A gentle introduction to the bootstrap

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Outline

- History
- Algorithms
- Software
- Examples

Here is the abstract that I provided. I am including it here to remind myself what I promised to talk about.

The bootstrap is a methodology derived by Bradley Efron in the 1980s that provides a reasonable approximation to the sampling distribution of various "difficult" statistics. Difficult statistics are those where there is no mathematical theory to establish a distribution. It is also useful when you don't trust the mathematical theory because of a small sample size or potential violations of the underlying assumptions. The bootstrap is also a mechanism used by many machine learning algorithms to avoid overfitting. This talk will orient you to the general mechanisms of the bootstrap algorithm and illustrate its application in a couple of simple settings.

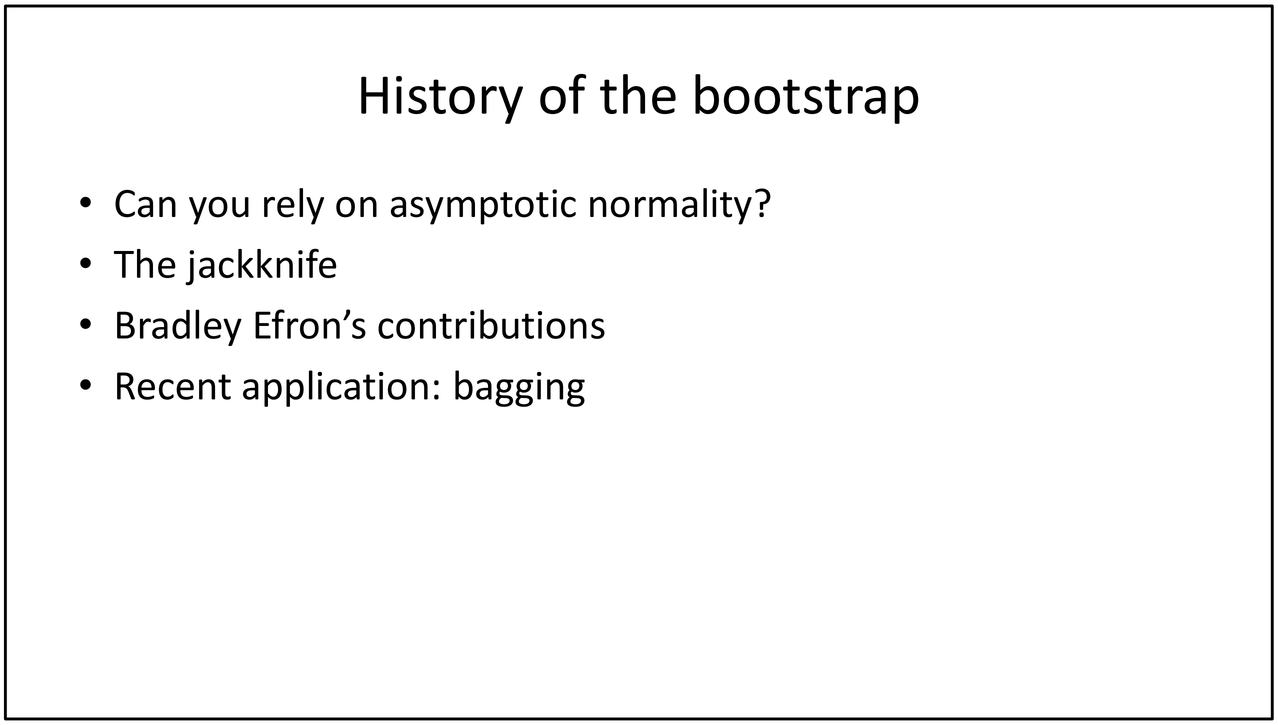
This talk will cover four major areas.

First, I will provide a historical overview, starting with a simpler method that the bootstrap was based on called the jackknife. Then I will talk about Bradley Efron's work to develop the bootstrap and establish its theoretical foundations. Then I will mention how bootstrapping has developed into a methodology used in machine learning called bagging.

Next, I will explain the reasons why you might want to use the bootstrap: to estimate bias, calculate standard errors, compute confidence intervals, test hypotheses, and to visualize variations in statistical plots.

I will illustrate the mechanics of the bootstrap and show briefly how to implement the bootstrap in SAS, Stata, and R.

Then I will discuss some special cases where you might consider more complex forms of bootstrapping.



History of the bootstrap

- Can you rely on asymptotic normality?
- The jackknife
- Bradley Efron's contributions
- Recent application: bagging

I want to provide a bit of historical context. Before the bootstrap came along, researchers relied on a variety of mathematical theorems like the Central Limit Theorem and extensions to the Central Limit Theorem to estimate bias, calculate standard errors, produce confidence intervals, and test hypotheses.

The bootstrap represents an early attempt to use the power of computer simulation to estimate bias, calculate standard errors, produce confidence intervals, and test hypotheses. The bootstrap provides these answers in many settings where you can't find a variation on the Central Limit Theorem that would apply or when you don't trust the approximation. I'll provide a brief overview of the jackknife, an earlier approach that the bootstrap was based on. Then I'll talk about Bradley Efron's work in the 1970's and 1980's to develop the bootstrap and to establish the mathematical principles that make the bootstrap work in so many different areas. Finally, I will talk about how bootstrapping came to be relied on in various machine learning algorithms.

Can we rely on asymptotic normality? (1/4)

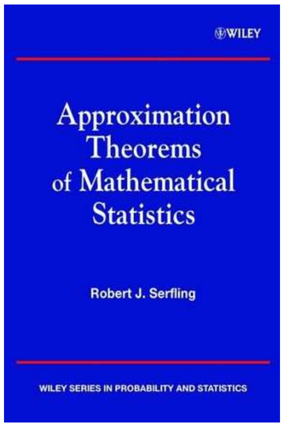

WILEY
Approximation Theorems of Mathematical Statistics
Robert J. Serfling
WILEY SERIES IN PROBABILITY AND STATISTICS

Figure 1. Cover of book by Robert Serfling

I need to start with a book that I used when I was in graduate school. The title is "Approximation Theorems in Mathematical Statistics" by Robert Serfling. It was all about the variety of ways to show that some statistic followed an asymptotic normal distribution.

Can we rely on asymptotic normality? (2/4)

- $\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$ is approximately normal if
  - The X_i all come from the same distribution
  - The X_i are all independent
  - The X_i have a finite second moment
- A more precise statement
  - $lim(n \to \infty)\ \frac{\bar{X}-\mu}{\sigma/\ \sqrt{n}} = N(0,1)$

I’m sure you’re all familiar with the Central Limit Theorem. It’s the graddaddy of all approximation theorems. It states that the average of independent identically distributed random variables is approximately normal.

The rule of thumb is that you can trust the normal approximation when the sample size is greater than 30. There is a lot that you can quibble about with respect to the cut-off of 30, but we’re not going to get too fussy about this.

Can we rely on asymptotic normality? (3/4)

Furthermore,

$$E[\bar{X}] = \mu$$

$$Var(\bar{X}) = \frac{\sigma^2}{n}$$

$$std.err(\bar{X}) = \frac{\sigma}{\sqrt{n}}$$

You can also show easily that the expected value of the sample mean is mu (the sample mean is an unbiased estimate of the population mean) and that the variance of the sample mean is the variance of an individual X value divided by the sample size n. Equivalently, the standard error of X=bar is the standard deviation of an individual value divided by the square root of the sample size.

Can we rely on asymptotic normality? (4/4)

What about:

$$MAD(X) = \frac{1}{n}\sum_{i=1}^{n}|X_i - \bar{X}|$$

$$IQR = X_{.75} - X_{.25}$$

$$n < 30$$

What about more complex settings?

What if you are measuring the mean absolute deviation (the average of the absolute values of each individual value minus the sample mean) or the interquartile range (the difference between the 75th percentile and the 25th percentile).

If you are really clever and if you understand all the approximation theorems in Robert Serfling's book, you will know how to establish an approximation to these statistics (usually a normal approximation, but sometimes there are other distributions like the chi-square distribution that represent a good approximation).

But an even more fundamental question is what do you do when the sample size is not large enough to justify the use of the Central Limit Theorem? I put down n<30 here, but in some settings (well behaved distributions without much skewness and only a weak tendency to produce outliers), you might get by with only 10 observations. Other times (extremely skewed distributions and/or a strong tendency to produce outliers), even a sample size of 300 is inadequate to assume an approximately normal distribution.

It turns out that you can use simulations involving the data itself to establish an underlying distribution.

You might find that the normal distribution is a reasonable approximation. If so, great! Consider the bootstrap to be a sensitivity check that you passed with flying colors.

If the results of the bootstrap are markedly different from the results assuming approximate normality, then investigate further. But you can rely on the bootstrap results to provide valid confidence intervals and hypothesis tests. Although there are a few settings where you shouldn’t rely on a bootstrap approach, it is a credible approach for a surpringly broad range of settings.

The jackknife (1/4)

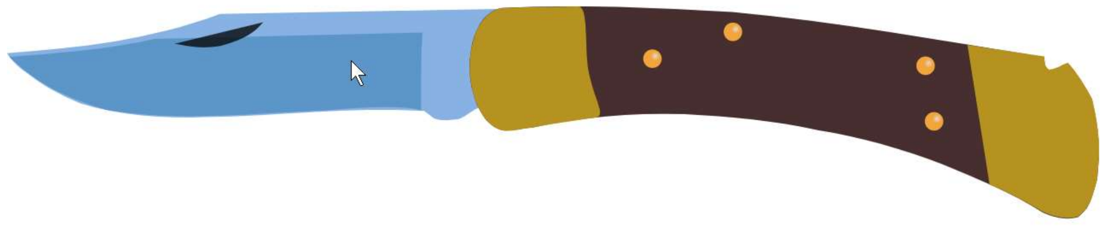


Figure 1. Image of a jackknife

To understand the bootstrap, you need to understand the approach that it was intended to improve upon, the jackknife.

The jackknife was first developed in 1949 by Maurice Quenouille and was extended to a more general setting by John Tukey in the 1950s. Dr. Tukey was fond of giving clever names to various statistical terms. He was the one, for example, who coined the term “bit” as a shorted form of binary digit. He chose the name “jackknife” for the Quenouille approach because the jackknife is an all-purpose tool.

The jackknife (2/4)

$$X \quad = (2,3,7,5,6)$$

$$\begin{aligned} X^{(-1)} &= (\ \ ,3,7,5,6) \\ X^{(-2)} &= (2,\ \ ,7,5,6) \\ X^{(-3)} &= (2,3,\ \ ,5,6) \\ X^{(-4)} &= (2,3,7,\ \ ,6) \\ X^{(-5)} &= (2,3,7,5,\ \ ) \end{aligned}$$

For the jackknife, you create subsamples by leaving one data point out.

The original data set in this small artificial example is 2, 3, 7, 5, 6. The first subsample leaves out the 2. The second subsample leaves out the 3. And so forth. With five data points, you have five subsamples.

The jackknife (3/4)

MAD (2, 3, 7, 5, 6) = 1.68

MAD (3, 7, 5, 6) = 1.25

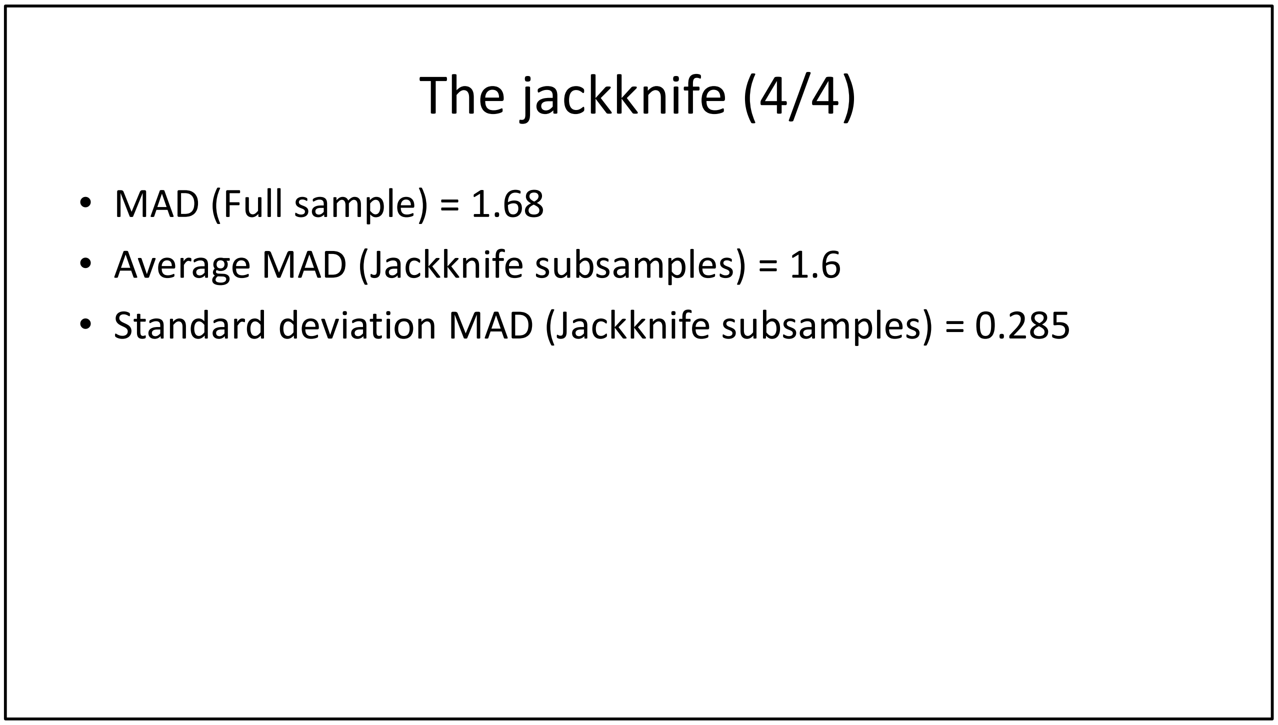
MAD (2, 7, 5, 6) = 1.5

MAD (2, 3, 5, 6) = 1.5

MAD (2, 3, 7, 6) = 2

MAD (2, 3, 7, 5) = 1.75

Then calculate a statistic (in this case, the mean absolute deviation). Do it first for the entire sample. Then do it for each jackknife subsample. Notice that there is some variation in the results from one jackknife subsample to another.



