Lecture 26: Bootstrapping linear regression

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Recap

- What is a regression model?
- Descriptive statistics – graphical
- Descriptive statistics – numerical
- Inference about a population mean
- Difference between two population means
- Some tips on R
- Simple linear regression (covariance, correlation, estimation, geometry of least squares)
  - Inference on simple linear regression model
  - Goodness of fit of regression: analysis of variance.
  - F-statistics.
  - Residuals.
  - Diagnostic plots for simple linear regression (graphical methods).

Recap

- Multiple linear regression
  - Specifying the model.
  - Fitting the model: least squares.
  - Interpretation of the coefficients.
  - Matrix formulation of multiple linear regression
  - Inference for multiple linear regression
    - T-statistics revisited.
    - More F statistics.
    - Tests involving more than one β.
- Diagnostics – more on graphical methods and numerical methods
  - Different types of residuals
  - Influence
  - Outlier detection
  - Multiple comparison (Bonferroni correction)
  - Residual plots:
    - partial regression (added variable) plot,
    - partial residual (residual plus component) plot.

Recap

- Adding qualitative predictors
  - Qualitative variables as predictors to the regression model.
  - Adding interactions to the linear regression model.
  - Testing for equality of regression relationship in various subsets of a population
- ANOVA
  - All qualitative predictors.
  - One-way layout
  - Two-way layout
- Transformation
  - Achieving linearity
  - Stabilize variance
  - Weighted least squares
- Correlated Errors
  - Generalized least squares

Bootstrapping linear regression

Outline

- Bootstrap method (Efron 1979)
  - Recommended reading: (Davison and Hinkley 1997), (Efron and Tibshirani 1994)
- Bootstrapping regression
- Motivation:
  - We've talked about correcting our regression estimator in two contexts: WLS (weighted least squares) and GLS (Generalized least squares).
  - Both require a model of the errors for the correction.
  - In both cases, we use a two stage procedure to "whiten" the data and use the OLS model on the "whitened" data.
  - **What if we don't have a model for the errors?**
  - We will use the bootstrap

The bootstrap

- Computer-based resampling procedure to access the statistical accuracy.
- Computes standard error or bias of a statistic or sampling distribution of a statistic or confidence intervals of parameters.
- No need a mathematical expression for the statistical accuracy such as bias or standard error.

The bootstrap

- $\boldsymbol{X} = (X_1, \cdots, X_n)^T \sim F$.
- $\theta = T(F)$, a parameter of interest.
- $\hat{\theta} = T(\hat{F}_n) = s(\boldsymbol{x})$, an estimate from $\boldsymbol{x} = (x_1, \cdots, x_n)^T$.
- Let $\hat{F}$ be the empirical distribution of the observed values x_i, $\hat{F}_n(t) = \dfrac{\sum_{i=1}^n I(x_i \leq t)}{n}$.
- A bootstrap sample $\boldsymbol{X}^* = (X_1^*, \cdots, X_n^*)$, a random sample of size n drawn with replacement from $\hat{F}_n$ (total of distinct bootstrap samples $\binom{2n-1}{n-1}$) see this link for the illustration.
- A bootstrap replication of $\hat{\theta}$ is $\hat{\theta}^* = s(\boldsymbol{x}^*)$.
- Bootstrap replicates $\hat{\theta}^{*1}, \cdots, \hat{\theta}^{*R}$, where R is the number of bootstrap samples.

The bootstrap (illustration)

