce non-identical resamples
- **Parametric bootstrap**: Assume the data comes from a known distribution and estimate the parameters given the data. Use this estimated distribution to draw samples.
- **Block bootstrap**: When the data is no longer iid, and correlations between data or errors exists.
  - For example, bootstrap on time-series data
  - See `boot::tsboot`

What can go wrong?

- If the data is skewed, need more bootstrap samples, and choose the confidence interval wisely
  - Very difficult in any situation to get CIs that are accurate
- Need to sample as the original data was sampled
  - This may involve resampling within groups
- Estimating parameters at the end of the parameter space
- Failure of $\hat{F}$ to estimate F.

Failing Example

$X_1, \ldots, X_n \sim \text{Uniform}(0, \theta)$. We want to estimate θ which has an MLE of

$$\hat{\theta} = X_{\max} = \max\{X_1, \ldots, X_n\}$$

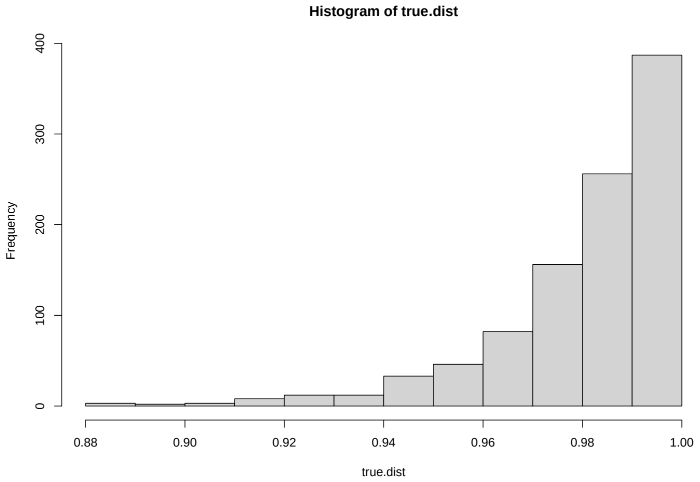
and it can be shown that

$$P(X_{\max} \leq x) = F_{X_{\max}}(x) = \left(\frac{x}{\theta}\right)^n$$

Uniform Max True Distribution

```r
true.dist <- replicate(1000, {
  x <- runif(50)
  max(x)
})
hist(true.dist)
```

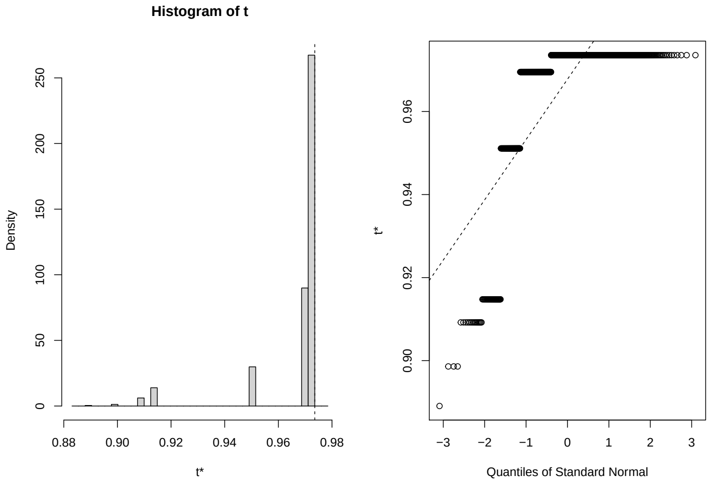
Uniform Max True Distribution



Bootstrap Uniform Max

```
x <- runif(50)
boot.max <- function(data, indices) max(data[indices])

results.max <- boot(data=x, statistic=boot.max, R=1000)
plot(results.max)
```

Bootstrap Uniform Max

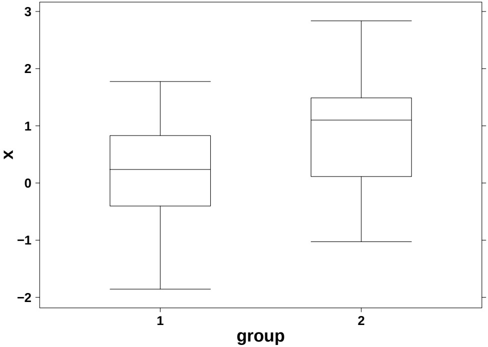


Permutation Tests

- We have seen how resampling can be used to quantify the uncertainty of an estimate
- Resampling methods can also be used to generate a null-distribution for a hypothesis test.
- Definition: **p-value** - The probability of obtaining test results *at least as extreme* as the observed results.
  - Easier conceptually to reason about with permutation tests than parameteric tests.

Simple Example - Comparing Means in Two Groups

- Two groups (each with 15 samples, unpaired) of normal distributions: $N(\mu_0 = 0, 1)$ and $N(\mu_1 = 1, 1)$.
- The null-hypothesis is that $\mu_0 = \mu_1$, one-sided alternative is $\mu_0 \neq \mu_1$.