The jackknife (4/4)

- MAD (Full sample) = 1.68
- Average MAD (Jackknife subsamples) = 1.6
- Standard deviation MAD (Jackknife subsamples) = 0.285

The average of the jackknife subsamples is a bit less than 1.68. This indicates a small amount of bias, though I would argue that the size of the bias is manageable. The standard deviation of the jackknife subsamples is around 0.3 (I'm rounding liberally here). This standard deviation is a reasonable estimate for the standard error of the mean absolute deviation. So plus or minus two standard errors gives you an approximate confidence interval from 1.0 to 2.2. A fair amount of imprecision, but hardly surprising for a dataset with a total sample size of 5.

Bradley Efron's contribution (1/5)

Figure 1. Photograph of Bradley Efron with President Bush

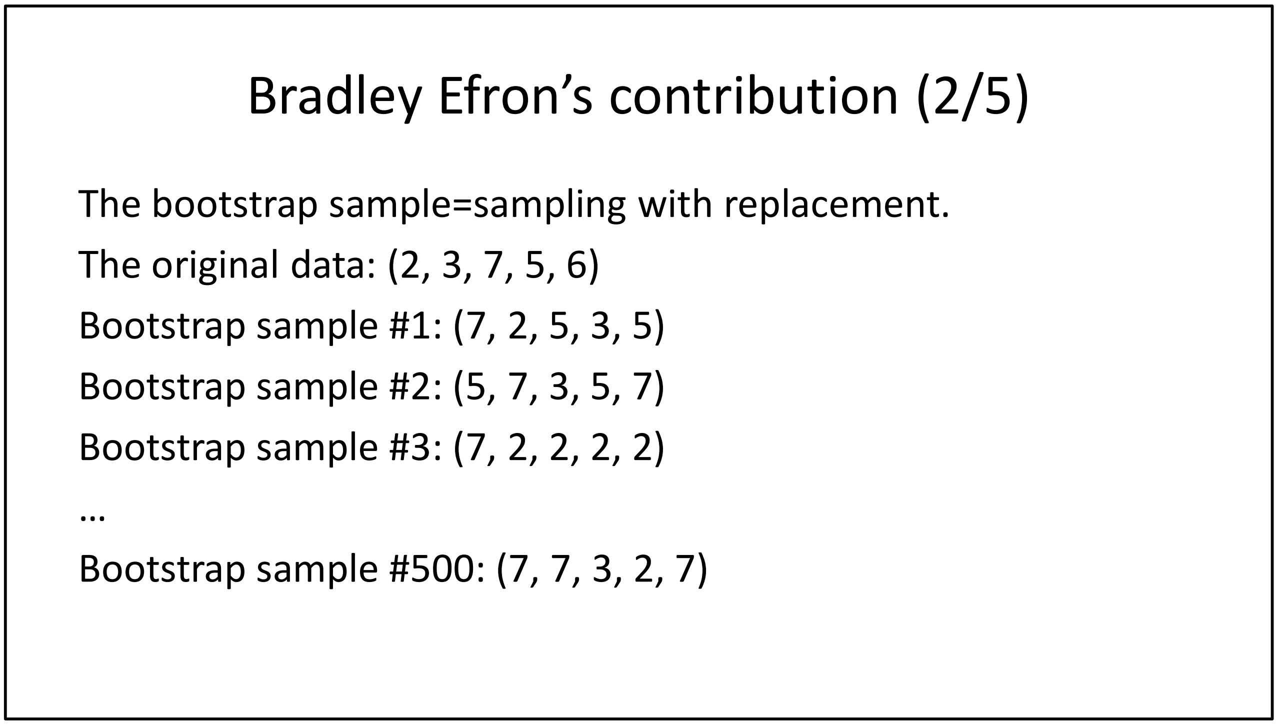
This image is from a White House ceremony where Bradley Efron received the President's National Medal of Science. I was quite shocked when I found this picture a few days ago, and I've been trying to call Joe Biden ever since to see where my medal is. Seriously, you have to be a really special statistician to deserve an honor like this.

Most of the information about Bradley Efron comes from

Denise LaFontaine. The History of Bootstrapping: Tracing the Development of Resampling With Replacement. The Mathematics Enthusiast 2021, 18(1). Available in pdf format.

Bradley Efron entered the PhD program in Statistics at Stanford University in 1960. He was influenced by one of the faculty at Stanford, Rupert Miller, who was working on establishing conditions under which the jackknife did or did not perform well. Shortly after graduating, Dr. Efron started working on an approach that would fix some of the shortcomings of the jackknife.

It turns out that the jackknife works in a variety of settings, but fails badly for certain statistics like the median and the interquartile range. The bootstrap handles all the cases that the jackknife handles but also handles quite a few that the jackknife can't.



Bradley Efron's contribution (2/5)

The bootstrap sample=sampling with replacement.

The original data: (2, 3, 7, 5, 6)

Bootstrap sample #1: (7, 2, 5, 3, 5)

Bootstrap sample #2: (5, 7, 3, 5, 7)

Bootstrap sample #3: (7, 2, 2, 2, 2)

…

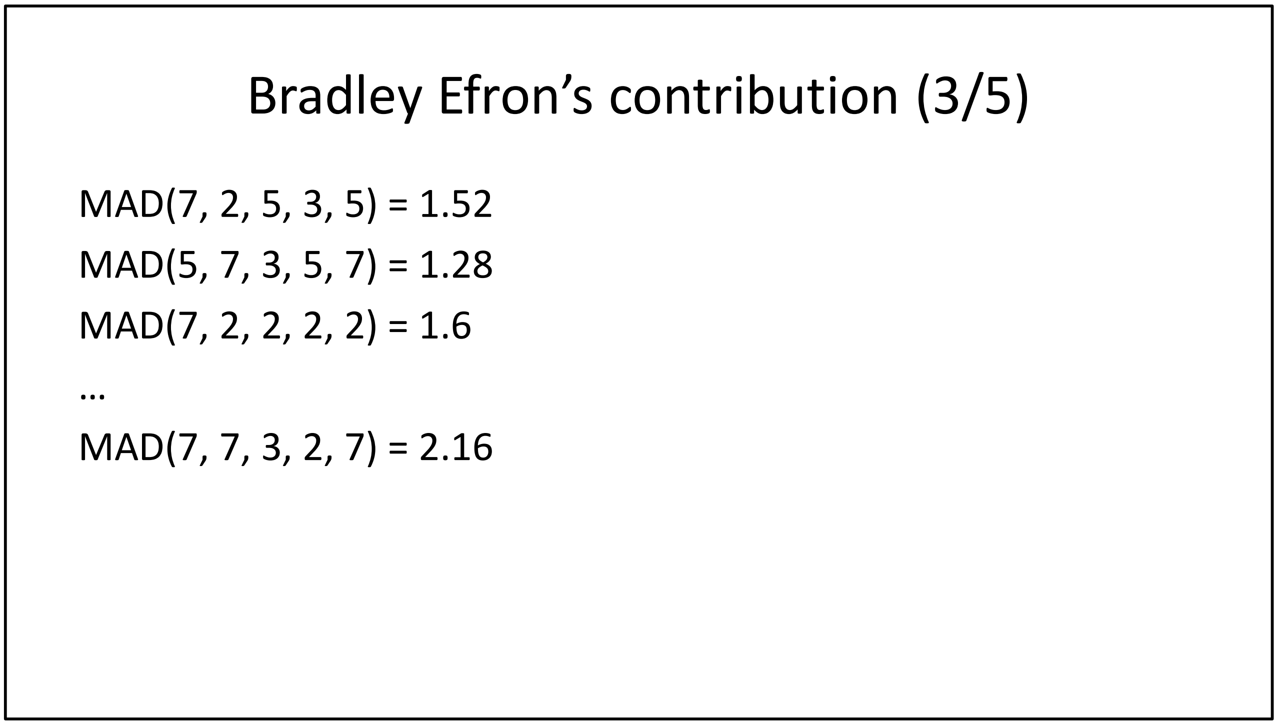
Bootstrap sample #500: (7, 7, 3, 2, 7)

Bradley Efron decided to create subsamples by sampling from the full data set, but with replacement.

Sampling with replacement means that the first data value selected gets tossed back into the pool and is available for selection later on. It might get selected a second, or even a third time. A consequence of this is that one or more of the original values might not make it into the bootstrap sample. If one data value is hogging two or three spots, that squeezes out room for another data value.

The first bootstrap sample picks the 5 twice and skips over the 6. The second bootstrap sample picks the 5 twice and the 7 twice and skips over the 2 and the 6.

One big advantage of the bootstrap samples is that you can do this hundreds or even thousands of times.



Bradley Efron’s contribution (3/5)

MAD(7, 2, 5, 3, 5) = 1.52

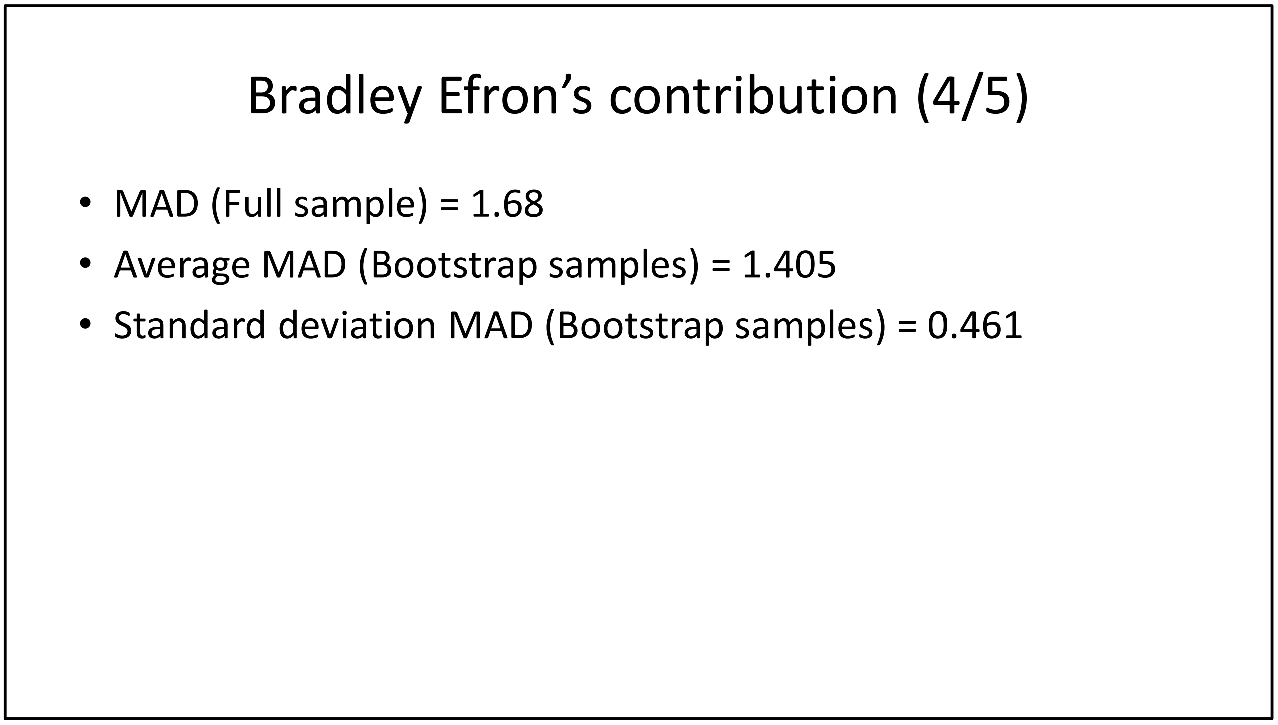
MAD(5, 7, 3, 5, 7) = 1.28

MAD(7, 2, 2, 2, 2) = 1.6

…

MAD(7, 7, 3, 2, 7) = 2.16

Here’s what you might do with the bootstrap samples. Suppose we are interested in the behavior of the mean absolute deviation for this particular dataset. You can calculate that statistic for each bootstrap sample. It is 1.52 for the first bootstrap sample, 1.28 for the second bootstrap sample, and so forth. Notice how much this statistic varies from one sample to the next.

