Lecture 12

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The jackknife

The bootstrap
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The bootstrap

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The jackknife

- The jackknife is a tool for estimating standard errors and the bias of estimators

- As its name suggests, the jackknife is a small, handy tool; in contrast to the bootstrap, which is then the moral equivalent of a giant workshop full of tools

- Both the jackknife and the bootstrap involve *resampling* data; that is, repeatedly creating new data sets from the original data

The jackknife

- The jackknife deletes each observation and calculates an estimate based on the remaining $n - 1$ of them
- It uses this collection of estimates to do things like estimate the bias and the standard error
- Note that estimating the bias and having a standard error are not needed for things like sample means, which we know are unbiased estimates of population means and what their standard errors are

The jackknife

- We'll consider the jackknife for univariate data
- Let $X_1, \ldots, X_n$ be a collection of data used to estimate a parameter θ
- Let $\hat{\theta}_n$ be the estimate based on the full data set
- Let $\hat{\theta}_{i,n}$ be the estimate of θ obtained by *deleting observation i*
- Let $\bar{\theta}_n = \frac{1}{n} \sum_{i=1}^{n} \hat{\theta}_{i,n}$

Continued

- Then, the jackknife estimate of the bias is

$$(n-1)\left(\bar{\theta}_n - \hat{\theta}_n\right)$$

  (how far the average delete-one estimate is from the actual estimate)

- The jackknife estimate of the standard error is

$$\left[\frac{n-1}{n}\sum_{i=1}^{n}(\hat{\theta}_{i,n} - \bar{\theta}_n)^2\right]^{1/2}$$

  (the deviance of the delete-one estimates from the average delete-one estimate)

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Jackknife: intuition

Consider the case when the estimator $\hat{\theta}_n$ has bias of order n:

$$E(\hat{\theta}_n) = \theta + \frac{b}{n}$$

Then $E(\hat{\theta}_{i,n}) = \theta + \frac{b}{n-1}$ and

$$E(\bar{\theta}_n) = \theta + \frac{b}{n-1}$$

with the Jackknife estimator of the bias

$$(n-1)\{E(\bar{\theta}_n) - E(\hat{\theta}_n)\} = (n-1)\left\{\frac{b}{n-1} - \frac{b}{n}\right\} = \frac{b}{n}$$

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Jackknife: bias correction

For all estimators with a bias of the type $E(\hat{\theta}_n) = \theta + \frac{b}{n}$

$$\hat{\theta}_n - (n-1)(\bar{\theta}_n - \hat{\theta}_n)$$

is unbiased

$$\mathrm{ps}_{i,n} = \hat{\theta}_n - (n-1)(\bar{\theta}_{i,n} - \hat{\theta}_n) = n\hat{\theta}_n - (n-1)\hat{\theta}_{i,n}$$

are called pseudo-values; Jackknife: treat pseudo-values as independent
If $\hat{\theta}_n = \bar{X}_n$ then $\mathrm{ps}_{i,n} = X_i$.

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Jackknife: variance estimation

Assume that the variance of $\hat{\theta}_n$ is of the type σ^2/n

Then an estimator of σ^2/n is

$$\frac{1}{n}\{\frac{1}{n-1}\sum_{i=1}^{n}(\mathrm{ps}_{i,n} - \bar{\mathrm{ps}}_n)^2\} \approx \frac{1}{n}\{\frac{1}{n-1}\sum_{i=1}^{n}(\mathrm{ps}_{i,n} - \hat{\theta}_n)^2\}$$

As $(\mathrm{ps}_{i,n} - \hat{\theta}_n) = (n-1)(\hat{\theta}_n - \hat{\theta}_{i,n})$ the Jackknife formula for the variance estimator follows

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Pseudo observations

- Another interesting way to think about the jackknife uses pseudo observations

- Let

$$\mathrm{ps}_{i,n} = n\hat{\theta}_n - (n-1)\hat{\theta}_{i,n}$$

- Think of these as "whatever observation i contributes to the estimate of θ"

- When $\hat{\theta}_n$ is the sample mean, the pseudo observations are the data themselves

- Then the sample standard error of these observations is the previous jackknife estimated standard error.