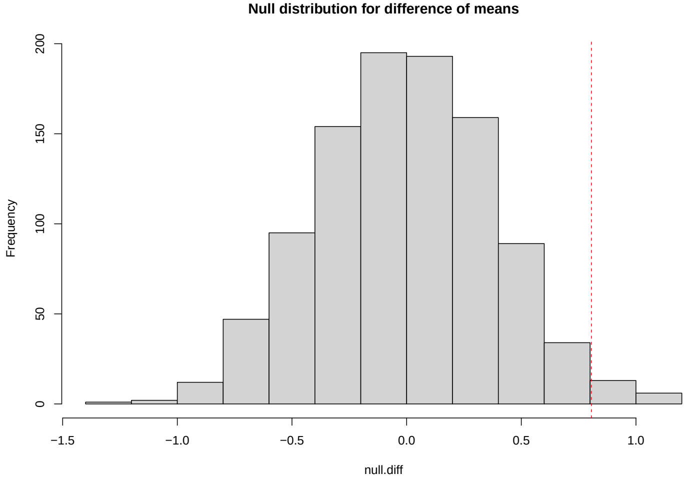
Simple Example - Comparing Means in Two Groups

- The difference in mean is 0.81
- Can perform a t-test (parametric)
  - t-statistic = -2.13
  - degrees of freedom $= 2n - 2 = 28$
- Can also use a permutation test

Permutation test example

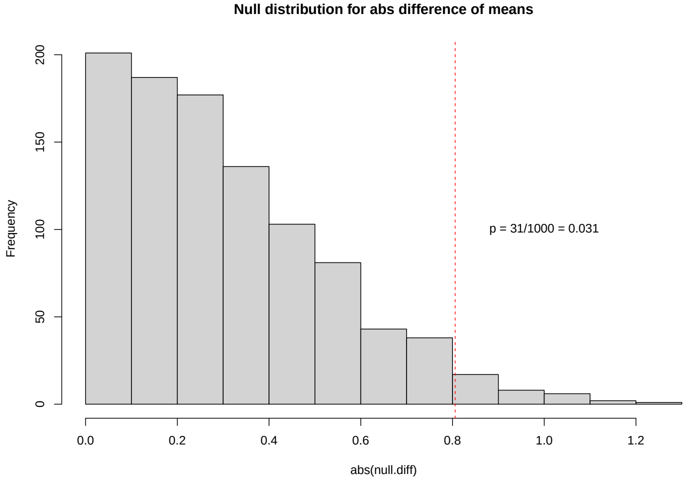
- Take the original data, shuffle (resample without replacement) either the data or the label
- Compute the test statistic for each permutation
- This distribution is the null distribution

Permutation - Null distribution



Permutation Test

- We can then compute the two-sided p-value by computing how many of the (absolute) null-differences are greater than the (absolute value) of the observed value



Permutation Test - two-sided

- Using a two-sided test in other cases is not as straightforward
- What is meant by “more extreme?”
- In the symmetric case, can just multiple by 2 times the smallest p-value
    - When the distribution is asymmetric, this can be completely incorrect and other methods need to be considered.

Example: Null is true (Rice 2008)

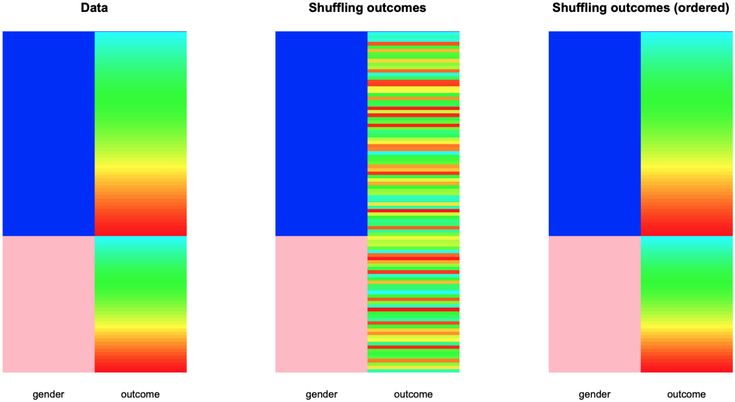


Figure 1: Null is true

Example: Null is false (Rice 2008)

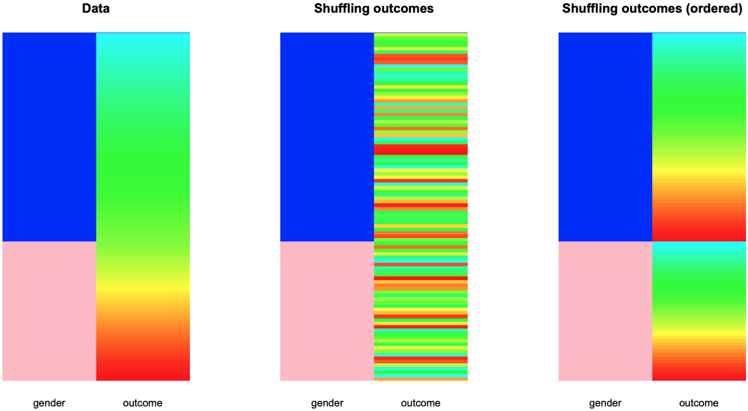


Figure 2: Null is false

Permutation Tests

- Using this simple example, it is easy to do either the t-test or the permutation test
- What parametric test would you do if we were comparing the medians across the groups? What about the skew between two groups?
  - Permutation test simplest option
- Even if sample size is quite large, if the data is largely skewed then t-test may completely inaccurate
  - $n \geq 5000$ for CLT to be accurate on exponential population

Summary

- Resampling methods are a simple way of:

1. Estimating the uncertainty of an estimator (bootstrapping, jackknife)
2. Performing significance tests by permuting data (permutation/randomization tests)
3. Validating models (bootstrapping, cross-validation)

References

- Bootstrap confidence intervals
- Permutation Tests
- What Teachers Should Know About the Bootstrap: Resampling in the Undergraduate Statistics Curriculum