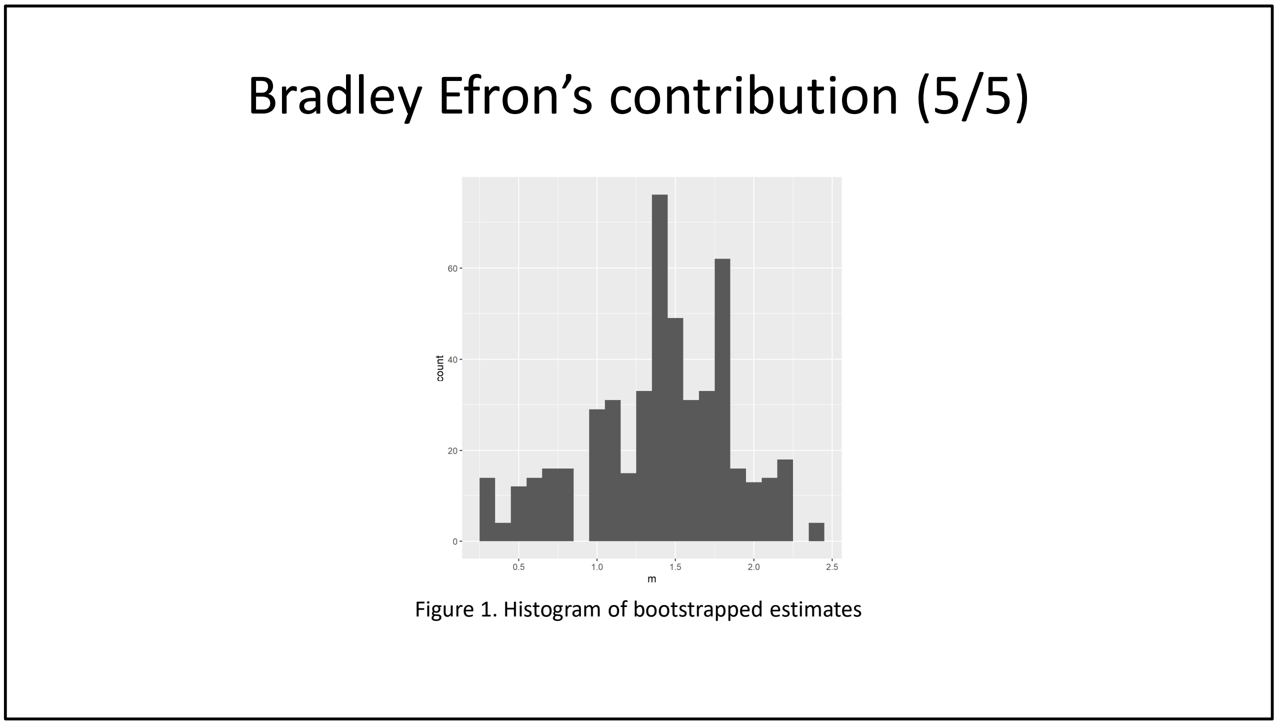


Bradley Efron’s contribution (4/5)

- MAD (Full sample) = 1.68
- Average MAD (Bootstrap samples) = 1.405
- Standard deviation MAD (Bootstrap samples) = 0.461

The average across all the bootstrap samples is a bit smaller than the estimate for the original data. This indicates, as we noticed before with the jackknife, a small amount of bias.

The standard deviation from the bootstrap mean absolute deviations is an estimate of the standard error of that statistic. It is fairly large, but as noted earlier, not too much of a surprise.



Bradley Efron’s contribution (5/5)

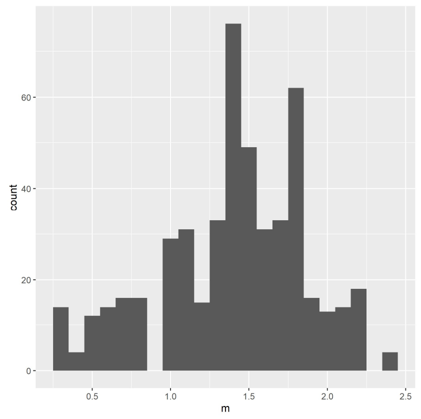


Figure 1. Histogram of bootstrapped estimates

This is a histogram of the 500 bootstrapped estimates of the mean absolute deviation. Notice that it is “patchy” and does not follow a smooth bell shaped curve. This is an important issue that we will address when computing confidence intervals.

A bit of intuition about the bootstrap (1/4)

```
##  [1] 0.1255651 0.2471120 0.4401903
0.4797214 0.6168521 0.6277533 0.6620774
##  [8] 0.7144533 0.8218821 0.9324032
##  [1] 0.09478332 0.20456205 0.28939346
0.37797642 0.46512980 0.55964851
##  [7] 0.65407535 0.74701894 0.88380306
0.98684128
```

A bit of intuition about the bootstrap (1/4)

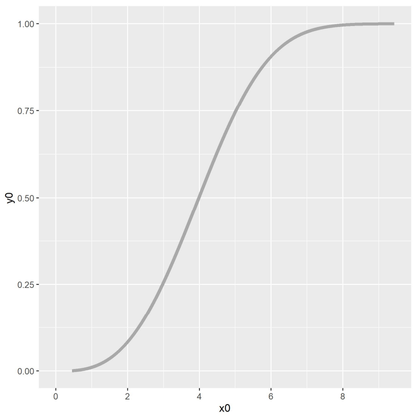


Figure 1. An example of a cumulative density function

Suppose we have inside knowledge about the true probabilities for the data in our sample. Here is a cumulative distribution function that can generate data for a particular distribution.

The cumulative distribution allows you to compute the cumulative probability for any data value. Select the data value on the X axis, project up to the curve and slide horizontally to read the cumulative probability on the Y axis.

You can also invert the process to get a percentile. Select a percentile level on the Y-axis, project horizontally until you intersect the curve, then drop down to the X-axis to get the percentile.

To get the median, for example, find 0.5 on the y-axis, project over to the curve and down to about 4.

It's subtle, but notice that the curve is a just a bit lopsided, indicating a tiny amount of a skewness in this data.

If you had inside knowledge, enough to specify the cumulative distribution function, you could generate random samples from this distribution and calculate statistics on those random samples. It is a basic tool in Statistics known as Monte Carlo simulation.

A bit of intuition about the bootstrap (2/4)

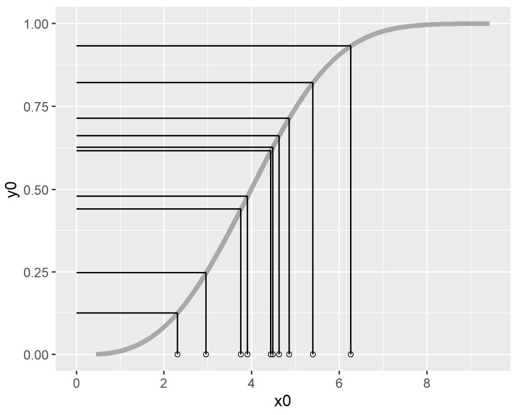


Figure 1. Using random uniform values to simulate data from a cumulative distribution function

The simplest way to generate random variables from a specific cumulative density function is to select values on the y-axis from a random variable uniformly distributed on the interval 0 to 1. Project those values horizontally until they intersect the curve and then drop down to the X-axis. What you're doing is picking random percentiles from the distribution.

So grab n uniform random variables, convert them into percentiles from the cumulative distribution function, and then calculate some statistic like the mean absolute deviation. Get another set of n uniform random variables and repeat the process. With computers as fast as they are today, you could do this a few hundred or even a few thousand times and not break a sweat.

Of course, most of the time, you can't run this Monte Carlo simulation without making some strong assumptions. If you have a particular set of data, do you ever really know what the cumulative distribution function is that created this data? Even if you were lucky enough to have some inside information–that it was associated with a normal random variable, for example–you wouldn't know which normal. You wouldn't know the mu and you wouldn't know the sigma.

A bit of intuition about the bootstrap (3/4)

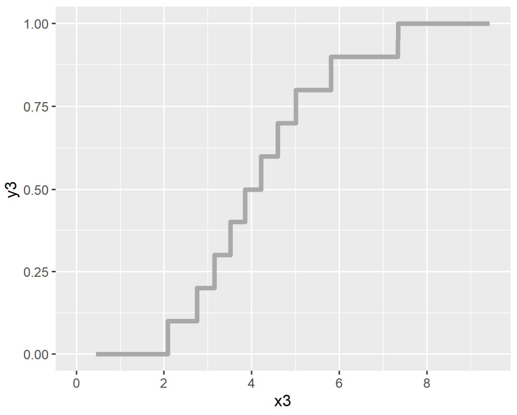


Figure 1. Estimate of cumulative density function from the data

You can get a good approximation to the cumulative distribution function using the data. Draw a step function with a jump of 1/n at each data point where n is the number of data points.

This step function is known as the empirical cumulative distribution function.

The empirical cumulative distribution function does a pretty good job. It is unbiased and converges to the true cumulative distribution function as the sample size increases.

A bit of intuition about the bootstrap (4/4)

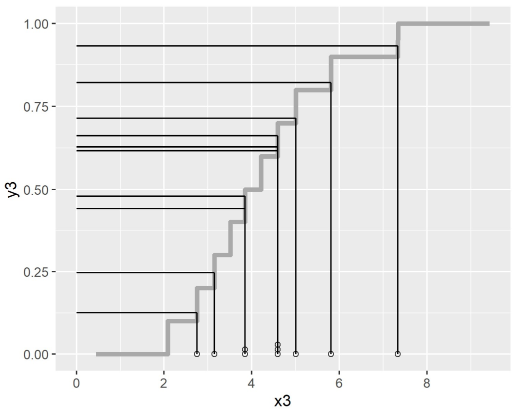
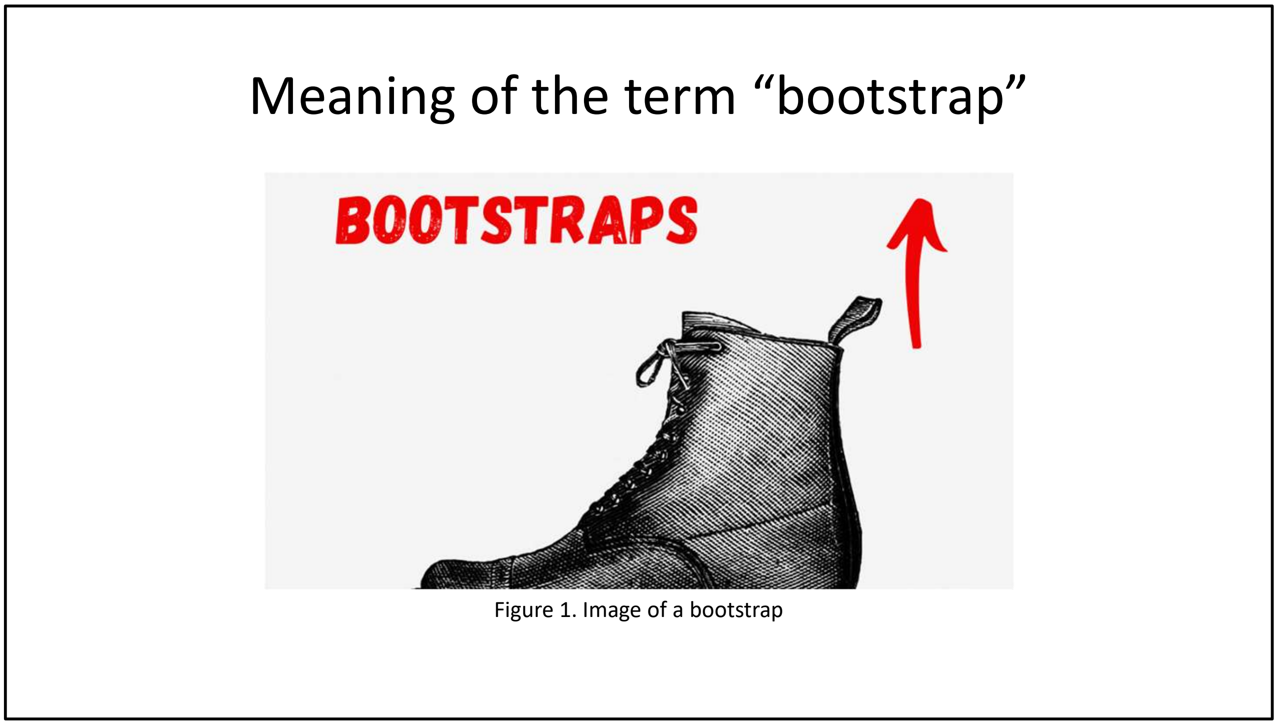


Figure 1. Random uniform values converted into a bootstrap

If you can't generate random variables from the true cumulative distribution function, then a good approximation would be to generate random variables from the empirical cumulative distribution function. Generate values on the Y-axis that are uniformly distributed on the interval 0 to 1, project over horizontally and then drop down to the X-axis.

What you're doing here is sampling from the data with replacement. So, at least intuitively, this is equivalent to an approximate Monte Carlo simulation based on the empirical cumulative distribution function.

Notice in this example that some of the data values



Meaning of the term "bootstrap"

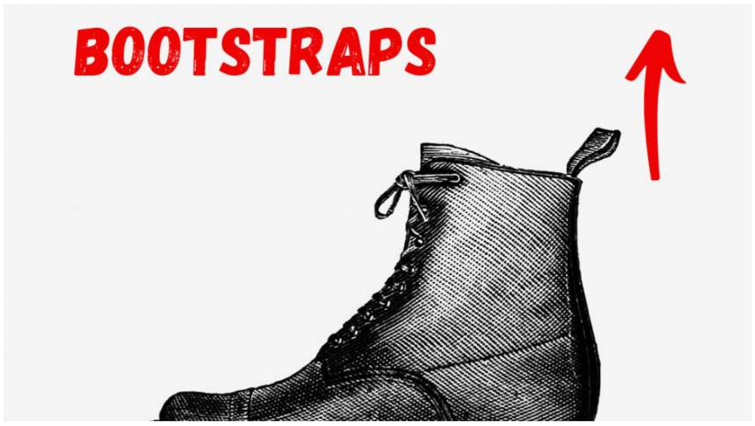
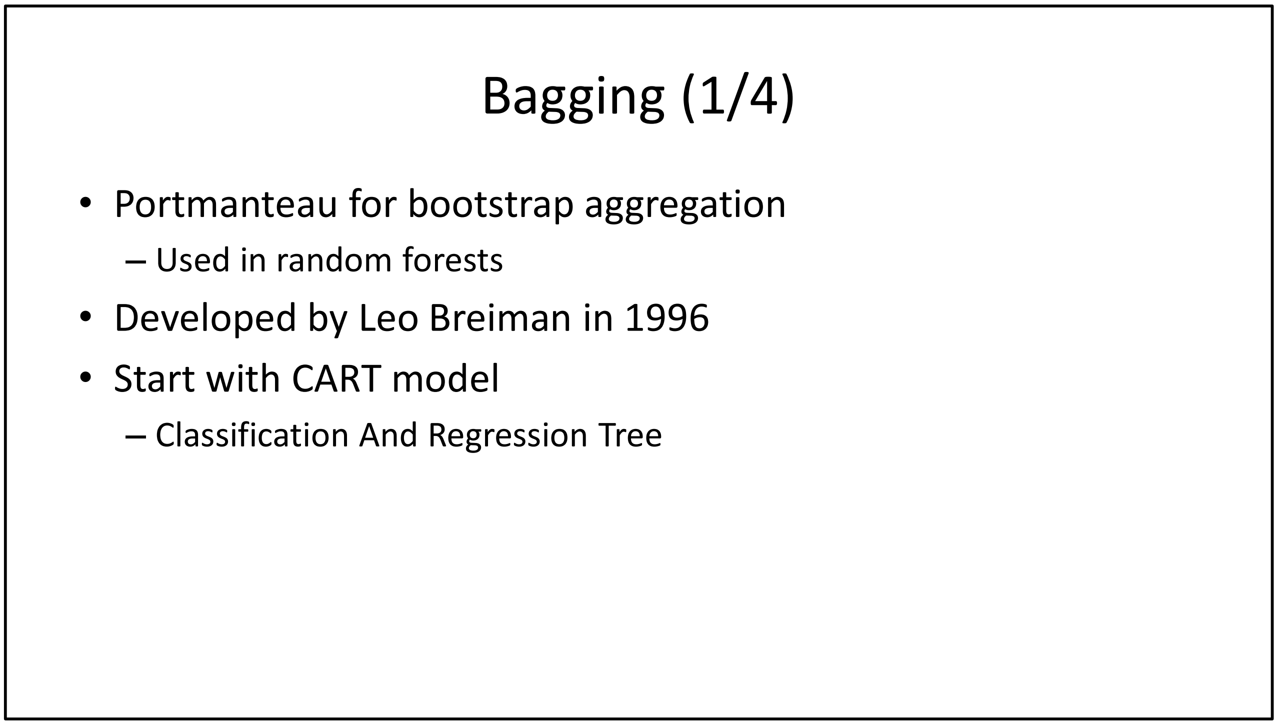


Figure 1. Image of a bootstrap

The name bootstrap comes from the saying "Pull yourself up by your bootstraps". It is a reference to getting something done without any help. This is analogous to the bootstrap produces results with just the data at hand and no outside help from an assumed distribution.

