Monte Carlo experiments and resampling methods

Statistical Programming with R

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Simulation, computer intensive statistical methods

- classical statistical methods are largely based on idealized assumptions (e.g. linear relations, normal distribution)
- the application of statistical methods to nonlinear, non-gaussian problems required the adoption of alternative statistical tools
- the advances in computational power of todays computers have enabled newer and more complicated statistical methods
- a new perspective in statistics: hard theoretical analysis is replaced by computationally intensive but simpler methods
- Monte Carlo simulation and resampling techniques are increasing in popularity.

Why use simulation?

- if classical inference theory fails, statistical inference is still possible using simulation to obtain standard errors, confidence intervals, and test hypotheses (example: median)
- to compare the quality of estimators
- to evaluate performance of models, algorithms
- to validate inferential and resampling methods
- to assess and select models

Monte Carlo as an experimental design

Monte Carlo method is a designed experiment

Criterion:

- Fit measure

Explanatory variables:

- structure of the data
- methods, algorithms

	F1			
F2		1	2	3
	1	r	r	r
	2	r	r	r
	3	r	r	r
	3	r	r	r

Monte Carlo simulation vs Resampling

Monte Carlo simulation

Sample from:

- distribution
- true model

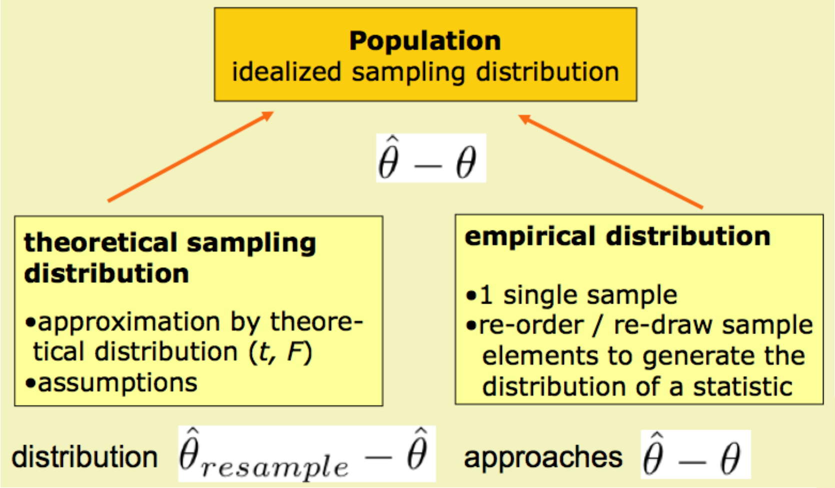
Strong assumptions on distribution of the data

Resampling

- **Re**sample from original sample
- no information on population characteristics or distribution

No assumptions on distribution of the data

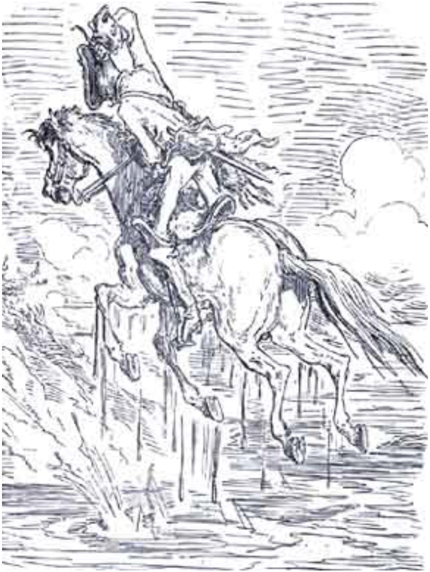
Paper Rodgers (1999)



Key concepts

- estimator
- bias and variance of an estimator (mean squared error)
- hypothesis testing
- confidence interval
- model
- model assessment
- model selection

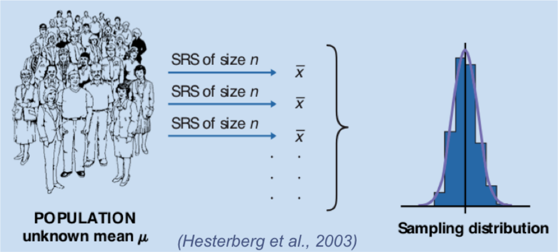
A resampling technique: the bootstrap

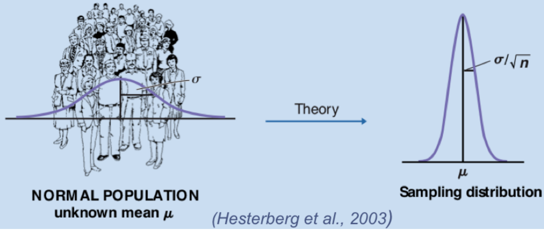


Baron Münchausen has fallen in a lake and pulls himself and his horse up by his bootstrap (or hair, depending on the version)

Rudolph Erich Raspe, *Münchausen* (1763)

Probability theory





Take many random samples from population and compute mean (sampling distribution of the mean)

Probability theory shortcut:
assume population follows normal distribution
sampling distribution of the mean approaches normal