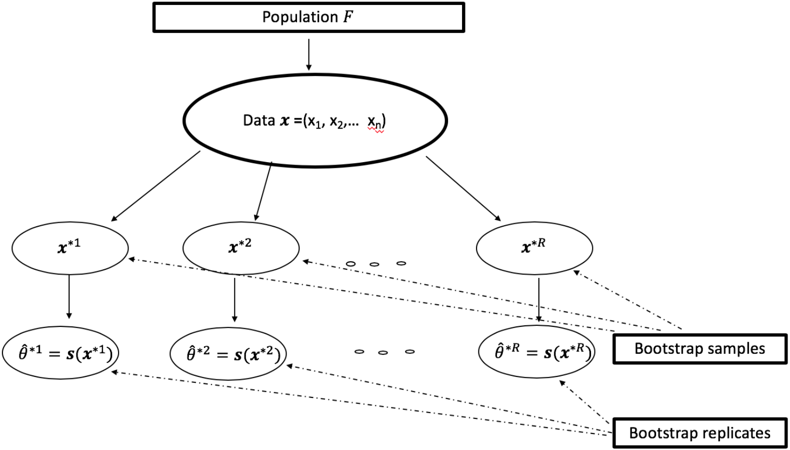


Figure 1: Bootstrap method

The bootstrap method for estimating standard error

- Draw R bootstrap samples $\boldsymbol{X}^{*1}, \cdots, \boldsymbol{X}^{*R}$ each with n values with replacement.
- Evaluate bootstrap replicate $\hat{\theta}^{*r} = s\left(\boldsymbol{x}^{*r}\right)$.
- Estimate the standard error $\mathrm{se}\left(\hat{\theta}\right)$

$$\hat{\mathrm{se}}_{\mathrm{boot}}\left(\hat{\theta}\right) = \left[\frac{\sum_{r=1}^{R}\left(\hat{\theta}^{*r} - \hat{\theta}^{*}(\cdot)\right)^{2}}{R-1}\right]^{1/2},$$

where $\hat{\theta}^{*}(\cdot) = \dfrac{\sum_{r=1}^{R}\hat{\theta}^{*r}}{R}$.

- How large should be R? The rules of thumb: $R = 50$ is often enough to give a good estimate of $\mathrm{se}\left(\hat{\theta}\right)$ (much larger values of R are required for confidence intervals).

Bootstrap percentile confidence interval

- Order bootstrap replicates $\hat{\theta}^*_{(1)}, \cdots, \hat{\theta}^*_{(R)}$.
- Let $m = [\alpha/2 \times R]$, $[u]$ is the largest integer less than or equal to u.
- Approximate $(1-\alpha)\,100\%$ confidence interval for θ is $\left(\hat{\theta}^*_{(m)}, \hat{\theta}^*_{(R-m)}\right)$.
- Choose $R = 1000$ or larger than 1000.

Assessing the error in bootstrap estimates

- Bootstrap estimates are not exact (nearly unbiased but can have substantial variance).
- Two sources of variability
  - Sampling variability: we have only a sample of size n rather than the entire population.
  - Bootstrap resampling variability: we only take R bootstrap samples rather than total of $\binom{2n-1}{n-1}$ distinct bootstrap samples.

Two sources of variability (illustration)

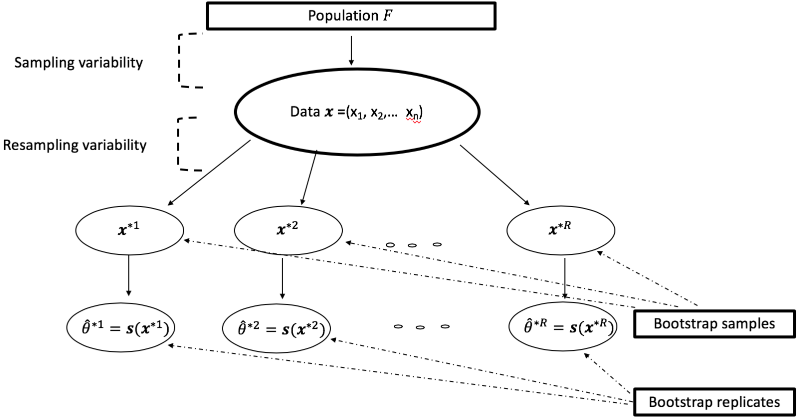


Figure 2: The sampling and resampling variability

Example

- An example from `bootstrap` package (Efron and Tibshirani 1994).
- The data are LSAT scores (for entrance to law school) and GPA. This data were used to illustrate the bootstrap by Bradly Efron, the inventor of the bootstrap.