But the image of lifting yourself into the air by yanking on a loop of your shoe is also an analogy to doing something that seems impossible. The Useless Etymology website has a nice discussion of this saying, and the image you see here is taken from their website.

The origin of this phrase is unclear. Several web pages trace this phrase back to a book, The Surprising Adventures of Baron Munchausen. This was a litany of tall tales somewhat akin to the Paul Bunyan character in American folklore. One of the improbable tasks that Baron Munchausen did was lifting himself out of a deep well by pulling on his bootstraps.



Bagging (1/4)

- Portmanteau for bootstrap aggregation
  - Used in random forests
- Developed by Leo Breiman in 1996
- Start with CART model
  - Classification And Regression Tree

I want to briefly address an important application of the bootstrap to machine learning. Bagging is a portmanteau, a combination and shortening of two words: bootstrap aggregation.

The basic building block for bagging in the random forest model is the CART model, Classification and Regression Trees.

Bagging (2/4)

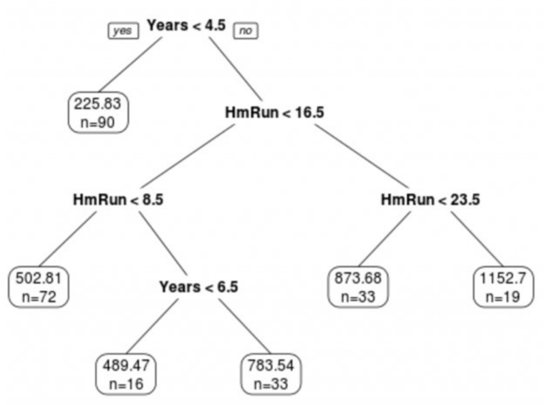


Figure 1. Illustration of a regression tree

A regression tree is a model used for continuous outcomes. It finds optimal splits of the data that create subgroups where the outcome variable shows very little variation. This is an example from the Statology blog on how to fit CART models.

Zach Bobbitt. How to Fit Classification and Regression Trees in R. Statology blog, 2020-11-22. Available in html format.

The graph shows a prediction model for baseball player salaries. If the numbers seem low, it is because the data comes form 1987. The first split is between years in the league. If it is less than 4.5, the node to the left shows a mean salary of 225.83 thousand dollars. If it is greater than 4.5, the node to the right shows an additional split: were the number of home runs less than 16.5, then another split is the number of home runs also less than 8.5 then the mean salary is 502.81 thousand dollars. I won't go through every branch, but each of the final nodes is a combination of splits involving years in the league or home runs.

Bagging (3/4)

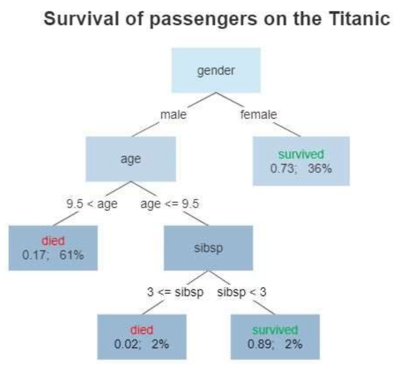


Figure 1. Image of a classification tree

This is an example of a classification tree. You use a classification tree when you are predicting a binary outcome.

This is an example from the Wikipedia page on decision tree learning. It is work by Gilgoldm and published under a Creative Commons open source license (CC BY-SA 4.0) and is available for download here.

Both classification trees and regression trees have a tendency to overfit the data. They are also highly sensitive to small changes in the data. In fact, I would have a hard time recommending the use of these models at all.

There is an approach, however, that largely overcomes these concerns. It is called an ensemble approach. You combine multiple regression or classification trees into a “forest.” And you do this with the help of the bootstrap.

Bagging (4/4)

Bootstrap sample b=1: CART model predictions, $\hat{Y}_{(1)}$

Bootstrap sample b=2: CART model predictions, $\hat{Y}_{(2)}$

Bootstrap sample b=3: CART model predictions, $\hat{Y}_{(3)}$

…

Bootstrap sample b=B: CART model predictions, $\hat{Y}_{(B)}$

Final prediction: $\frac{1}{B}\sum_{b=1}^{B} \hat{Y}_b$

In bagging, you fit a model (in the case of Random Forests, you fit a CART model) to a few hundred or thousand bootstrap samples. Get predicted values for each model. Average those predicted values across all the bootstrap samples.

There are some additional enhancements to the Random Forest models, but the key element is the bagging step.

Note: Each bootstrap sample might produce a different set of independent variables, so you can’t say anything directly about which variables help the most in predicting the outcome. You can’t get p-values or confidence intervals for individual independent variables. There are some indirect ways to assess this, but I will not talk about these.

Break #1

- What have you learned
  - History of the bootstrap
- What's coming next
  - Algorithms

Algorithms

- Estimate bias
- Calculate standard errors
- Compute confidence intervals
- Test hypotheses
- Visualizations
- How many bootstraps

I want to show the algorithms used in bootstrapping. These fall into four categories: estimating bias, calculating standard errors, computing confidence intervals, and testing hypotheses.

Evaluate estimates on bootstrapped samples

- $\hat{\theta} = \hat{\theta}(X_1, X_2, \ldots, X_n)$ is an estimate of θ.
- Recalculate for B bootstrap samples
  - $\hat{\theta}^{(1)} = \hat{\theta}\left(X_1^{(1)}, X_2^{(1)}, \ldots, X_n^{(1)}\right)$
  - $\hat{\theta}^{(2)} = \hat{\theta}\left(X_1^{(2)}, X_2^{(2)}, \ldots, X_n^{(2)}\right)$
  - …
  - $\hat{\theta}^{(B)} = \hat{\theta}\left(X_1^{(B)}, X_2^{(B)}, \ldots, X_n^{(B)}\right)$

For all of the proposed uses of the bootstrap, you start with an estimate based on the full dataset. Call that estimate theta-hat.

Then for each bootstrap sample, you calculate the same estimate.

Estimate bias

- Compare the bootstrap average to the original estimate
  - $\bar{\theta} - \hat{\theta}$
  - where $\bar{\theta} = \frac{1}{B}\sum_{b=1}^{B} \hat{\theta}^{(b)}$

To estimate bias, see how much the average of the bootstrapped estimates differs from the estimate based on the full sample.

For what it's worth, many people (including myself) consider concerns about bias to be overblown. There are times when a biased estimate can be quite serious, especially if the bias is caused by a flaw in the sampling process. But debates about whether you should divide n versus n-1 in the formula for variance are a bit silly.

Furthermore, a small amount of bias in an estimator may be worth it if you can get less sampling error in return.

There's no correct answer about if and when you should adjust for bias, but I am presenting it here as a simple application of the bootstrap. In all candor, the use of the bootstrap for calculating standard errors, computing confidence intervals, and testing hypotheses are far more common uses of the bootstrap.

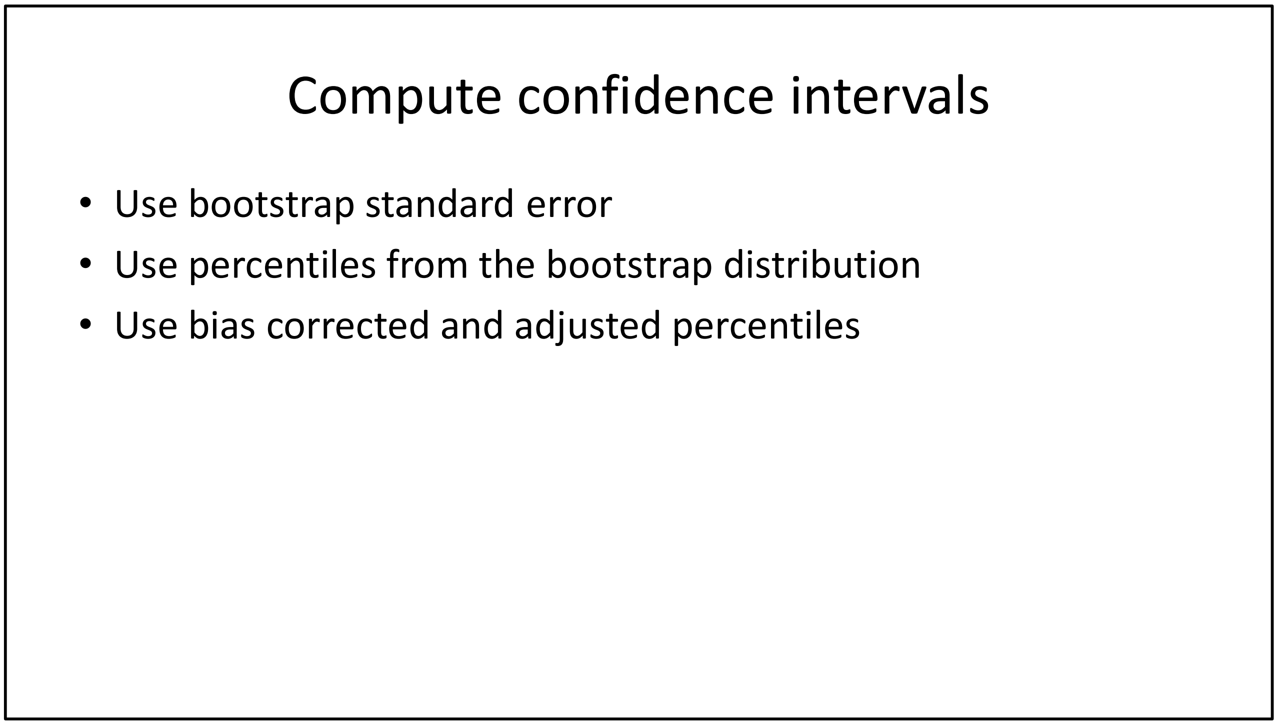
Calculate standard errors

- Calculate the standard deviation of the bootstrap estimates
  - $\sigma^{(B)} = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}\left(\hat{\theta}^{(b)} - \bar{\theta}\right)^2}$

You can use the standard deviation of the bootstrapped estimates as an estimate of the standard error of your statistic.

We'll talk next about confidence intervals and hypothesis tests. But the question arises: why would you want a bootstrap estimate of the standard error if not to use it in a confidence interval or a hypothesis test?

Perhaps there is some value in getting the standard error using a classic approach and comparing it to the bootstrap estimate of the standard error. If the two are close, that gives you some reassurance that the classic approach is appropriate. If they differ, then examine things like whether the sample size is large enough to justify the normal approximation or if other assumptions that you need are justifiable.



