

Lecture 10 - Key

The Bootstrap

Our final section takes a slight diversion from the textbook to focus on another important (re)sampling technique known as the bootstrap.

Situation: Let y_1, y_2, \dots, y_n be a SRS of size n taken from a distribution F that is unknown. Let θ be a parameter of interest associated with this distribution and let $\hat{\theta} = S(y_1, y_2, \dots, y_n)$ be a statistic used to estimate θ . The notation $S(y_1, y_2, \dots, y_n)$ denotes a statistic based on the data y_1, y_2, \dots, y_n .

- Ex. The sample mean $\bar{y} = \hat{\theta} = S(y_1, y_2, \dots, y_n)$ is a statistic used to estimate the true mean.

Similar to our other sampling procedures, with the point estimate $\hat{\theta}$ we are interested in determining:

1. the *standard error of the estimator*,
2. the *bias of $\hat{\theta}$* ,
3. the *confidence interval for $\hat{\theta}$* .

Bootstrap methods are computer intensive methods for estimating these quantities using bootstrap samples.

A bootstrap sample is a SRS of size n taken with replacement from the original data y_1, y_2, \dots, y_n .

We denote a bootstrap sample as $y_1^*, y_2^*, \dots, y_n^*$ which consists of *members of the original data set y_1, y_2, \dots, y_n with some members appearing zero times, some appearing one time, some appearing twice,...*

A bootstrap sample replication of $\hat{\theta}$, denoted $\hat{\theta}^*$, is the value of $\hat{\theta}$ evaluated *using the bootstrap sample $y_1^*, y_2^*, \dots, y_n^*$* .

The bootstrap algorithm requires that a large number (B) of bootstrap sample be taken. The bootstrap sample replication $\hat{\theta}^*$ is then calculated for each of the B bootstrap samples. *We will denote the b^{th} bootstrap replication as $\hat{\theta}^*(b)$ for $b = 1, 2, \dots, B$.*

Example. Consider six data points that correspond to the inches of snowfall on your scheduled exam dates: $\{y_1 = 9, y_2 = 4, y_3 = 13, y_4 = 5, y_5 = 6, y_6 = 8\}$.

Using the snowfall dataset, write R pseudocode for taking bootstrap samples from the snowfall dataset.

sample 1	sample 2	sample 3	sample 4	sample 5	sample 6
6	8	8	6	8	8
4	6	13	9	6	6
4	9	6	6	6	4
5	6	9	5	9	4
13	8	9	8	6	8
8	8	5	8	8	5
6	6	6	9	9	13
13	6	8	9	8	5
6	5	9	5	5	9
6	8	4	5	4	5
13	9	9	4	9	5
8	8	8	13	13	13
4	4	6	4	5	13
6	4	4	9	6	13
6	6	8	4	9	13
9	6	8	6	8	9
6	5	4	5	5	4
9	13	4	4	8	8
4	4	5	8	8	4
4	8	9	8	9	13

Bootstrap Estimate of Standard Error

The bootstrap estimate of the standard error of $\hat{\theta}$ is

$$SE_b(\hat{\theta}) = \sqrt{\frac{\sum_{b=1}^B [\hat{\theta}^*(b) - \hat{\theta}^*]^2}{B-1}},$$

where $\hat{\theta}^* = \sum_{b=1}^B \hat{\theta}^*(b) / B$ is the sample mean of the B bootstrap replications. We have actually done something very similar. Recall our approximate sampling distributions constructed using repeated samples (Lab 2 - bird data). In a similar fashion the bootstrap procedure approximates the distribution for $\hat{\theta}$.

Note that the previous equation for $SE_B(\hat{\theta})$ is simply the standard deviation of the B bootstrap replications.

Under many circumstances, as the sample size n increases, the sampling distribution of $\hat{\theta}$ becomes more normally distributed. Under this assumption, an approximate t-based bootstrap confidence interval can be generated using $SE_B(\hat{\theta})$ and a t-distribution:

$$\hat{\theta} \pm t^* SE_B(\hat{\theta}),$$

where t^* has $n - 1$ degrees of freedom. Note n corresponds to the number of original samples, not the number of bootstrap replicates

Bootstrap Estimate of Bias

The bias of $\hat{\theta} = S(Y_1, Y_2, \dots, Y_N)$ as an estimator of θ is defined as:

$$bias(\hat{\theta}) = E[\hat{\theta}] - \theta.$$

The bootstrap estimate of the bias of $\hat{\theta}$ as an estimate of θ is calculated by replacing the distribution F with the empirical distribution function \hat{F} . In other words the expectation (with respect to F) is unknown, but can be estimated using the empirical CDF \hat{F} using the bootstrap samples. This yields

$$bias_b(\hat{\theta}) = \hat{\theta}^* - \hat{\theta}.$$

Then, the bias-corrected estimate of θ is

$$\tilde{\theta}_B = \hat{\theta} - bias_b(\hat{\theta}) = 2\hat{\theta} - \hat{\theta}^*.$$

One suggestion is to center confidence intervals at $\tilde{\theta}$ such that bias corrected t-based confidence intervals can be expressed as $\tilde{\theta}_B \pm t^* SE_B(\hat{\theta})$.

