# Stat 435 Lecture Notes 4

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## Contents



# Bootstrap: motivation

## Overview

- The *bootsrtap* is mainly used to *estimate and quantify the uncertainty associated with a given estimate or statistical learning methed*
- For example, it can be used to estimate the standard error of an estimate (such as an estimated coefficient in a regression model)

- The bootstrap *may not work well when sample size is small or when sample comes from a relatively small region of the distribution of an unknown data generating process*

## Illustration I: problem

Problem formulation:

- suppose we wish to invest a fixed sum of money into two financial assets that yield (random) returns of $X$ and $Y$, respectively
- we will invest a fraction $\alpha$ of our money in $X$, and the rest $1-\alpha$ in $Y$
- we need to choose $\alpha$ that minimizes the risk, or variance, of our investment.

Namely, we need to find $\alpha$ that minimizes

$$\mathrm{Var}(\alpha X + (1-\alpha)Y)$$

## Illustration I: solution

- By calculus, we know that

  $$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}$$

  minimizes

  $$\mathrm{Var}(\alpha X + (1-\alpha)Y),$$

  where $\sigma_X^2 = \mathrm{Var}(X)$, $\sigma_Y^2 = \mathrm{Var}(Y)$ and $\sigma_{XY} = \mathrm{Cov}(X,Y)$
- However, in reality, the quantities $\sigma_X^2$, $\sigma_Y^2$ and $\sigma_{XY}$ are unknown, and need to be estimated

## Illustration I: estimate

- With estimates $\hat{\sigma}_X^2$, $\hat{\sigma}_Y^2$ and $\hat{\sigma}_{XY}$ for $\sigma_X^2$, $\sigma_Y^2$ and $\sigma_{XY}$, respectively, we have the *plug-in estimate*

  $$\hat{\alpha} = \frac{\hat{\sigma}_Y^2 - \hat{\sigma}_{XY}}{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2 - 2\hat{\sigma}_{XY}}$$

  for the *optimal but unknown* solution

  $$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}$$

- How accurate is $\hat{\alpha}$? Can we estimate the standard error of $\hat{\alpha}$?

## Illustration I: estimate

- If $\hat{\sigma}_X^2$, $\hat{\sigma}_Y^2$ and $\hat{\sigma}_{XY}$ are accurate, then so should be $\hat{\alpha}$
- How to assess the accuracy of $\hat{\alpha}$ (via the accuracy of $\hat{\sigma}_X^2$, $\hat{\sigma}_Y^2$ and $\hat{\sigma}_{XY}$) if we have only a sample of size $n$ at hand?
- Mini discussion on the question above: Case 1 "$n$ small", Case 2 "$n$ moderate", and case 3 "$n$ large"

## Illustration I: simulated samples

If we know the population distribution, we can simulate samples:

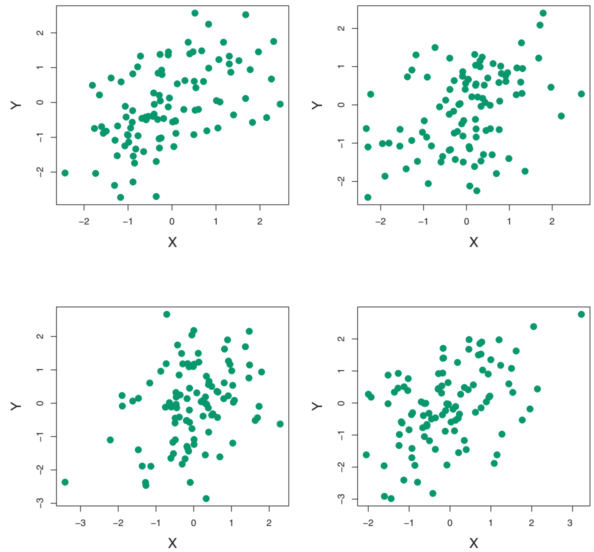


**FIGURE 5.9.** *Each panel displays* 100 *simulated returns for investments* $X$ *and* $Y$*. From left to right and top to bottom, the resulting estimates for* $\alpha$ *are* 0.576*,* 0.532*,* 0.657*, and* 0.651*.*

## Illustration I: simulated samples

- Suppose we simulate $B = 1000$ *independent* samples for $(X, Y)$ (if we knew the truth), we will have $B$ estimates $\hat{\alpha}_j, j = 1, \ldots, B$ of $\alpha$
- The sample mean $\bar{\alpha} = \frac{1}{B}\sum_{j=1}^{B}\hat{\alpha}_j$ (of $\hat{\alpha}_j$'s) should be close to $\alpha$
- The sample standard deviation

$$s\left(\hat{\alpha}\right) = \sqrt{\frac{1}{B-1}\sum_{j=1}^{B}\left(\hat{\alpha}_j - \bar{\alpha}\right)^2}$$

  (of of $\hat{\alpha}_j$'s) should be close to $\sigma_{\hat{\alpha}} = \sqrt{\widehat{\mathrm{Var}(\alpha)}}$

## Illustration I: truth and estimate

- Truth: $\sigma_X^2 = 1$, $\sigma_Y^2 = 1.25$, $\sigma_{XY} = 0.5$ and $\alpha = 0.6$
- Estimates based on $B = 1000$ simulated, independent samples: $\bar{\alpha} = 0.5996$ and $s\left(\hat{\alpha}\right) = 0.083$
- Interpretation: for a random sample from the population, we would expect $\hat{\alpha}$ to differ from $\alpha$ by approximately 0.08 on average

*Note:* is the "1 standard deviation" rule sensible?

