MONASH University

ETC3250

Business Analytics

Week 6

Resampling methods

31 August 2017

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3	Regression for prediction	3,7	Tas & David
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6	Model selection and resampling methods	5	Souhaib
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10	Clustering	10	Souhaib
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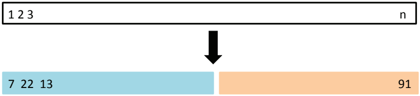
Resampling methods

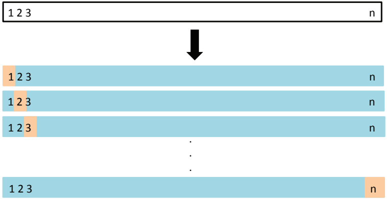
Resampling methods are used in

1. **validating models** by using (random) subsets of the data (e.g cross validation and bootstrapping),
2. **estimating uncertainty** in sample statistics by drawing randomly with replacement from the data set (e.g. bootstrapping),
3. performing **(non-parametric) significance tests** (permutation tests).

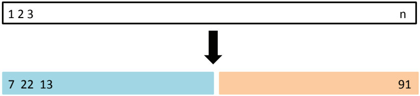
Outline

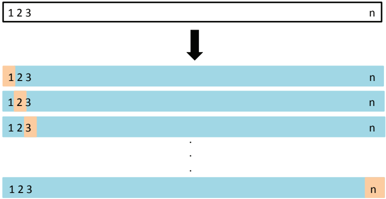
Validation set and Leave-one-out

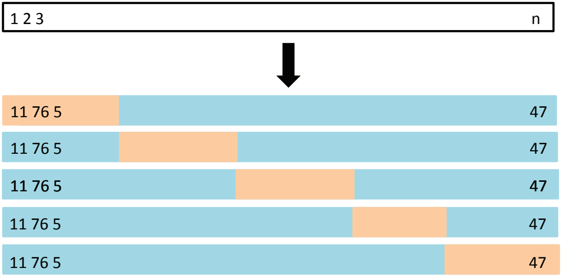




Cross-validation







k-fold Cross-validation

- Divide the data set into k different parts.
- Remove one part, fit the model on the remaining $k-1$ parts, and compute the MSE on the omitted part.
- Repeat k times taking out a different part each time

By averaging the k MSEs we get an estimated validation (test) error rate for new observations.

$$\mathrm{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k}\mathrm{MSE}_i$$

LOOCV is a special case where $k = n$.

k-fold Cross-validation

- Each training set is only $(k-1)/k$ as big as the original data set. So the estimates of prediction error will be biased upwards.
- Bias minimized when $k = n$ (LOOCV).
- But variance increases with k (as there are overlapping observations in each part).
- $k = 5$ or $k = 10$ provide a good compromise for this bias-variance tradeoff.

Outline

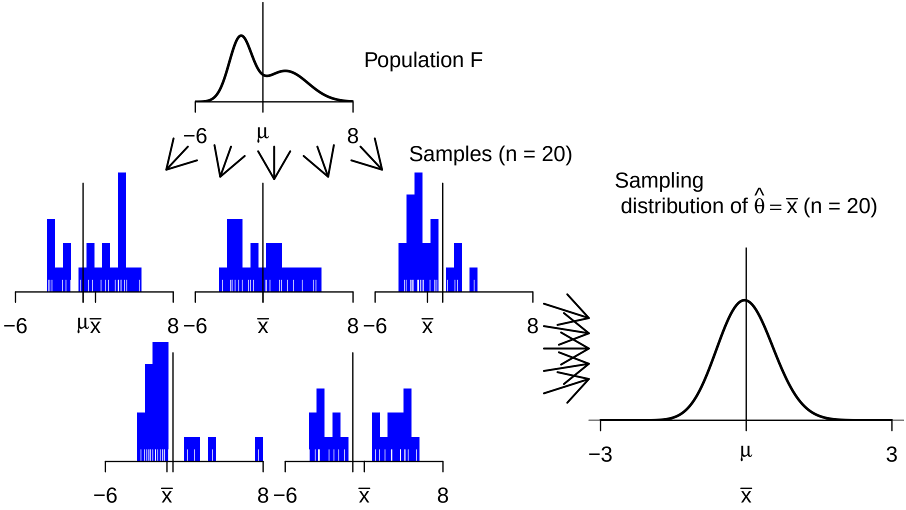
Pull yourself up by your bootstraps

What is the bootstrap?

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

- 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
- We 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).