Compute confidence intervals

- Use bootstrap standard error
- Use percentiles from the bootstrap distribution
- Use bias corrected and adjusted percentiles

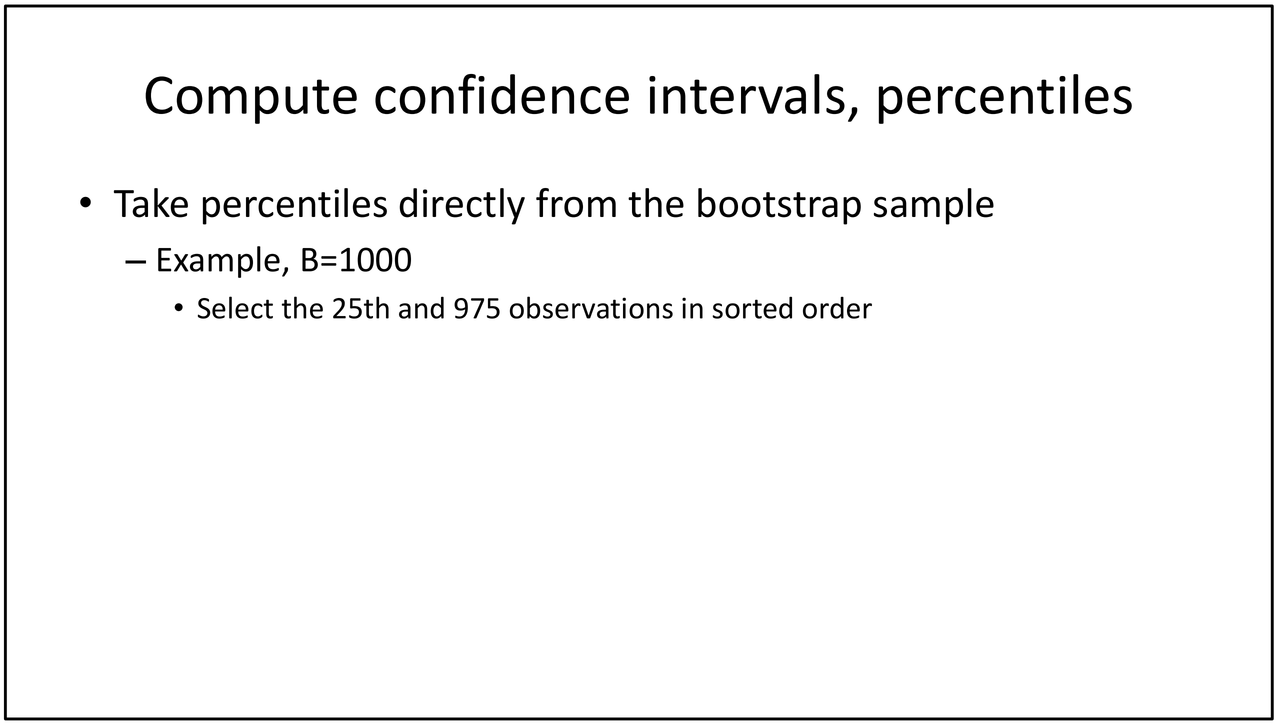
The most frequent use of the bootstrap, by far, is the creation of confidence intervals. There are many ways to do this, but three of the most common approaches are a classical interval using the bootstrap standard error, an interval that relies on percentiles from the bootstrap distribution, and some corrections that improve the accuracy of percentile confidence interval.

Compute confidence intervals, bootstrap standard error

- Easy, once you have a standard error
  - $\hat{\theta}^{(b)} \pm z_{1-\alpha/2}\sigma^{(B)}$
- Should you use a t-distribution?
  - Uncertain degrees of freedom

Once you have a standard error, the simplest confidence interval is going use the bootstrap estimate plus or minus a percentile from the standard normal distribution times the bootstrap standard deviation.

There is some controversy about whether you should use a t distribution here. I personally do not recommend it, because it is unclear what the degrees of freedom should be.



Compute confidence intervals, percentiles

- Take percentiles directly from the bootstrap sample
  - Example, B=1000
    - Select the 25th and 975 observations in sorted order

An even simpler approach is to take percentiles directly from the bootstrap sample. For this, you need a pretty large number of bootstrap samples. Although some sources say that a few hundred might be okay, I would recommend at least a thousand.

With a thousand bootstrap samples, you would select the 25th and 975th observations, after sorting the data.

Compute confidence intervals, BCa (1/5)

- Bias adjustment (using bootstrap estimates)
  - $\hat{z}_0 = \Phi^{-1}\left(\frac{1}{B} H\left(\hat{\theta}^{(b)} - \hat{\theta}\right)\right)$ where
    - H(x)=1 for zero or positive values, 0 for negative values
    - Φ^{-1} is the percentile function for the standard normal distribution
- Acceleration (using jackknife)
  - $\hat{a} = \frac{\sum_{i=1}^{n}\left(\hat{\theta}_{(.)} - \hat{\theta}_{(i)}\right)^3}{6\left(\sum_{i=1}^{n}\left(\hat{\theta}_{(.)} - \hat{\theta}_{(i)}\right)^2\right)^{3/2}}$

Every reference that I reviewed showed these equations and immediately apologized for their complexity. There appears to be little intuition that you can discern from these formulas. The formula for z-hat-0 is a bit easier to follow, perhaps. It is an adjustment for bias.

The H function effectively counts the number of bootstrap estimates that are greater than the estimate based on the original data. Divide by the number of bootstrap samples to get a proportion. Phi inverse converts this proportion into a percentile from a standard normal distribution. If exactly half of the bootstrap estimates are greater than the estimate based on the original data, then you get a big fat zero which means no bias adjustment.

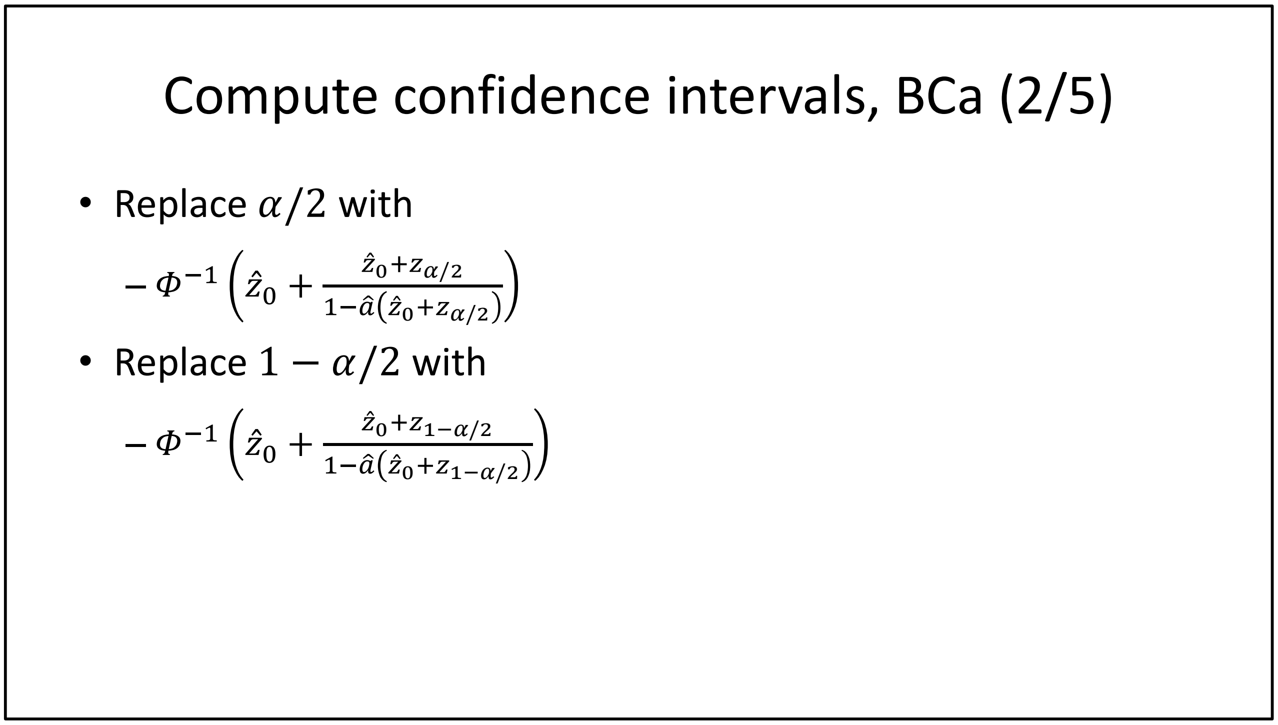
The formula for a-hat is a bit trickier. Notice that it involves deviations from the mean raised to the third power, which seems to be akin to a measure of skewness.

Dr. Efron refers to it as an acceleration, because it relates to the second derivative of the score function. Don't ask me what the score function represents. Also don't ask me why the acceleration relies on a jackknife sample rather than a bootstrap sample.

Remember that in Calculus, the first derivative is analogous to speed and the second derivative is analogous to acceleration.

If z-hat-sub-0 is equal to zero, there is no adjustment to the confidence interval based on bias.

If the jackknife estimates are perfectly symmetric, then a-hat is a big fat zero, meaning no adjustment to the confidence interval based on skewness.



Compute confidence intervals, BCa (2/5)

- Replace $\alpha/2$ with

  $-\Phi^{-1}\left(\hat{z}_0 + \frac{\hat{z}_0 + z_{\alpha/2}}{1 - \hat{a}\left(\hat{z}_0 + z_{\alpha/2}\right)}\right)$
- Replace $1 - \alpha/2$ with

  $-\Phi^{-1}\left(\hat{z}_0 + \frac{\hat{z}_0 + z_{1-\alpha/2}}{1 - \hat{a}\left(\hat{z}_0 + z_{1-\alpha/2}\right)}\right)$

The percentiles that you select from the bootstrap distribution are no longer at alpha/2 and 1-alpha/2, but are moved to account for bias and skewness in the bootstrap distribution.

Percentiles with no adjustment (3/5)

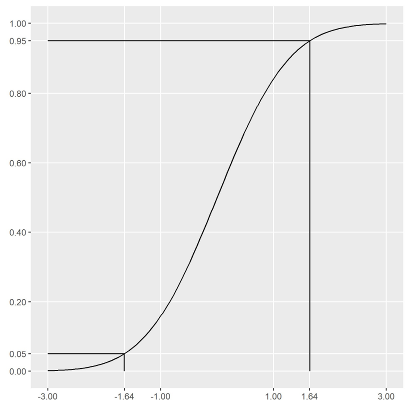


Figure 1. Graph of unadjusted percentiles

Here’s a picture showing what the unadjusted percentiles look like for a 90% confidence interval. Z-0-hat is zero, so no bias adjustment and a-hat is also zero, so no adjustment for skewness. You would just choose the 5th and 95th percentiles of the bootstrapped estimates.

Percentiles with bias adjustment (4/5)

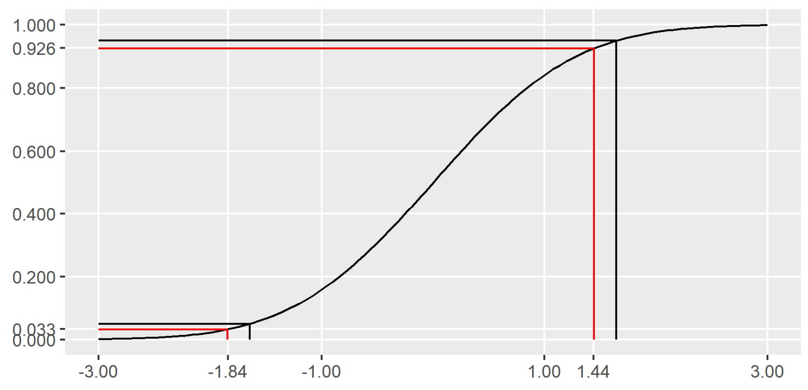


Figure 1. Percentiles with bias adjustment

A bias adjustments shifts the z values to the left or the right. In this hypothetical case, the z values are shifted left by 0.2 units, and instead of using the instead of the 5th and the 95th percentiles, you would use would be the 3.3 percentile and the 92.6 percentile.

Percentiles with acceleration adjustment (5/5)

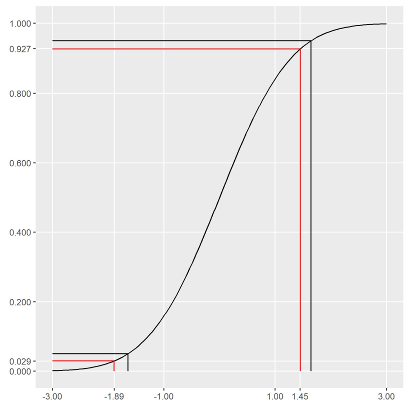


Figure 1. Histogram of bootstrapped estimates

An adjustment for skewness also shifts the z values to the left or the right, though the shift is stronger on one side versus the other. In this hypothetical case, you would use would be the 2.9 percentile and the 92.7 percentile.

These formulas are messy, and easy to get wrong, so I would recommend if you are programming from scratch that you stick one of the simpler approaches.

Test hypotheses

- Test
  - \$H_0: geq =0\$
  - H_1: $\theta > 0$
- Reject H_0 if fewer than α of the $\hat{\theta}^{(b)}$'s are less than 0.
  - Could also test using a bootstrap confidence interval

To test a hypothesis, count the proportion of bootstrap values that agree with the null hypothesis. If it is less than alpha, then you reject the null hypothesis. Extension to two sided hypotheses is not difficult.

You could also look at any one of the bootstrap confidence intervals and see whether that interval includes or excludes the null value.