# Bootstrap: definition and applications

## Simulation and double-dipping

- *Simulated from the truth*: when we know a data generating process, we can simulate samples to estimate a statistic on the process. However, if we know the truth, why do we need to estimate the statistic?
- *Simulated from the estimate*: with a sample from a data generating process, we can estimate the process, use the estimated process to generate samples, and use the generated samples to estimate a statistic
- *Resampling from the sample*: sample randomly from a sample from a data generating process, regard the sampled observations as a new data set, and use them to estimate a statistic

## Bootstrap: definition

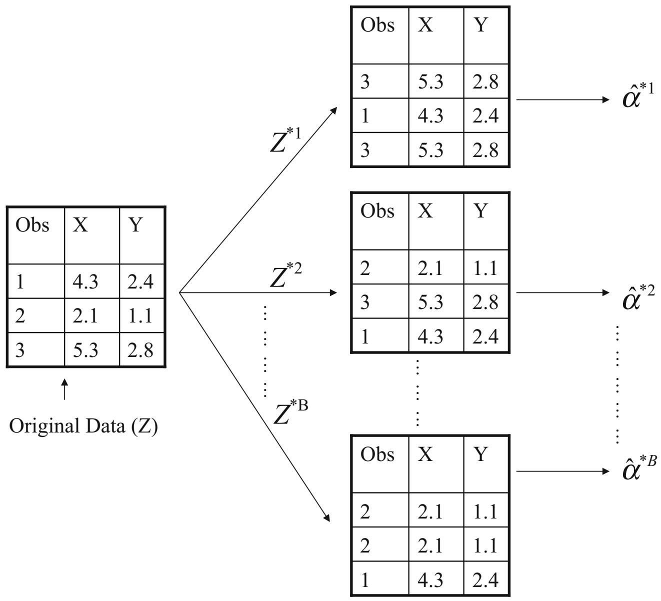
In order to assess the distributional properties of an estimate of a statistic, the bootstrap

- takes a subset of a given data set *as if it is a set of new observations independent of the given data set*
- uses the subset to obtain an estimate of the statistic
- does so *repeatedly and independently using different subests of the given data set*
- take the *empirical distribution of estimates obtained from these subsets as an estimate of the distribution of the estimate* of the statistic

## Bootstrap: procedure

- Given a sample of size $n$, let $\hat{\alpha}$ be an estimate of a statistic $\alpha$ obtained from the sample
- *Sample randomly with replacement* from the sample to obtain $n$ observations, and do this independently $B$ times to obtain $B$ bootstrap samples $S_j, j = 1, \dots, B$
- Let $\hat{\alpha}_j$ be the estimate of $\alpha$ obtained from $S_j$. Then *the empirical distribution $G$ of $\hat{\alpha}_j, j = 1, \dots, B$ is used as the (true) distribution of $\hat{\alpha}$, and statistics about $\hat{\alpha}$ are obtained from $G$*

## Bootstrap: graphical illustration




## Bootstrap: statistics

- The *(bootstrap) estimated mean* of $\hat{\alpha}$ is $\bar{\alpha} = \frac{1}{B}\sum_{j=1}^{B} \hat{\alpha}_j$
- The *(bootstrap) estimated variance* of $\hat{\alpha}$ is

$$\mathrm{SE}^2\left(\hat{\alpha}\right) = (B-1)^{-1}\sum_{j=1}^{B}\left(\hat{\alpha}_j - \bar{\alpha}\right)^2$$

- For $\alpha \in (0,1)$, the *(bootstrap)* $(1-\alpha) \times 100$ *percent confidence interval* for $\hat{\alpha}$ is $(c_L, c_U)$, where $c_L$ is the $\{0.5\alpha \times 100\}$th percentile of $G$, and $c_L$ is the $\{(100 - 0.5\alpha) \times 100\}$th percentile of $G$

## Illustration of bootstrap

Bootstrap applied to a sample; $\mathrm{SE}^2\left(\hat{\alpha}\right) = 0.087$: illusion or excellence?