- The mean of these observations is a bias-corrected estimate of θ

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Example

- Consider the data set of 630 measurements of gray matter volume for workers from a lead manufacturing plant
- The median gray matter volume is around 589 cubic centimeters
- We want to estimate the bias and standard error of the median

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Example

The gist of the code

```
n <- length(gmVol)
theta <- median(gmVol)
jk <- sapply(1 : n,
             function(i) median(gmVol[-i])
             )
thetaBar <- mean(jk)
biasEst <- (n - 1) * (thetaBar - theta)
seEst <- sqrt((n - 1) * mean((jk - thetaBar)^2))
```

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Example

Or, using the bootstrap package

```
library(bootstrap)
out <- jackknife(gmVol, median)
out$jack.se
out$jack.bias
```

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Example

- Both methods (of course) yield an estimated bias of 0 and a se of 9.94

- Fact: the jackknife estimate of the bias for the median is always 0 when the number of observations is even

- It has been shown that the jackknife is a linear approximation to the bootstrap

- Do not use the jackknife for sample quantiles like the median; it has been shown to have some poor properties

The bootstrap

- The bootstrap is a tremendously useful tool for constructing confidence intervals and calculating standard errors for difficult statistics

- For example, how would one derive a confidence interval for the median?

- The bootstrap procedure follows from the so called bootstrap principle

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Example: nonparametric bootstrap

- Given a vector of *n* subjects (rows, ...)
- "Nonparametric bootstrap": *B* resamples "with replacement"; each resample is done exactly *n* times

```
a=c("John","Sarah","Gina","Victor","Jimmy")
for (i in 1:6)
{print(sample(a,replace=TRUE))}

[1] "John"   "Jimmy"  "Sarah"  "Sarah"  "Victor"
[1] "Jimmy"  "Sarah"  "Victor" "Victor" "Victor"
[1] "Sarah"  "Jimmy"  "Sarah"  "John"   "Gina"
[1] "Victor" "Jimmy"  "Gina"   "Sarah"  "Jimmy"
[1] "John"   "Sarah"  "John"   "Victor" "Gina"
[1] "Sarah"  "John"   "Victor" "Jimmy"  "Victor"
```

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Set theory: an example

PID	BMI	SEX	AGE
1	22	1	45
2	27	0	57
3	31	1	66
4	24	1	49
5	23	0	33
6	18	0	40
7	21	0	65
8	26	1	59
9	34	1	65
10	20	0	42

Q: Construct a bootstrap CI for the difference in the mean BMI of women and men

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Example: nonparametric bootstrap

```
data_bmi=read.table(file=file.name,header=TRUE)
attach(data_bmi)

women_bmi<-BMI[SEX==1]
men_bmi<-BMI[SEX==0]
n_women<-length(women_bmi)
n_men<-length(men_bmi)

B_boot<-10000
mean_diff=rep(NA,B_boot)
for (i in 1:B_boot)
{#Begin bootstrap
mw<-mean(women_bmi[sample(1:n_women,replace=TRUE)])
mm<-mean(men_bmi[sample(1:n_men,replace=TRUE)])
mean_diff[i]<-mw-mm
}#End bootstrap
```

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Example: nonparametric bootstrap

```
mBoot<-mean(mean_diff)
sdBoot<-sd(mean_diff)

CI1<-c(mBoot-1.96*sdBoot,mBoot+1.96*sdBoot)
CI2<-quantile(mean_diff,probs=c(0.025,0.975))

>CI1
[1]  0.8176955 10.3444245

>CI2
 2.5% 97.5%
  0.8  10.4
```
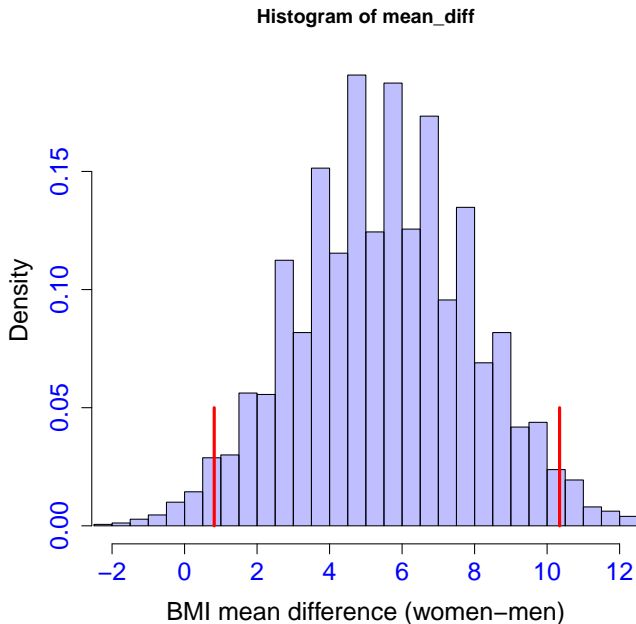
Histogram of mean_diff