Visualization (1/2)

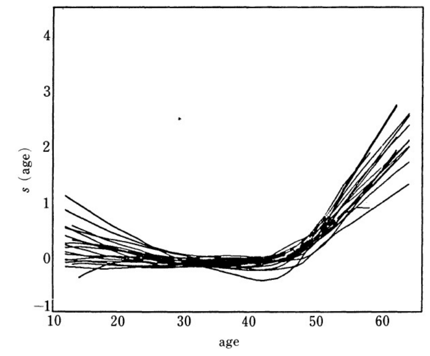


FIG. 7. *20 bootstraps of the local likelihood estimate for the Stanford heart transplant data.*

Figure 1. Age changes in risk for heart transplant patients

Visualization (2/2)

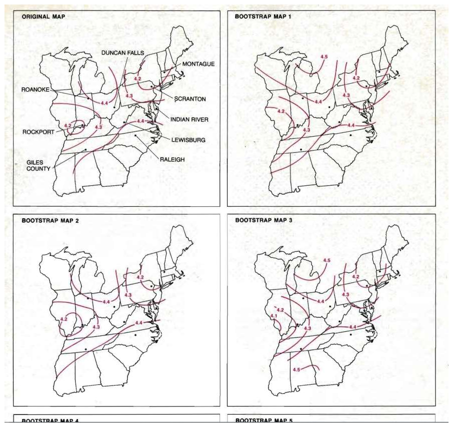


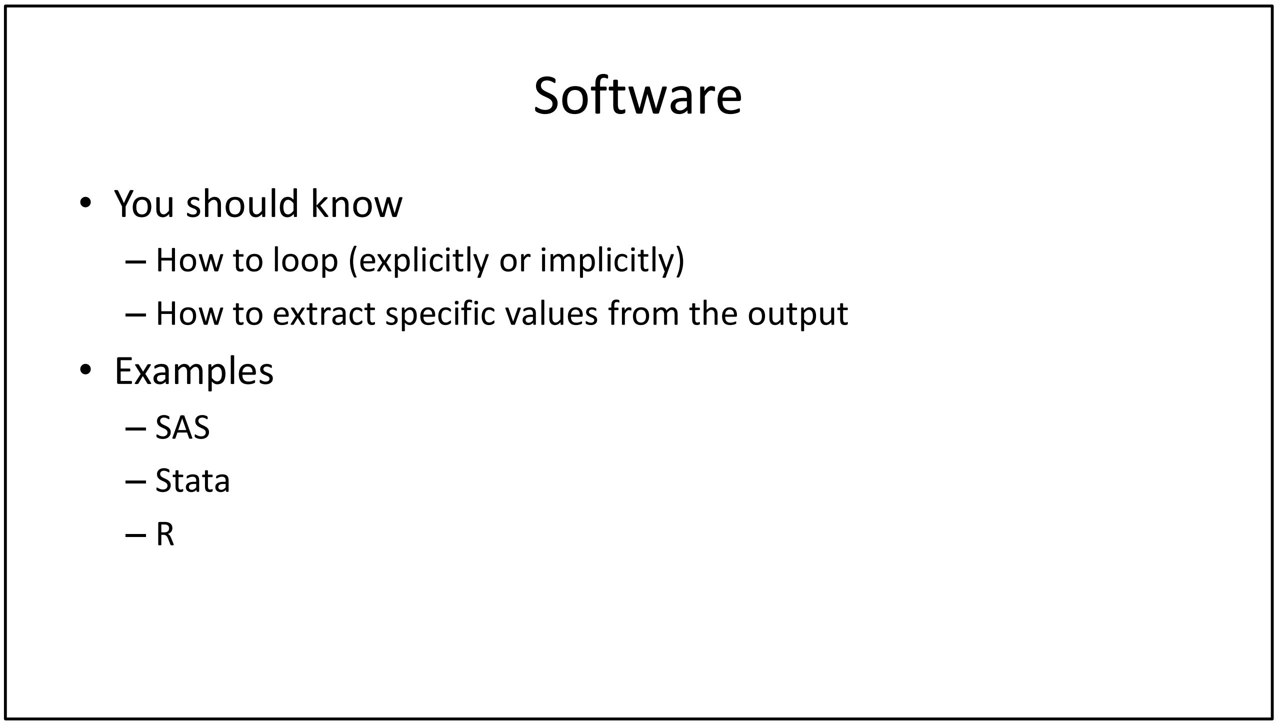
Figure 1. Map

How many bootstraps?

- For visualization: 10 to 50
- For estimating a standard error: 50 to 100
- For confidence intervals and hypothesis tests: 500 to 1000

Break #2

- What you have learned
  - Purposes of the bootstrap
- What's coming next
  - Software

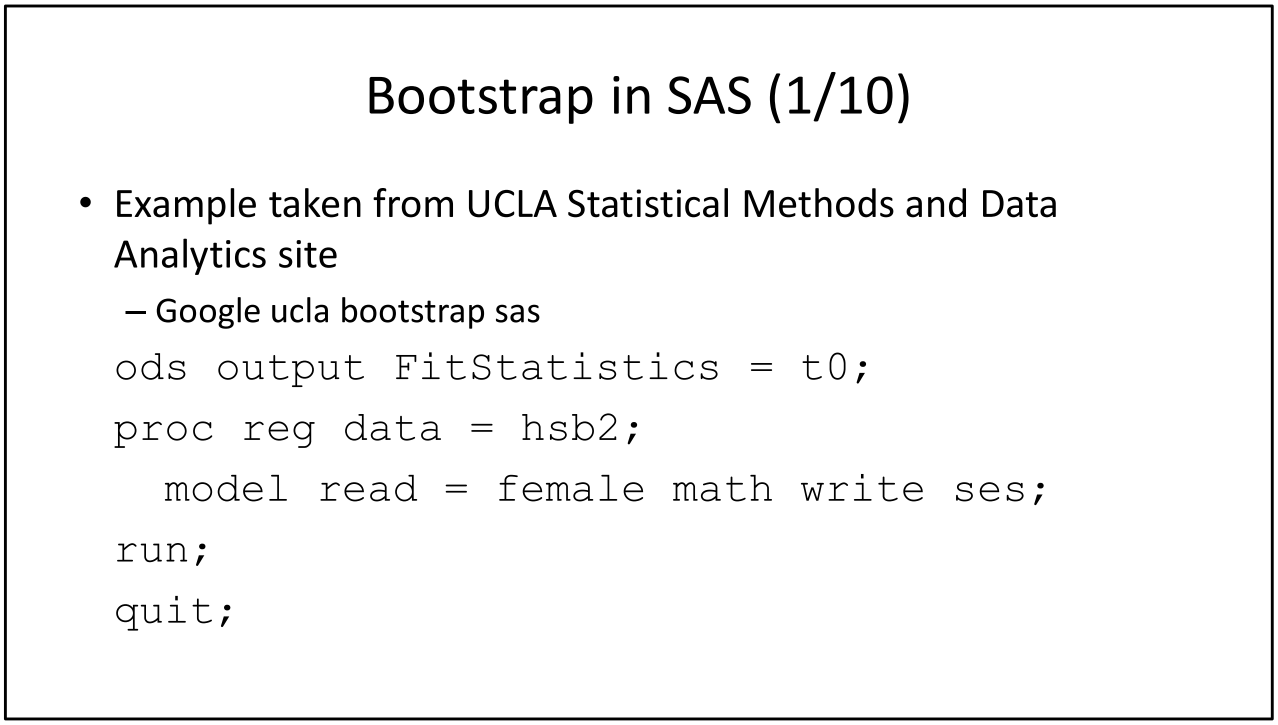


Software

- You should know
  - How to loop (explicitly or implicitly)
  - How to extract specific values from the output
- Examples
  - SAS
  - Stata
  - R

If you want to program a bootstrap, you need to have enough familiarity with your statistical software to run a loop and extract specific values from the output.

I want to show briefly, how to do a simple bootstrap in SAS, Stata, and R. It may be possible to do this in SPSS, but I am not familiar enough with SPSS to outline how the approach might work.



Bootstrap in SAS (1/10)

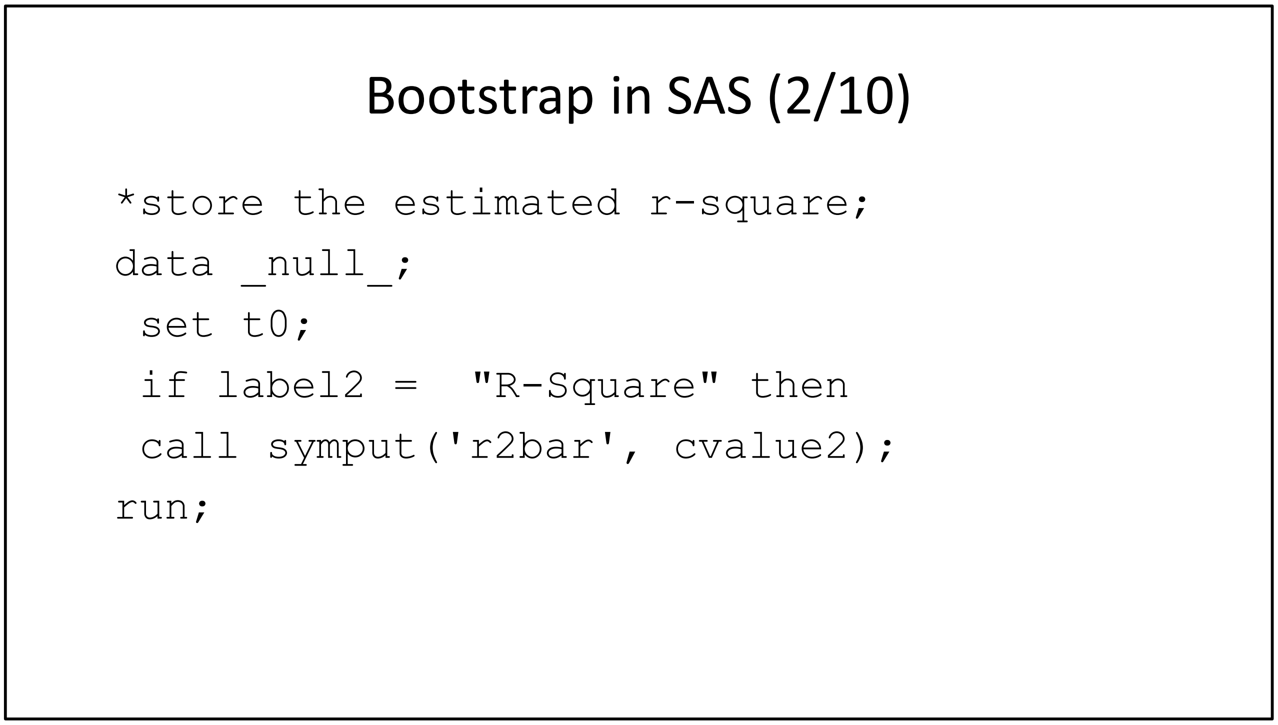
- Example taken from UCLA Statistical Methods and Data Analytics site
  - Google ucla bootstrap sas

```
ods output FitStatistics = t0;
proc reg data = hsb2;
  model read = female math write ses;
run;
quit;
```

This example is taken from the UCLA Statistical Methods and Data Analytics site. It pops up easily on a simple google search.

The first statement tells SAS that it should take the output from the following procedure, pull out a particular number from the output called “FitStatistics” and store it in a dataset with the name t0.

I’m guess that the “quit” statement is important here because of the way you are handling output with the ods statement.



Bootstrap in SAS (2/10)

```
*store the estimated r-square;
data _null_;
 set t0;
 if label2 =  "R-Square" then
 call symput('r2bar', cvalue2);
run;
```

The data step here creates a dataset with the sole purpose of moving the r-squared value to a macro variable. The key function here is symput and if you are not familiar with it, check out the SAS documentation.

Bootstrap in SAS (3/10)

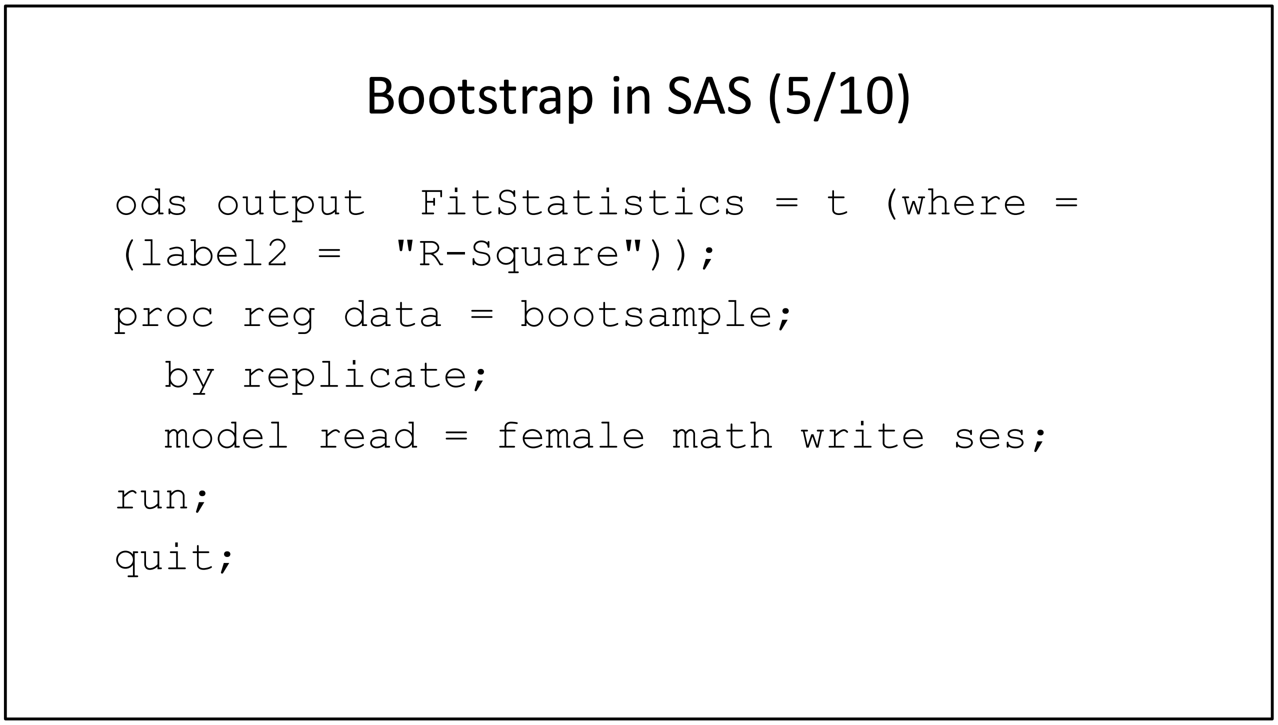
```
%let rep = 500;
proc surveyselect data= hsb2
out=bootsample
     seed = 1347 method = urs
     samprate = 1 outhits rep = &rep;
run;
ods listing close;
```

Although you could use a loop here, the surveyselect procedure allows you to create 500 bootstrap samples and store them all in a single dataset.

Bootstrap in SAS (4/10)

```
Sample Size                           200
Expected Number of Hits                 1
Sampling Weight                         1
Number of Replicates                  500
Total Sample Size                  100000
Output Data Set                BOOTSAMPLE
```

Here is part of the output from surveyselect. The original dataset has 200 observations. We are creating 500 replicates using sampling with replacement. That creates a dataset of 100,000 observations.



Bootstrap in SAS (5/10)

```
ods output  FitStatistics = t (where =
(label2 =  "R-Square"));
proc reg data = bootsample;
  by replicate;
  model read = female math write ses;
run;
quit;
```

The ods statement on the first line of code on this slide tells SAS to look at the output from the following procedure and store the result in a dataset called t.

The “by replicate” statement tells SAS to run a separate regression for each bootstrap sample.