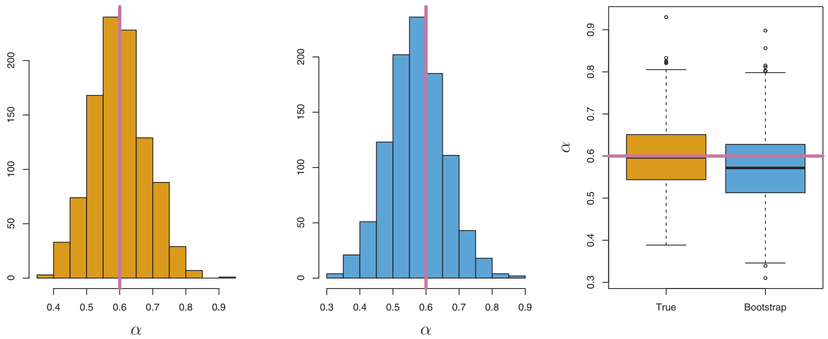



**FIGURE 5.10.** Left: *A histogram of the estimates of $\alpha$ obtained by generating 1,000 simulated data sets from the true population.* Center: *A histogram of the estimates of $\alpha$ obtained from 1,000 bootstrap samples from a single data set.* Right: *The estimates of $\alpha$ displayed in the left and center panels are shown as boxplots. In each panel, the pink line indicates the true value of $\alpha$.*

# Boostrapping linear regression

## Linear regression

- Model: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p + \varepsilon$ with $E(\varepsilon) = 0$ and $\mathrm{Var}(\varepsilon) = \sigma^2$
- Observations: $(y_i, x_{1i}, x_{2i}, \ldots, x_{pi}), i = 1, \ldots, n$, where $x_{ji}$ is the $i$th observation for $X_j$
- Estimate: $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \ldots + \hat{\beta}_p X_p$
- Fit: $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{1i} + \hat{\beta}_2 x_{2i} + \ldots + \hat{\beta}_p x_{pi} + \varepsilon_i$
- Residuals: $e_i = y_i - \hat{y}_i$

## Bootstrapping from sample

Set $\boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_p)$ and $\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p)$

- Sample from data generating process:

$$S = \{\mathbf{z}_i = (y_i, x_{1i}, x_{2i}, \ldots, x_{pi}), i = 1, \ldots, n\}$$

- Sample with replacement $n$ observations from $S$ and repeat this independently to obtain $B$ subsets $S_j, j = 1, \ldots, B$
- Obtain $\hat{\boldsymbol{\beta}}_j$ from $S_j$ for each $j = 1, \ldots, B$
- Use the empirical distribution of $\hat{\boldsymbol{\beta}}_j, j = 1, \ldots, B$ as the distribution of $\hat{\boldsymbol{\beta}}$

## Bootstrapping residuals

- Residuals: $R = \{e_i = y_i - \hat{y}_i, i = 1, \ldots, n\}$
- Sample with replacement $n$ observations from $R$ to obtain $B$ sets of residuals $R_j = \{e_i^{(j)}, i = 1, \ldots, n\}$
- For each $j$, set $y_i^{(j)} = \hat{y}_i + e_i^{(j)}$ and fit the model with observations

$$S_j = \{\mathbf{z}_i^{(j)} = (y_i^{(j)}, x_{1i}, x_{2i}, \ldots, x_{pi}), i = 1, \ldots, n\}$$

and obtain estimate $\hat{\boldsymbol{\beta}}_j$

- Use the empirical distribution of $\hat{\boldsymbol{\beta}}_j, j = 1, \ldots, B$ as the distribution of $\hat{\boldsymbol{\beta}}$

### Bootstrapping samples or residuals

- Asymptotically (and under some conditions), bootstrapping samples and bootstrapping residuals are equivalent
- Bootstrapping samples is less sensitive to model misspecification
- Bootstrapping samples may be less sensitive to the assumptions concerning independence or exchangeability of the error terms

## Boostrap: failures

### Boostrap failures

Bootstrap can fail

- when sample size is too small
- for estimating extremal statistics
- when observations are dependent
- for survey sampling

*Note:* the book "Bootstrap methods: a guide for practitioners and researchers" by Michael R. Chernick contains more information on this.

### License and session Information

License

```
> sessionInfo()
R version 3.5.0 (2018-04-23)
Platform: x86_64-w64-mingw32/x64 (64-bit)
Running under: Windows 10 x64 (build 19041)

Matrix products: default

locale:
[1] LC_COLLATE=English_United States.1252
[2] LC_CTYPE=English_United States.1252
[3] LC_MONETARY=English_United States.1252
[4] LC_NUMERIC=C
[5] LC_TIME=English_United States.1252

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods
[7] base

other attached packages:
[1] knitr_1.21
```

```
loaded via a namespace (and not attached):
 [1] compiler_3.5.0  magrittr_1.5    tools_3.5.0
 [4] htmltools_0.3.6 yaml_2.2.0      Rcpp_1.0.3
 [7] stringi_1.2.4   rmarkdown_1.11  stringr_1.3.1
[10] xfun_0.4        digest_0.6.18   evaluate_0.12
```