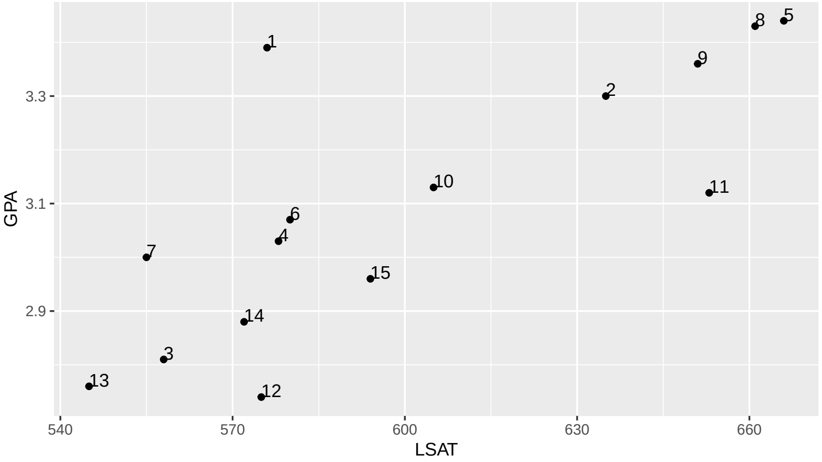
```r
data(law) # in the bootstrap package
head(law)
```

```
##   LSAT  GPA
## 1  576 3.39
## 2  635 3.30
## 3  558 2.81
## 4  578 3.03
## 5  666 3.44
## 6  580 3.07
```

Example (scatterplot)

```r
library(ggplot2)
ggplot(data = law, aes(x= LSAT, y= GPA))
```

Example (scatterplot)



Example (Plug-in estimate of the correlation coefficient)

- Let X = LSAT and Y = GPA, F be a joint distribution of (X, Y).
- Correlation coefficient $= \theta = \theta(F)$.
- Sample correlation coefficient $= \hat{\theta} = \theta(\hat{F})$.

```
theta.hat = cor(law$LSAT, law$GPA)
theta.hat
```

```
## [1] 0.7763745
```

Example (bootstrap replicates)

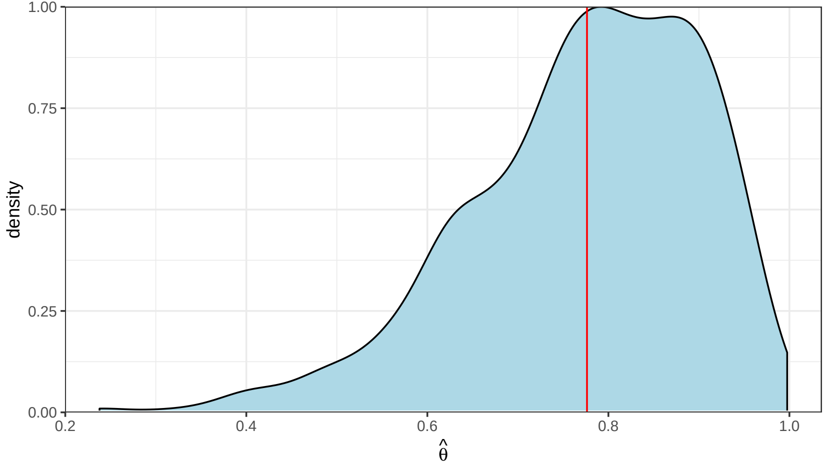
- Compute bootstrap replicates: $\hat{\theta}^*$

```
com.theta.hat = function(df, ind){
  cor(df$LSAT[ind], df$GPA[ind])
}
theta.hat.star = boot(data = law,
                      com.theta.hat,
                      R = 1000)$t
```

Example (bootstrap approximation for the sampling distribution of the estimator)

```r
theta.hat.star.df =
  data.frame(theta.hat.star = theta.hat.star)
p = ggplot(theta.hat.star.df) +
  geom_density(aes(x = theta.hat.star,
                   y = ..scaled..),
    fill = "lightblue") +
  geom_hline(yintercept=0, colour="white", size=1) +
  theme_bw() +
  ylab("density") +
  xlab(bquote(hat(theta))) +
  geom_vline(xintercept = theta.hat, col = "red")+
  scale_y_continuous(expand = c(0,0))
```

Example (bootstrap approximation for the sampling distribution of the estimator)



Example (standard error of $\hat{\theta}$ using bootstrap)

```r
sd(theta.hat.star)
```

```
## [1] 0.1342333
```

Example (percentile interval for θ using bootstrap)

- 95% bootstrap percentile interval

```
quantile(theta.hat.star, probs = c(.025, .975))
```

```
##      2.5%     97.5% 
## 0.4742893 0.9598190
```

- Learn about different types of bootstrap confidence interval: STAT205 Notes

Bootstrapping linear regression

- Suppose we think of the pairs (X_i, Y_i) coming from a joint distribution F – this is a joint distribution for *both the predictors and the response.*
- Note: this is different than our usual model up to this point. Our usual model says that

$$Y_{n\times 1}|X_{n\times p} \sim N(X\beta, \sigma^2 I)$$

  (or our WLS / GLS models for error).
- **We have essentially treated X as fixed.**
- In our usual model, β is clearly defined. What is β without this assumption that X is fixed?
- Can we write β as a function of F: $\beta(F)$?