Bootstrap in SAS (6/10)

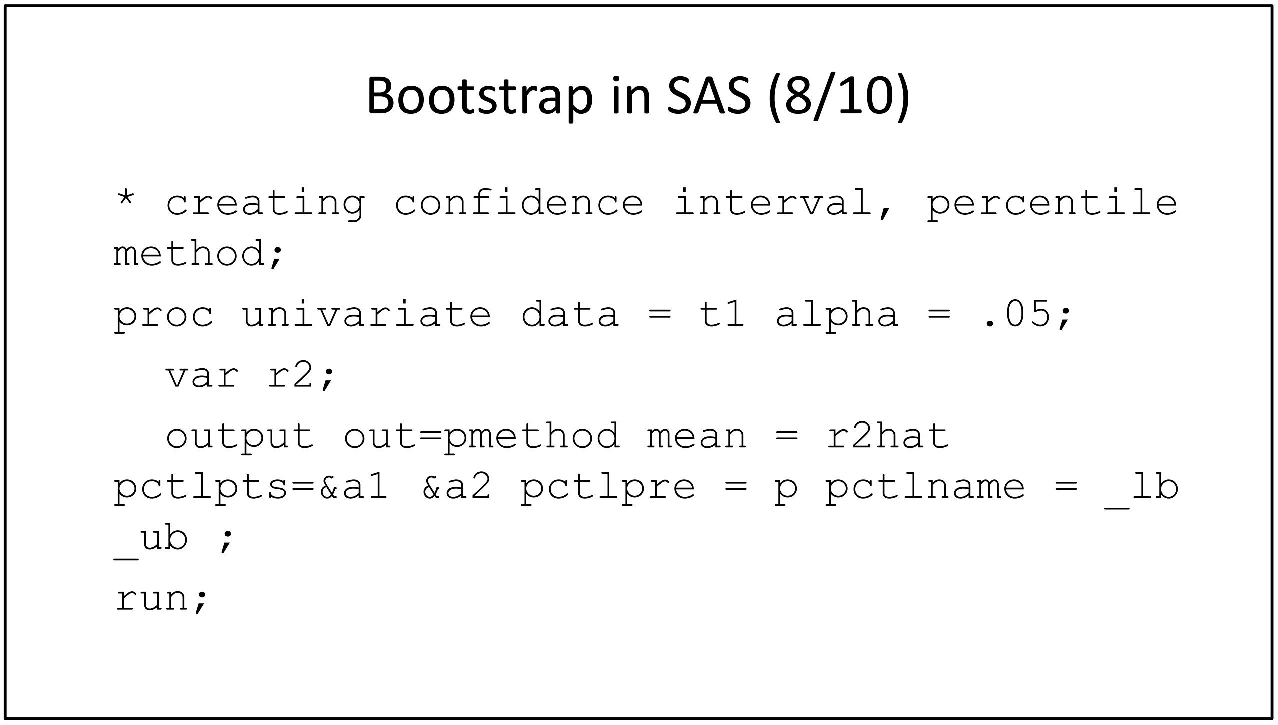
```
* converting character type to numeric
type;
data t1;
  set t;
  r2 = cvalue2 + 0;
run;
```

The output stored in the dataset, however, is a string, and you have to convert it to a numeric value by adding zero. This is a classic SAS hack.

Bootstrap in SAS (7/10)

```
%let alphalev = .05;
%let a1 = %sysevalf(&alphalev/2*100);
%let a2 = %sysevalf((1 -
&alphalev/2)*100);
```

The first three lines are just a fancy way of getting from a 0.05 alpha level to selecting the 2.5 percentile and the 97.5 percentile.



Bootstrap in SAS (8/10)

```
* creating confidence interval, percentile
method;
proc univariate data = t1 alpha = .05;
  var r2;
  output out=pmethod mean = r2hat
pctlpts=&a1 &a2 pctlpre = p pctlname = _lb
_ub ;
run;
```

proc univariate produces the mean as well as the 2.5 and 97.5 percentiles. The pctlpre and pctlname make the variable names of the output dataset look nice.

Although the folks at UCLA take great pains to make everything look nice, they should have used a noprint option for proc univariate to keep the output cleaner.

Bootstrap in SAS (9/10)

```
data t2;
  set pmethod;
  bias = r2hat - &r2bar;
  r2 = &r2bar;
run;
ods listing;
```

That &r2bar is a macro variable of the estimate of R-squared from the original dataset. You subtract it from the mean of the bootstrap samples (r2hat) to get the estimated bias.

Bootstrap in SAS (10/10)

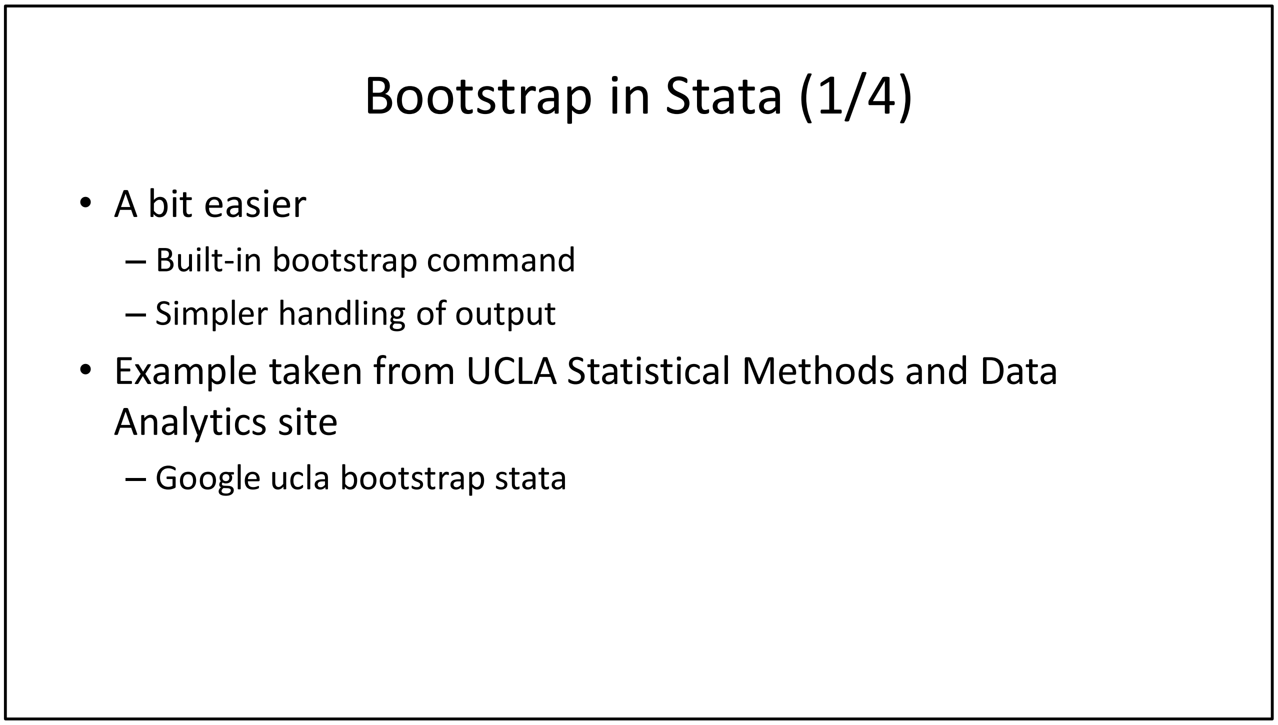
```
proc print data  = t2;
  var r2 bias p_lb p_ub;
run;

Obs      r2         bias        p_lb
p_ub
 1     0.5189    .0066164    0.436
0.6017
```

After all this careful work, you now have the original estimate of R-squared (52% after rounding), the estimated bias (less than 1%) and the confidence interval (44% to 60%).

As a quick recap, knowledge of the output delivery system (ods) and macro variables were critical. Thankfully, you did not need a loop here, but familiarity with looping mechanisms in SAS is probably worth knowing for other bootstrap examples.

If you want to learn more, Rick Wicklin of SAS Institute has a nice series of blog posts. Start with this one.



Bootstrap in Stata (1/4)

- A bit easier
  - Built-in bootstrap command
  - Simpler handling of output
- Example taken from UCLA Statistical Methods and Data Analytics site
  - Google ucla bootstrap stata

I am not an expert on Stata, but it was created in 1985 about two decades later than SAS. So it did not have any holdovers from the restricted options available in the age of IBM mainframe computers.

This example is taken from the UCLA Statistical Methods and Data Analytics site. It pops up easily on a simple google search.

Bootstrap in Stata (2/4)

```
use
http://statistics.ats.ucla.edu/stat/stata/
notes/hsb2, clear
regress read female math write ses
```

Here is the Stata code to get the estimates from the original data.

Bootstrap in Stata (3/4)

```
bootstrap rmse=e(rmse), reps(100)
seed(12345): regress read female math
write ses
```

Stata has a bootstrap function built-in. It is both a good thing and a bad thing. It is good in that it simplifies your code. It is bad in that it can only bootstrap on prespecified parts of the output. In fairness, this is also a limitation with the output delivery system in SAS. Both systems are pretty good at letting you pick out the pieces of the output that you are most interested in.

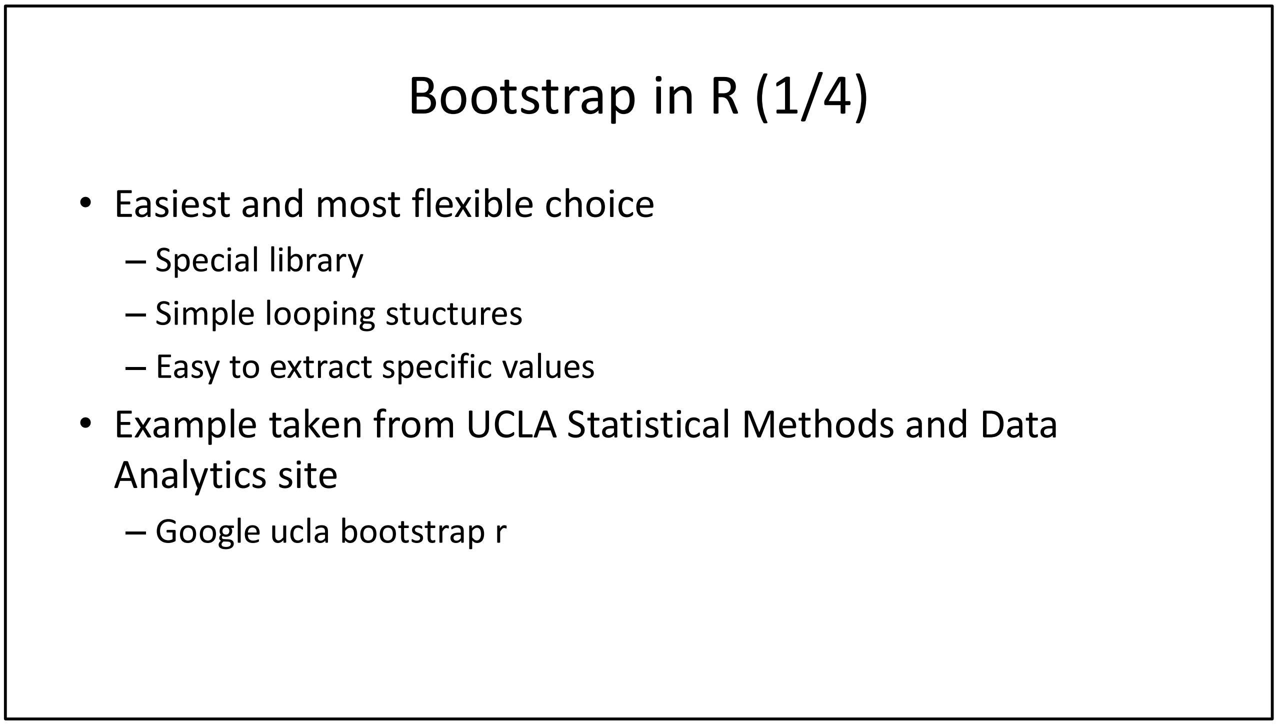
Bootstrap in Stata (4/4)

```
----------------------------------------
             |   Observed   Bootstrap
             |      Coef.   Std. Err.
-------------+--------------------------
        rmse |   7.184202   .2594069
---------------------------------------


---------------------------------------
                       Normal-based
```

Here is the output. By default, it provides a confidence interval based on the bootstrap standard error, but you can get other confidence intervals as well.

In this example, the original data produced a root mean squared error of 7.2 and the bootstrap 95% confidence interval goes from 6.7 to 7.7.



Bootstrap in R (1/4)

- Easiest and most flexible choice
  - Special library
  - Simple looping stuctures
  - Easy to extract specific values
- Example taken from UCLA Statistical Methods and Data Analytics site
  - Google ucla bootstrap r

R was created in 1999, and relied on a modular approach that makes it ideal for bootstrapping. There is a special library that works for most cases, even some very exotic ones. Looping in R is easy as is extracting specific values.

Again, I am using an example from the UCLA Statistical Methods and Data Analytics site. It pops up easily on a simple google search.

