MONASH University

ETC3250

Business Analytics

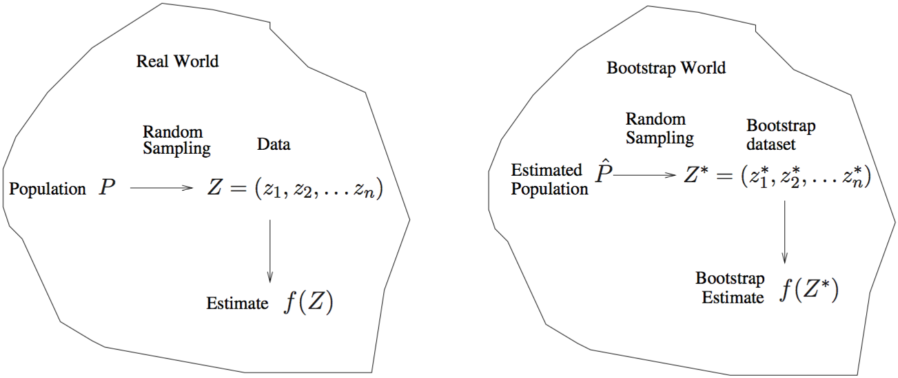
Week 4.
The Bootstrap

20 August 2015

Pull yourself up by your bootstraps

What is the bootstrap?

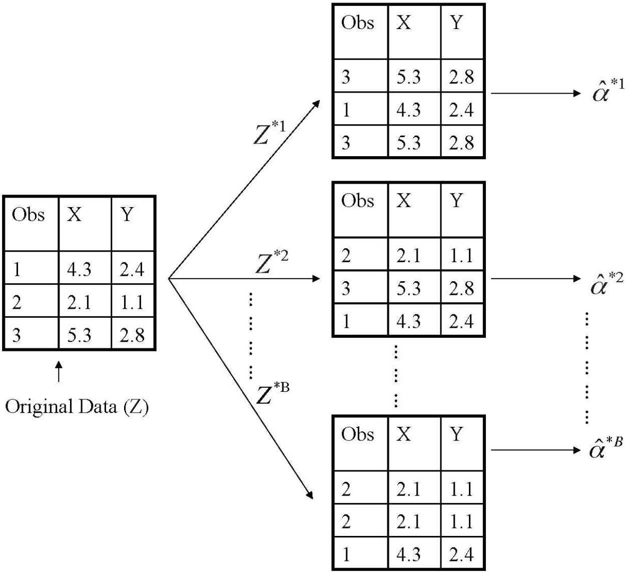
The bootstrap is a flexible statistical tool to **quantify the uncertainty** associated with a *given estimator* or *statistical learning method*.


Real World
Random Sampling
Data
Population $P \longrightarrow Z = (z_1, z_2, \ldots z_n)$
Estimate $f(Z)$
Bootstrap World
Random Sampling
Bootstrap dataset
Estimated Population $\hat{P} \longrightarrow Z^* = (z_1^*, z_2^*, \ldots z_n^*)$
Bootstrap Estimate $f(Z^*)$

What is the bootstrap?

- The bootstrap allows us to use a computer to **mimic the process of obtaining new data sets**, so that we can estimate the variability of our estimate without generating additional samples
- Rather than repeatedly obtaining independent data sets from the population, we instead obtain distinct data sets (with the same size as our original dataset) by repeatedly sampling observations **from the original data set with replacement** (nonparametric) or **from an estimated model** (parametric).

Illustration of the bootstrap



Obs	X	Y
1	4.3	2.4
2	2.1	1.1
3	5.3	2.8

Obs	X	Y
3	5.3	2.8
1	4.3	2.4
3	5.3	2.8

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2	2.1	1.1
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The bootstrap procedure

- Find a good estimate $\hat{P}$ of P
  - Parametric bootstrap
  - Nonparametric bootstrap
- Draw B independent bootstrap samples $X^{*(1)}, \ldots, X^{*(B)}$ from $\hat{P}$:

$$X_1^{*(b)}, \ldots, X_n^{*(b)} \sim \hat{P} \quad b = 1, \ldots, B.$$

- Evaluate the bootstrap replications:

$$\hat{\theta}^{*(b)} = s(X^{*(b)}) \quad b = 1, \ldots, B.$$

- Estimate the quantity of interest from the simulated distribution of the $\hat{\theta}^{*(b)}$

Examples

What is the standard error of $\hat{\theta}$ (i.e., the standard deviation of the sampling distribution of $\hat{\theta}$)?

1. $\hat{\theta} =$ sample mean
2. $\hat{\theta} =$ sample median
3. $\hat{\theta} =$ expected shortfall at 5%
4. $\hat{\theta} =$ lag 1 autocorrelation.

Prediction error estimation

- Fit the model on a set of bootstrap samples, and then keep track of how well it predicts the original training set

$$\mathrm{Err}_{\mathrm{boot}} = \frac{1}{B}\frac{1}{N}\sum_{b=1}^{B}\sum_{i=1}^{N} L(y_i, \hat{f}^{*b}(x_i))$$

- Each of these bootstrap data sets is created by sampling with replacement, and is the same size as our original dataset. As a result some observations may appear more than once in a given bootstrap data set and some not at all.

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Prediction error estimation

- Training and validation sets have observations in common! Overfit predictions will look very good.

$$
\begin{aligned}
&\mathrm{P}(\text{observation } i \in \text{ bootstrap sample } b)\\
&= 1 - (1 - \frac{1}{n})^n\\
&\approx 1 - \frac{1}{e}\\
&= 0.632
\end{aligned}
$$

- Remember that cross-validation uses *non-overlapping* data for the training and validation samples

Prediction error estimation

Better bootstrap version: we only keep track of predictions from bootstrap samples not containing that observation. The leave-one-out bootstrap estimate of prediction error can be defined as

$$\mathrm{Err}_{\text{loo-boot}} = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{|C^{-i}|}\sum_{b\in C^{-i}} L(y_i, \hat{f}^{*b}(x_i))$$

where C^{-i} is the set of indices of the bootstrap samples b that do not contain observation i. Problem of overfitting with $\mathrm{Err}_{\text{boot}}$ solved but training-set-size bias as with cross-validation.

Many applications

- Computing standard errors for complex statistics
- Prediction error estimation
- Bagging (Bootstrap aggregating)
- ...

Variations

There are several types of bootstrap based on different assumptions:

- block bootstrap
- sieve bootstrap
- smooth bootstrap
- residual bootstrap
- wild bootstrap

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