Population least squares

- For the joint distribution F, we can define

$$E_F[\boldsymbol{X}\boldsymbol{X}^T], \qquad E_F[\boldsymbol{X} \cdot \boldsymbol{Y}]$$

where $(\boldsymbol{X}, \boldsymbol{Y}) \sim F$ leading to

$$\beta(F) = \left(E_F[\boldsymbol{X}\boldsymbol{X}^T]\right)^{-1} E_F[\boldsymbol{X} \cdot \boldsymbol{Y}].$$

- In fact, our least squares estimator is $\beta(\hat{F}_n)$ where $\hat{F}_n$ is the *joint empirical distribution* of our sample of n observations from F.

Population least squares

- As we take a larger and larger sample,

$$\beta(\hat{F}_n) \to \beta(F)$$

and

$$n^{1/2}(\beta(\hat{F}_n) - \beta(F)) \to N(0, \Sigma(F))$$

for some covariance matrix $\Sigma = \Sigma(F)$ depending only on F.

- Recall the variance of OLS estimator (with X fixed):

$$(X^TX)^{-1}\mathrm{Var}(X^TY)(X^TX)^{-1}.$$

- With X random and n large this is approximately

$$\frac{1}{n}\left(E_F[\boldsymbol{X}\boldsymbol{X}^T]\right)^{-1}\mathrm{Var}_F(\boldsymbol{X}\cdot\boldsymbol{Y})\left(E_F[\boldsymbol{X}\boldsymbol{X}^T]\right)^{-1}.$$

Population least squares

- In usual model, $\mathrm{Var}(X^TY) = \sigma^2 X^TX \approx nE_F[\boldsymbol{X}\boldsymbol{X}^T]$. In WLS model it is $X^TW^{-1}X$ (or, rather, its expectation) where W might come from some model.
- **In this setting we will use OLS estimate – but correct its variance!**
- **Can we get our hands on Var(X^TY) or Var$(\hat{\beta})$ without a model?**

Basic algorithm for bootstrapping pairs

- There are many variants of the bootstrap, most using roughly this structure.
- Estimate $\text{Cov}\left(\hat{\beta}\right)$ using the bootstrap.

```
boot_replicate = c()
for (b in 1:B) {
    idx_star = sample(1:n, n, replace=TRUE)
    X_star = X[idx_star,]
    Y_star = Y[idx_star]
    boot_replicate = rbind(boot_replicate,
                           coef(lm(Y_star ~ X_star)))
}
cov_beta_boot = cov(boot_replicate)
```

Bootstrapping pairs

- Estimated covariance `cov_beta_boot` can be used to estimate $\text{Var}(\boldsymbol{a}^T\hat{\beta}) = \boldsymbol{a}^T\text{Cov}\left(\hat{\beta}\right)\boldsymbol{a}$ for confidence intervals or general linear hypothesis tests.
- Software does something slightly different – using percentiles of the bootstrap sample: *bootstrap percentile intervals*.

Bootstrapping regression (Using `Boot` function in `car` package)

- Reference for more R examples
- Example (Simulation)

```
library(car)# Boot() wraper function
n = 50
X = rexp(n)
# our usual model is false here! W=X^{-2}
Y = 3 + 2.5 * X + X * (rexp(n) - 1)
Y.lm = lm(Y ~ X)
```

- Confidence intervals for the regression partial coefficients.

```
confint(Y.lm)
```

```
##                 2.5 %   97.5 %
## (Intercept) 2.509889 3.486932
## X           2.188180 2.853384
```

Boot function in car package

```
pairs.Y.lm = Boot(Y.lm, coef,
                  method='case', R=1000)
```

Boot function in car package

```r
# bootstrap standard confidence interval
confint(pairs.Y.lm, type='norm')
```

```
## Bootstrap normal confidence intervals
##
##                2.5 %   97.5 %
## (Intercept) 2.476667 3.515178
## X           1.899959 3.152024
```

```r
# bootstrap percentile interval
confint(pairs.Y.lm, type='perc')
```

```
## Bootstrap percent confidence intervals
##
##                2.5 %   97.5 %
## (Intercept) 2.540548 3.490207
## X           1.925935 3.110014
```

Using the `boot` package

- The `Boot` function in `car` is a wrapper around the more general `boot` function.
- Here is an example using `boot`.