Bootstrap in R (2/4)

```
library(boot)
hsb2 <-
read.table("https://stats.idre.ucla.edu/st
at/data/hsb2.csv", sep=",", header=T)
```

Bootstrap in R (3/4)

```
fc <- function(d, i){
    d2 <- d[i,]
    return(cor(d2$write, d2$math))
}

set.seed(626)
bootcorr <- boot(hsb2, fc, R=500)
```

Bootstrap in R (4/4)

```
Bootstrap Statistics :
     original        bias    std. error
t1* 0.6174493 -0.001528707  0.04020362
```

Break #3

- What have you learned
  - Software
- What's coming next
  - Special issues

Special issues

- Multiple groups
- Time series
- Regression models

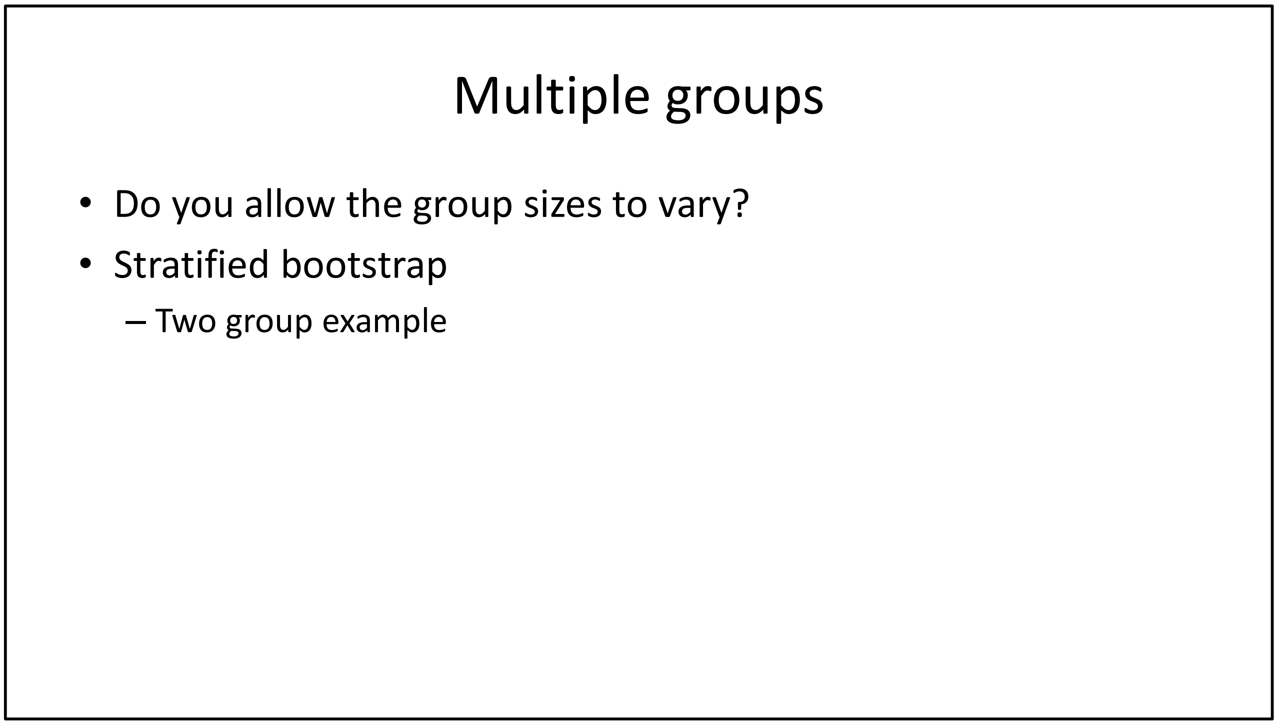
In more complex settings, you need to consider some modifications to the bootstrap. I have almost no experience in these settings and there is scant guidance in the published literature and on the web.

If you find yourself in one of these settings, I would encourage you to find a few publications that use the bootstrap in a setting reasonably similar to yours and emulate their approach.

I call this the "lemming school of research" which is a reference to the warning about peer pressure that almost every parent has nagged their children with ("If all your friends jumped off a cliff, would you jump off the cliff as well?").

It actually is not as bad as I make it sound. If a certain methodology has survived the peer reviewe process, that gives you a bit more confidence that you can survive the peer review process as well if you emulate their approach. There are no guarantees, of course, but this is perhaps an illustration of a more positive message: "there is safety in numbers."

The three settings I want to discuss are multiple groups, time series, and regression models.



Multiple groups

- Do you allow the group sizes to vary?
- Stratified bootstrap
  - Two group example

Suppose you have two or more groups and want to estimate a statistic across all of the groups. For example, you have a treatment and a control group and you want to estimate the difference in medians between the two groups.

You have two options. The first is to apply a simple bootstrap. This allows the relative sizes in the groups to vary. If one of the groups has a small relative sample size, then you run a slight risk having zero observations in that group for one or more of your bootstrap samples.

If the group sizes are all reasonably large, this is not a serious problem.

An alternative is to use a stratified bootstrap sample. It’s easy enough to envision with two groups. Let’s say that the two groups have sample sizes n1 and n2. Sample n1 observation with replacement from the first group, sample with n2 observations with replacement from the second group and then combine.

The stratified bootstrap answers a different question than the simple bootstrap. The simple bootstrap calculates uncertainty in a setting where you are collecting a single sample and that sample has a random number of subjects in each group. The stratified bootstrap calculates uncertainty where you are collecting samples from multiple groups, each with a fixed quota.

Is this a huge difference? I’m not sure, but my guess is that it is not all that important except when one or more of the group sizes is small. By small, I mean 10 or less. I should note, however, that I have not seen an “official” guidance on this question.

Time series

- Simple bootstrap destroys important features of time series models
  - Evenly spaced observations
  - Serial correlation
  - Seasonality
  - Temporal trends
- Solutions
  - Bootstrap blocks of consecutive observations
  - Detrend/decompose the time series

There are special features of time series data that make them difficult to use with a simple bootstrap. The first and most obvious feature is that most time series have a nice neatly ordered pattern or even spacing over time. A bootstrap sample is going to have gaps in some places and multiple observations at the same time point.

Most time series also exhibit serial correlation, seasonality, and/or temporal trends. These features are either seriously distorted or totally destroyed in a bootstrap sample.

There are several possible solutions. One is to bootstrap consecutive blocks of observations. This preserves time series features within a block and appears to perform reasonably well.

A second option is to remove any trend and decompose the time series into independent components, take a bootstrap sample of the independent components, and then recompose a new series from the bootstrap sample.

The approach you take largely depends on the context of your problem and what statistic you are trying to characterize. For example, if you detrend the data and remove seasonality, then any bootstrapped estimate from the reconstructed time series will be fine if it is modeling a feature of the data other than the trend or seasonality.

Regression models

- Subsample may have perfect collinearity
- Are the independent variables fixed or random?
- Solution: bootstrap residuals

The regression model has some of the same issues as the setting with multiple groups described earlier. If some of the independent variables are very strongly correlated, you might end up with a setting where the correlation is exactly 1 for one or more of the bootstrap samples. This is not a serious issue unless you have both a strong correlation and a small sample size.

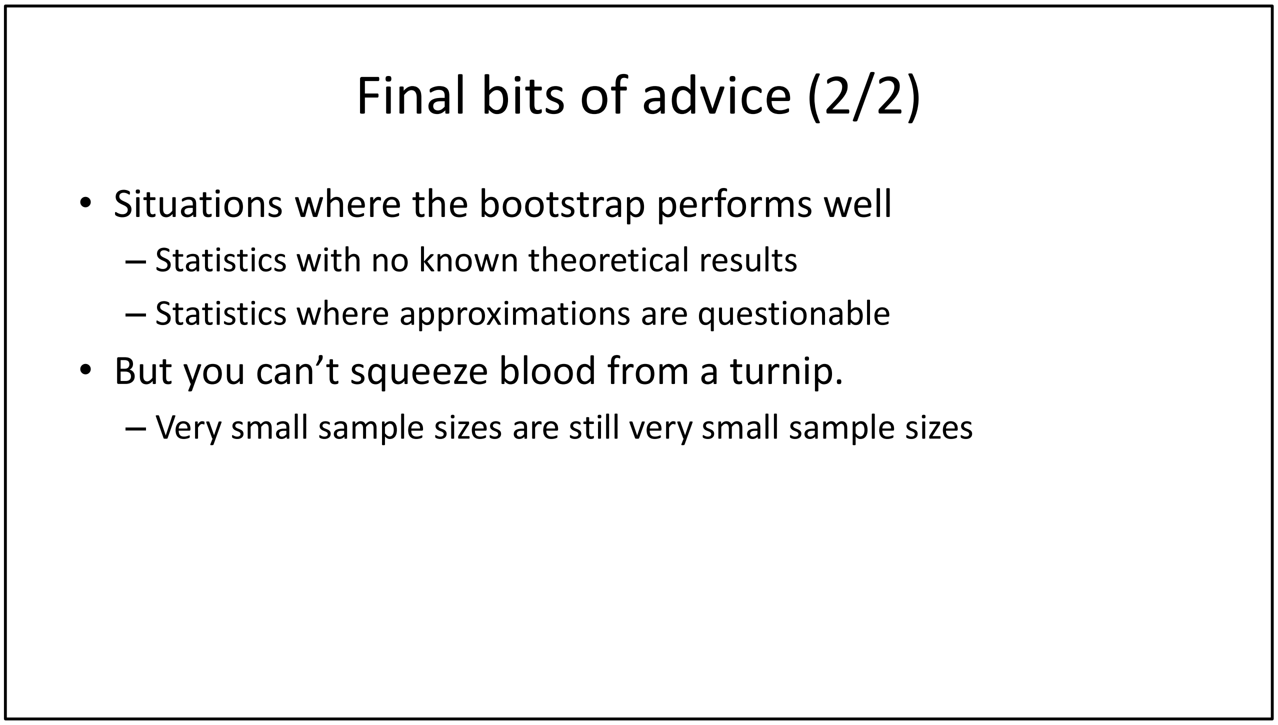
But another consideration is that the bootstrap sample treats the independent variables as if they are selected randomly along with the dependent variable. This may be the case, but there are some datasets where the X values are fixed in advance and the dependent variable is the only thing being sampled.

One possible solution is to compute the residuals and reconstruct a new dependent variable from the bootstrapped residuals.

Context is important here. If you bootstrap the residuals, you can’t use the reconstructed dependent variable as an estimate of the regression slopes themselves. You could use them to reconstruct a statistic that is independent of those slopes.

Final bits of advice (1/2)

- Situations where the bootstrap performs poorly
  - Small sample size
  - Data from "weird" distributions
  - Statistics at or near the extremes
- Situations where a simple bootstrap performs poorly
  - Multiple groups with small sample sizes
  - Time series models
  - Complex regression models

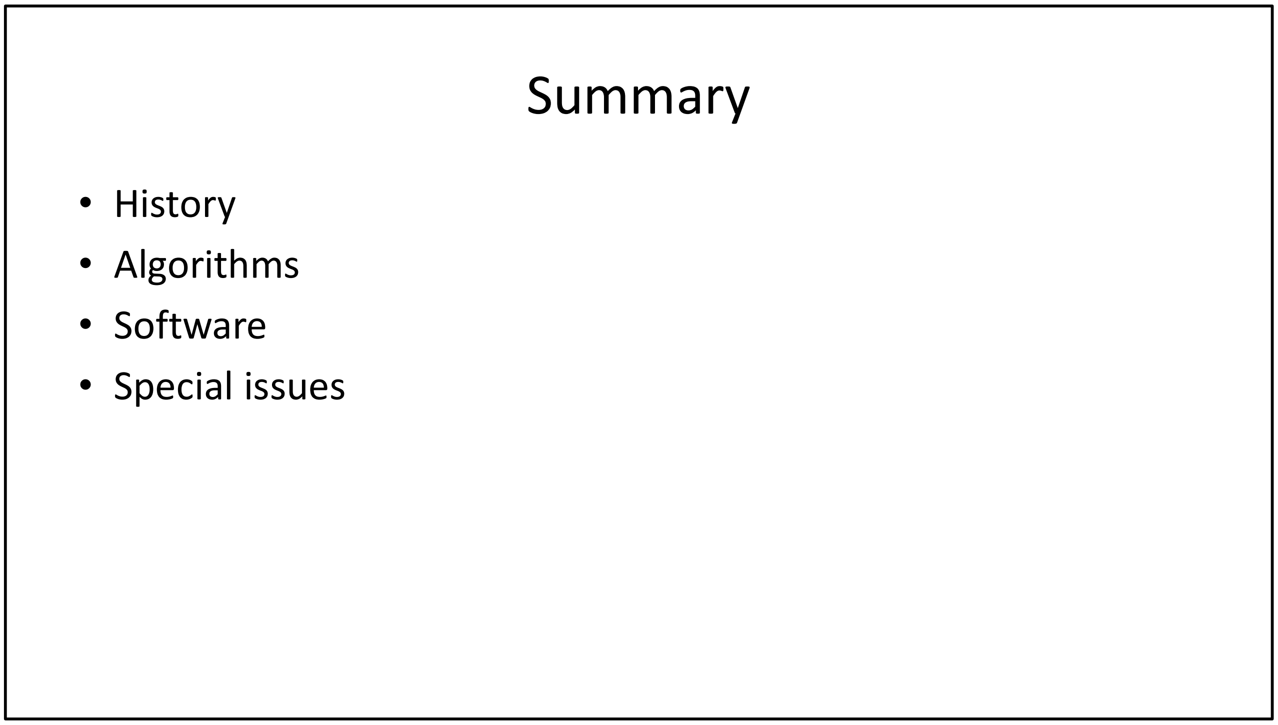


Final bits of advice (2/2)

- Situations where the bootstrap performs well
  - Statistics with no known theoretical results
  - Statistics where approximations are questionable
- But you can’t squeeze blood from a turnip.
  - Very small sample sizes are still very small sample sizes

The bootstrap performs well in settings where you do not have any theoretical results to guide your work. It also works well when the normal approximations that you rely on are questionable, either because the sample size is small or because the underlying distribution of the data is troublesome. By troublesome, I mean extreme skew or high probability of producing outliers. Both will tend to slow down the asymptotic approximation to normality.

Keep in mind, though, that the bootstrap can’t compensate for a limited sample size. The confidence intervals may be valid, but often they will be so wide as to be meaningless. There’s a saying that you can’t squeeze blood from a turnip. That’s an attempt to explain that you can’t get something from nothing.



Summary

- History
- Algorithms
- Software
- Special issues

So we've covered the history of the bootstrap, illustrated some algorithms, showed how to compute a bootstrap in SAS, Stata, and R, and discussed some special issues where you might want to modify the bootstrap approach.

I'd be glad to take any questions you might have.