Bootstrapping: Ideal world



Bootstrapping: Bootstrap world

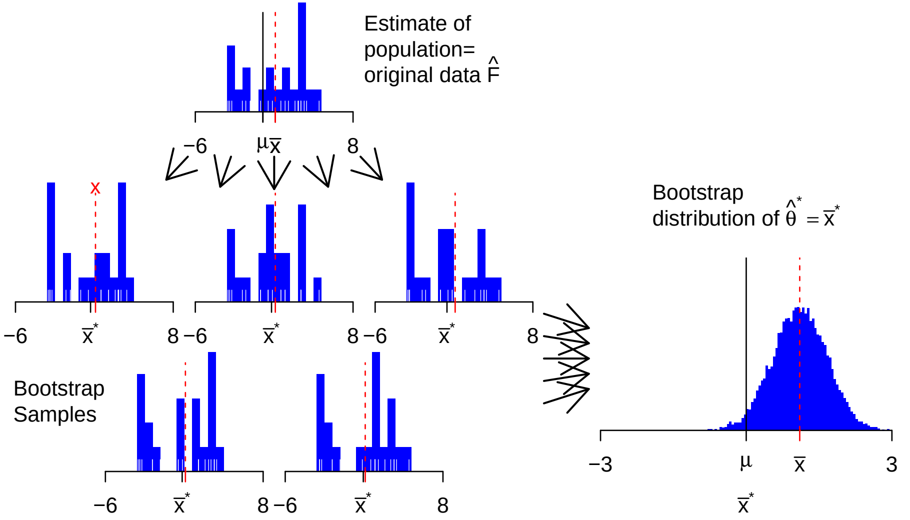
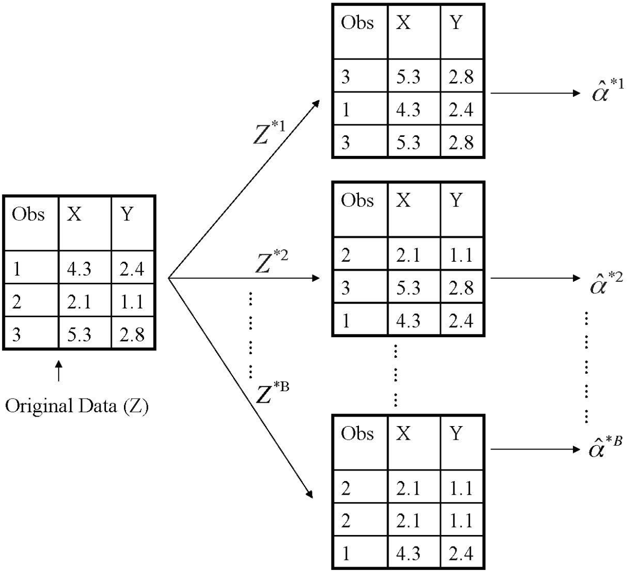


Illustration of the bootstrap



The bootstrap procedure

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

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

- Evaluate the bootstrap replications:

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

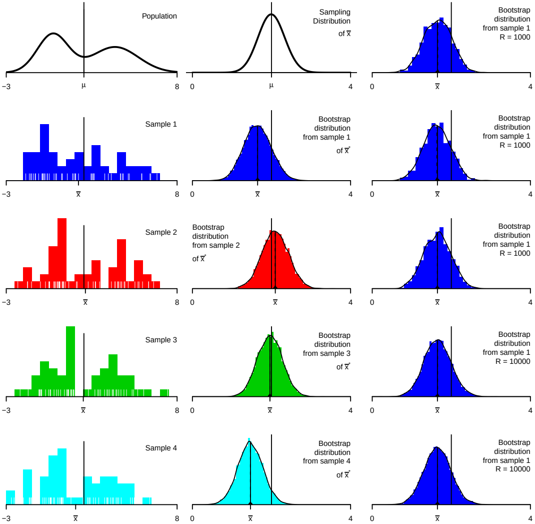
- Estimate the quantity of interest from the distribution of the $\hat{\theta}^{*(b)}$

Examples

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

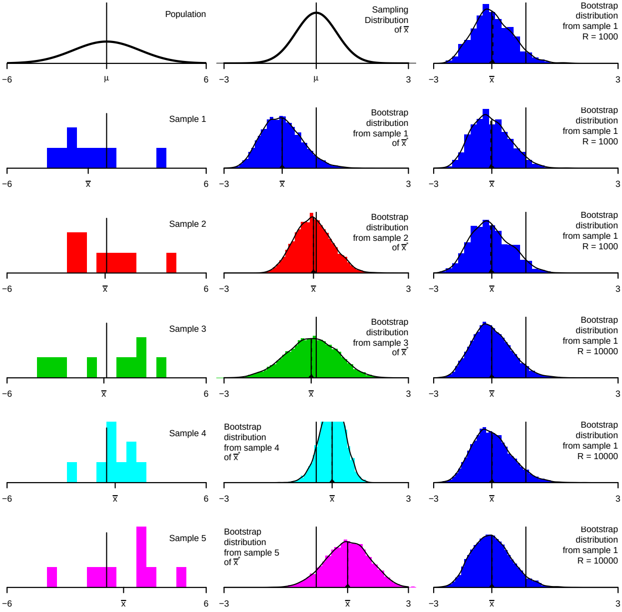
1. $\hat{\theta} =$ sample mean
2. $\hat{\theta} =$ sample median
3. $\hat{\theta} =$ expected shortfall at 5%
4. $\hat{\theta} =$ lag 1 autocorrelation.

Sample mean: $n = 50$



- Two types of random variation

Sample mean: $n = 9$



Prediction error estimation

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

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

- 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.

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

- 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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