Using the boot package

```
D = data.frame(X, Y)
bootstrap_stat = function(D, bootstrap_idx) {
    return(summary(lm(Y ~ X,
                      data=D[bootstrap_idx,]))$coef[,1])
}
boot_results = boot(D, bootstrap_stat, R=500)
```

Using the boot package

```r
# bootstrap standard confidence interval
confint(boot_results, type='norm')
```

```
## Bootstrap normal confidence intervals
##
##      2.5 %   97.5 %
## 1 2.481306 3.553691
## 2 1.848860 3.141992
```

```r
# bootstrap percentile interval
confint(boot_results, type='perc')
```

```
## Bootstrap percent confidence intervals
##
##      2.5 %   97.5 %
## 1 2.465994 3.505010
## 2 1.964832 3.160705
```

How is the coverage?

- First we'll use the standard regression model but errors that aren't Gaussian.
- Construct 95% confidence interval for the slope.

```
noise = function(n) { return(rexp(n) - 1) }
```

How is the coverage?

```
simulate_correct = function(n=20, b=0.5) {
  X = rexp(n)
  Y = 3 + b * X + noise(n)
  Y.lm = lm(Y ~ X)
  # parametric interval
  int_param = confint(Y.lm)[2,]
  # pairs bootstrap interval
  pairs.Y.lm = Boot(Y.lm, coef, method='case', R=1000)
  int_pairs = confint(pairs.Y.lm, type='perc')[2, ]
  names(int_pairs) = NULL
  result = c((int_param[1] < b) * (int_param[2] > b),
             (int_pairs[1] < b) * (int_pairs[2] > b))
  names(result) = c('parametric', 'bootstrap')
  return(result)
}
```

Check one instance

```r
simulate_correct()
```

```
## parametric  bootstrap
##          1           1
```

Check coverage

```r
nsim = 100
coverage = c()
for (i in 1:nsim) {
    coverage = rbind(coverage, simulate_correct())
}
print(apply(coverage, 2, mean))
```

```
## parametric  bootstrap
##       0.96       1.00
```

- Parametric method has coverage close to .95.

Misspecified model

- Now we make data for which we might have used WLS **but we don't have a model for the weights!**
- Construct 95% confidence interval for the slope.

Misspecified model

```
simulate_incorrect = function(n=20, b=0.5) {
  X = rexp(n)
  # the usual model is
  # quite off here -- Var(X^TY) is not well
  # approximated by sigma^2 * X^TX...
  Y = 3 + b * X + X * noise(n)
  Y.lm = lm(Y ~ X)
  # parametric interval
  int_param = confint(Y.lm)[2,]
  # pairs bootstrap interval
  pairs.Y.lm = Boot(Y.lm, coef, method='case', R=1000)
  int_pairs = confint(pairs.Y.lm, type='perc')[2, ]
  names(int_pairs) = NULL
  result = c((int_param[1] < b) * (int_param[2] > b),
             (int_pairs[1] < b) * (int_pairs[2] > b))
  names(result) = c('parametric', 'bootstrap')
  return(result)
}
```

Check one instance

```r
simulate_incorrect()
```

```
## parametric  bootstrap
##          1           1
```

Check coverage

```r
nsim = 100
coverage = c()
for (i in 1:nsim) {
    coverage = rbind(coverage, simulate_incorrect())
}

print(apply(coverage, 2, mean))
```

```
## parametric  bootstrap
##       0.57       0.95
```

- Bootstrap method has coverage close to .95.

Reference

- Chapter 9 (Regression models): Efron, Bradley, and Robert J Tibshirani. 1994. An Introduction to the Bootstrap. CRC press.
- Lecture notes of Pratheepa Jeganathan
- Lecture notes of Jonathan Taylor .

Davison, Anthony Christopher, and David Victor Hinkley. 1997. *Bootstrap Methods and Their Application*. Vol. 1. Cambridge university press.

Efron, B. 1979. "Bootstrap Methods: Another Look at the Jackknife." *Ann. Statist.* 7 (1). The Institute of Mathematical Statistics: 1–26. https://doi.org/10.1214/aos/1176344552.

Efron, Bradley, and Robert J Tibshirani. 1994. *An Introduction to the Bootstrap*. CRC press.