Density

BMI mean difference (women–men)

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The bootstrap principle

- Suppose that I have a statistic that estimates some population parameter, but I don't know its sampling distribution

- The bootstrap principle suggests using the distribution defined by the data to approximate its sampling distribution

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The bootstrap in practice

- In practice, the bootstrap principle is always carried out using simulation
- We will cover only a few aspects of bootstrap resampling
- The general procedure follows by first simulating complete data sets from the observed data with replacement
- This is approximately drawing from the sampling distribution of that statistic, at least as far as the data is able to approximate the true population distribution
- Calculate the statistic for each simulated data set
- Use the simulated statistics to either define a confidence interval or take the standard deviation to calculate a standard error

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Example

- Consider again, the data set of 630 measurements of gray matter volume for workers from a lead manufacturing plant
- The median gray matter volume is around 589 cubic centimeters
- We want a confidence interval for the median of these measurements

- Bootstrap procedure for calculating for the median from a data set of n observations
    - *i.* Sample n observations **with replacement** from the observed data resulting in one simulated complete data set
    - *ii.* Take the median of the simulated data set
    - *iii.* Repeat these two steps B times, resulting in B simulated medians
    - *iv.* These medians are approximately draws from the sampling distribution of the median of n observations; therefore we can
        - Draw a histogram of them
        - Calculate their standard deviation to estimate the standard error of the median
        - Take the 2.5^{th} and 97.5^{th} percentiles as a confidence interval for the median

Example code

```
B <- 1000
n <- length(gmVol)   n observations
resamples <- matrix(sample(gmVol,
                           n * B,
                           replace = TRUE),
                    B, n)
medians <- apply(resamples, 1, median)
sd(medians)
[1] 3.148706
quantile(medians, c(.025, .975))
    2.5%    97.5%
582.6384 595.3553
```

density

Gray Matter Volume

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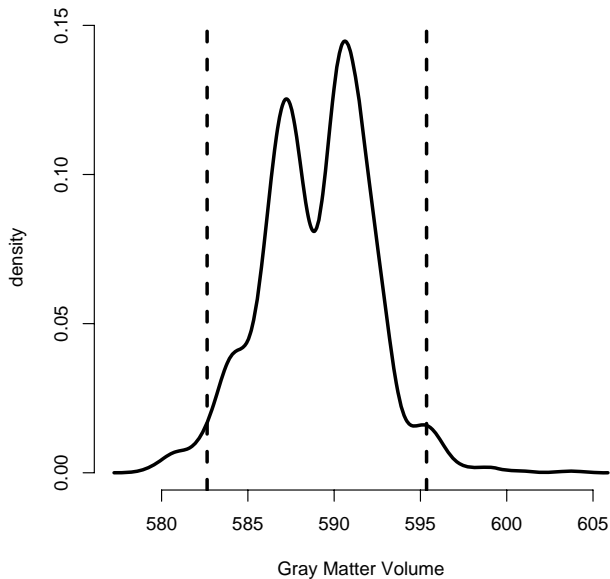
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Notes on the bootstrap

- This bootstrap procedure is non-parametric
- Essentially: 1) sample with replacement the population to create a similar population *of the same size*; 2) apply whatever procedure you want to this resampled population; 3) repeat; 4) aggregate results; 5) report results.
- Theoretical arguments proving the validity of the bootstrap rely on large samples
- There are lots of variations on bootstrap procedures; the book "An Introduction to the Bootstrap" by Efron and Tibshirani is a great place to start for both bootstrap and jackknife information

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```
library(boot)
stat <- function(x, i) {median(x[i])}
boot.out <- boot(data = gmVol,
                 statistic = stat,
                 R = 1000)
boot.ci(boot.out)
Level     Percentile          BCa
95%   (583.1, 595.2 )    (583.2, 595.3 )
```

Bradley Efron

- Bootstrap: Efron B (1979). Bootstrap methods: Another look at the jackknife. Annals of Statistics. 7, 126

- One of the most influential methods in Statistics

- A fundamental method based on understanding randomization

- B. Efron is Professor of Statistics at Stanford University