Bootstrapping

Mathematical Biostatistics Boot Camp

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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 $\hat{\theta}$ be the estimate based on the full data set
- Let $\hat{\theta}_i$ be the estimate of θ obtained by *deleting observation* i
- Let $\bar{\theta} = \frac{1}{n} \sum_{i=1}^{n} \hat{\theta}_i$

Continued

- Then, the jackknife estimate of the bias is

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

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

- The jackknife estimate of the standard error is

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

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

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

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))
```

Example

Or, using the `bootstrap` package

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

Example

- Both methods (of course) yield an estimated bias of 0 and a se of 9.94
- Odd little 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
- Generally do not use the jackknife for sample quantiles like the median; as it has been shown to have some poor properties

Pseudo observations

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

$$\text{Pseudo Obs} = n\hat{\theta} - (n-1)\hat{\theta}_i$$

- Think of these as ``whatever observation i contributes to the estimate of θ"
- Note when $\hat{\theta}$ 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

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

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

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

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 confidence interval 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

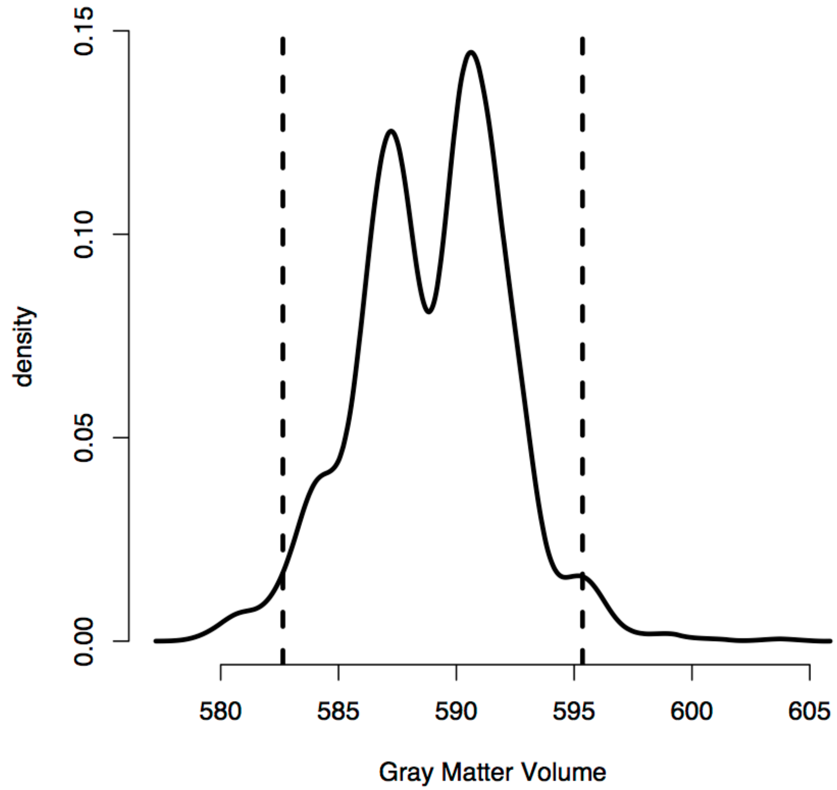
  iii. Repeat these two steps B times, resulting in B simulated medians

  iv. These medians are approximately drawn 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)
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
```


0.15
0.10
0.05
0.00
density
580
585
590
595
600
605
Gray Matter Volume

Notes on the bootstrap

- The bootstrap is non-parametric
- However, the theoretical arguments proving the validity of the bootstrap rely on large samples
- Better percentile bootstrap confidence intervals correct for bias
- 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 )
```