Bootstrap Confidence Intervals

There are a few options for generating confidence intervals from bootstrap replications.

The first option uses the normal approximation. An approximate $100(1 - \alpha)\%$ confidence interval for θ is

$$\hat{\theta} \pm t^* SE_B(\hat{\theta}) \quad \text{or} \quad \hat{\theta} \pm z^* SE_B(\hat{\theta}),$$

where t^* is an $\alpha/2$ critical value from a t -distribution with $n - 1$ degrees of freedom and z^* is the $\alpha/2$ critical value from a normal distribution.

Recall, the confidence intervals can also be centered at the bias corrected point estimate $\tilde{\theta}$.

For an approximate 95% confidence interval for θ to be useful, it is expected that 95% of the confidence intervals from this method would contain θ . The same principle holds for other confidence levels.

If the sample size is not large enough and the distribution sampled from is highly skewed (or not close to a normal distribution), *then the confidence interval stated above will not be reliable. That is the nominal confidence level is not close to the true confidence level.*

Another option for calculating bootstrap based confidence intervals uses the percentiles from the bootstrap samples.

If the sample size is *relatively small or it is suspected that the sampling distribution of $\hat{\theta}$ is skewed or non-normal*, an alternative to confidence intervals using the normal distribution are preferred.

The simplest alternative is to use percentiles from the B bootstrap replications.

The approximate bootstrap percentile-based confidence interval for θ is

$$(\hat{\theta}_L^*, \hat{\theta}_U^*)$$

where $\hat{\theta}_L^*$ and $\hat{\theta}_U^*$ are the lower $\alpha/2$ and upper $(1 - \alpha/2)$ percentiles of the B bootstrap replications respectively.

Practically to find $\hat{\theta}_L^*$ and $\hat{\theta}_U^*$ you:

1. Order the B bootstrap replications $\hat{\theta}^*(1), \hat{\theta}^*(2), \dots, \hat{\theta}^*(B)$ from smallest to largest.
2. Calculate $L = B \times \alpha/2$ and $U = B \times (1 - \alpha/2)$.
3. Find the L^{th} and U^{th} values in the ordered list of bootstrap replications.
4. The L^{th} value is the lower confidence interval endpoint $\hat{\theta}_L^*$ and the U^{th} value is the upper confidence interval endpoint $\hat{\theta}_U^*$.

Note the function `quantile(theta.star, probs=c(alpha/2, (1-alpha/2)))` in R will return $\hat{\theta}_L$ and $\hat{\theta}_U$.

Bootstrap Examples in R

We will work through the code in class. Now continue with the snowfall dataset to create confidence intervals using the normal approach (t-dist) and the quantile-based approach.

```
# Enter Data
snowfall <- c(9,4,13,5,6,8)
theta.hat <- mean(snowfall)
n <- length(snowfall)

B <- 5000 # number of bootstrap replicates
theta.boot <- rep(0,B)

# take bootstrap replications
for (i in 1:B){
  boot.samples <- sample(snowfall,replace=T)
  theta.boot[i] <- mean(boot.samples)
}

head(theta.boot,10)

## [1] 7.833333 6.333333 7.166667 8.666667 6.833333 8.833333 5.333333
## [8] 7.166667 6.666667 9.833333

# visualize distribution from bootstrap draws
hist(theta.boot,probability=T,main=expression("Histogram of " ~ hat(theta)),
      xlab=expression(hat(theta)))

# compute standard error
se.b <- sd(theta.boot)

# compute bias corrected estimate
theta.boot.mean <- mean(theta.boot)
tilde.theta <- 2 * theta.hat - theta.boot.mean

# normality based confidence intervals
upper.norm <- theta.hat + qt(.975,n-1)* se.b
lower.norm <- theta.hat - qt(.975,n-1)* se.b

abline(v=upper.norm,col='red',lwd=2)
abline(v=lower.norm,col='red',lwd=2)

# percentile based confidence intervals
upper.per <- quantile(theta.boot,probs=.975)
lower.per <- quantile(theta.boot,probs=.025)

abline(v=upper.per,col='blue',lwd=2)
abline(v=lower.per,col='blue',lwd=2)

legend('topright',c('normal','quantile'),col=c('red','blue'),lty=1,lwd=2)
```