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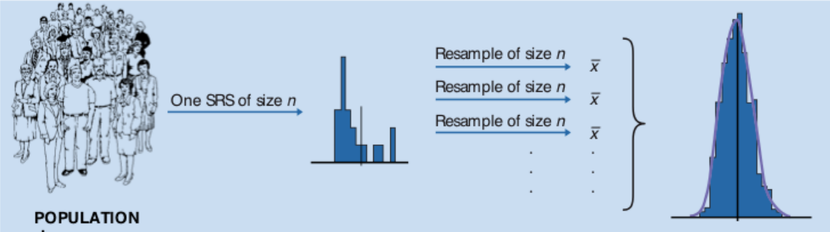
Basic idea bootstrap resampling

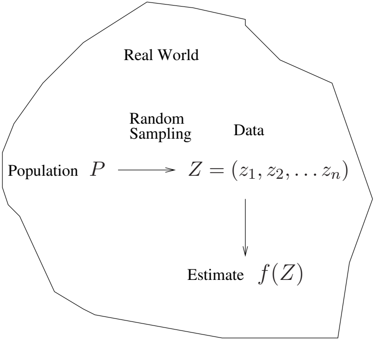


(Hesterberg et al., 2003)

The bootstrap idea

When there is **only one sample** and theory fails:

- the sample stands for the population
- the bootstrap distribution stands for sampling distribution
- substitute computing power for theoretical analysis


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

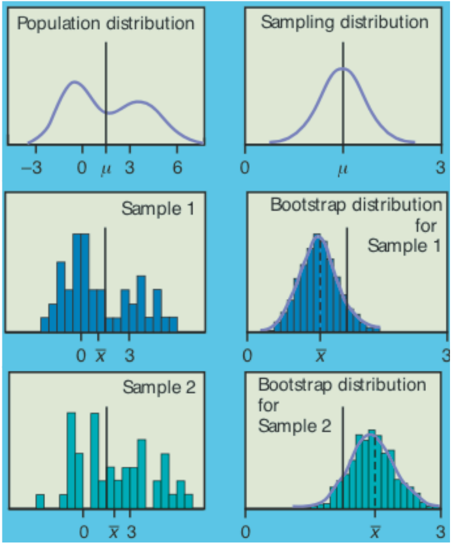
Basic idea bootstrap resampling

Use resampling to estimate how the sample statistic of a sample of size *n* from a certain population varies because of random sampling.

The bootstrap distribution does not reveal the center of the sampling distribution directly, but reveals the bias.

A statistic is biased when its sampling distribution is not centered at the true value of the parameter

How resampling works



The sampling distribution is centered at population mean μ

The bootstrap distributions are centered close to value of the sample mean $\bar{x}$

Almost all the variation in bootstrap distributions comes from selection of original sample

The shape and spread of bootstrap distributions resemble those of sampling distribution

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Bias and random sampling error

Sampling distribution of a statistic:

centered at true value + bias

bias = mean sampling distribution - true value

$= \hat{\theta} - \theta$

$= \bar{x} - \mu$

Bootstrap distribution of a statistic:

centered at sample value + bias

bias = mean bootstrap distribution - mean original sample

$= \hat{\theta}_{\text{resampling}} - \hat{\theta}$

$= \frac{1}{B} \sum_{b=1}^{B} \bar{x}^{\star} - \bar{x}$

($\bar{x}^{\star}$ = B replications of the statistic)

The two biases are similar even though the centers are not

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Use bootstrap distribution

The *bootstrap* is used for *estimation* to obtain the following measures of a statistic:

- bias ($\hat{\theta}_{\text{resampling}} - \hat{\theta}$):

$$\frac{1}{B}\sum_{b=1}^{B} \bar{x}^{\star} - \bar{x}$$

- standard error = standard deviation of bootstrap distribution

$$\hat{\sigma}_b(\hat{\theta}) = \hat{\sigma}_{b,\bar{x}} = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}\left(\bar{x}^{\star} - \frac{1}{B}(\bar{x}^{\star})\right)^2}$$

- confidence interval (percentile method)
  quantile(bootstrap distribution, p = c(0.025, 0.975))

RMSE: bias and variance combined

The *root mean squared error* of a statistic is a variability measure that combines bias and variance (*cf.* Efron & Gong, 1983):

$$\begin{aligned}\sqrt{\text{MSE}} &= \sqrt{E_F[(\hat{\theta} - \theta)]} \\ &= \sqrt{bias^2 + st.dev^2} \\ &= \sqrt{(\hat{\theta} - \theta)^2 + \hat{\sigma}_b(\hat{\theta})^2}\end{aligned}$$

Also useful to compare the distributions of a statistic obtained with several methods

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Resampling methods

Resampling methods can be used for different goals:

1. estimation (bias, standard errors, confidence intervals)
   - bootstrap
   - jacknife
2. hypothesis testing
   - bootstrap
   - permutation
3. model assessment and selection
   - cross-validation

Bootstrap vs Cross-validation

- In cross-validation, each of the K validation folds is distinct from the other $K-1$ folds used for training: *there is no overlap*. This is crucial for its success.
- To estimate prediction error using the bootstrap, we could think about using each bootstrap dataset as our training sample, and the original sample as our validation sample.
- But each bootstrap sample has significant overlap with the original data. About two-thirds of the original data points appear in each bootstrap sample.
- This will cause the bootstrap to seriously underestimate the true prediction error.