

Advanced statistics and modelling

6. week

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Parameter inference in statistics Hypothesis testing, MLE, Bootstrap

Calculating c and T in general

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Recap: Calculate parameters for a model (3 approaches):

- assume normal distribution,
- assume all possible values to be observed
- assume the observation is the most probable realization

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Calculating c and T in general

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Approach No. 1:

The Wald test assumes normal distributions: $N(\mu, \sigma^2)$ needs the expected value and the variance of the quantity.

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Calculating c and T in general

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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The Wald test assumes normal distributions: $N(\mu, \sigma^2)$ needs the expected value and the variance of the quantity.

How to calculate $\overline{()}$, $\hat{s}e$ and how to derive $T(x)$ functions in general?

Calculating c and T in general

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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How to calculate $\overline{(\cdot)}$, $\hat{s}e$ and how to derive $T(x)$ functions in general?
Three methods:

- **Bootstrap** – all observed
- **Method of Moments** – all observed weakly
- **Maximum Likelihood Estimation** – most probable observed

Bootstrap

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Theory behind this method:

$$\mathbb{E}(Y) = \lim_{B \rightarrow \infty} \frac{1}{B} \sum_{i=1}^B Y_i$$

For each function h with a finite mean

$$\mathbb{E}(h(Y)) = \lim_{B \rightarrow \infty} \frac{1}{B} \sum_{i=1}^B h(Y_i) = \langle h \rangle_B$$

Here B is the number of independent measurements (sampling with replacement) on the original dataset.

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Bootstrap

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Here B is the number of independent measurements (sampling with replacement) on the original dataset.

• In case the function h has $k > 1$ arguments, we simply draw k data with replacement (due to independence) from the original dataset.

• This delivers the expectation value as $\langle \cdot \rangle_B$
The standard error is just another function: $se^2 = \langle (\cdot - \langle \cdot \rangle_B)^2 \rangle_B$

Bootstrap

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Formal definition:

Bootstrap method is used for approximating the expected value and the standard error of any function from a measured dataset. E.g. if the $T(X)$ test statistics is approximated, then X is distributed according to a fixed, but unknown F distribution.

Steps for any $T(X)$ function:

- Draw k points from the measured dataset: this follows the F distribution, since the measured dataset has values according to F .
- Compute $T(X)$ where X is k dimensional vector.
- Repeat B times the above steps
- $E_{bootstrap} = \frac{1}{B} \sum_b^B T_b$
- $SE_{bootstrap} = \frac{1}{B} \sum_b^B (T_b - \frac{1}{B} \sum_r^B T_r)^2$

Note: Jackknife was a similar, replica based method.

Note2: if $T(X)$ is the test function for the mean,

then $T(X) = \sum_i^n X_i/n$ is the average, using all values of the sample.

Bootstrap for confidence intervals

Hypothesis
testing, MLE,
Bootstrap

Using bootstrap for confidence intervals $C(a, b)$:

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Bootstrap for confidence intervals

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Using bootstrap for confidence intervals $C(a, b)$:

- Normal method: $\hat{T} \pm z_{\alpha/2} \hat{se}_{bootstrap}$, so

$$a = \hat{T} - z_{\alpha/2} \hat{se}_{bootstrap}, b = \hat{T} + z_{\alpha/2} \hat{se}_{bootstrap}$$

Bootstrap for confidence intervals

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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$$a = \hat{T} - z_{\alpha/2} \hat{se}_{bootstrap}, b = \hat{T} + z_{\alpha/2} \hat{se}_{bootstrap}$$

- Pivotal method: $C = (a, b)$

$$a = \hat{T} + H^{-1}(1 - \alpha/2) \text{ and } b = \hat{T} + H^{-1}(\alpha/2)$$

$$\text{where } H(r) = \mathbb{P}_F(\hat{T} - T \leq r)$$

Bootstrap for confidence intervals

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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$$\text{where } H(r) = \mathbb{P}_F(\hat{T} - T \leq r)$$

- good approximation: $a = 2\hat{T} - T_{1-\alpha/2}^*$, $b = 2\hat{T} - T_{\alpha/2}^*$,
where T_{β}^* is β -sample-quantile of T_1, T_2, \dots, T_B replicas.

Bootstrap for confidence intervals

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- good approximation: $a = 2\hat{T} - T_{1-\alpha/2}^*$, $b = 2\hat{T} - T_{\alpha/2}^*$,
where T_{β}^* is β -sample-quantile of T_1, T_2, \dots, T_B replicas.
- Percentile interval: $(T_{\alpha/2}^*, T_{1-\alpha/2}^*)$

Parameter inference

Hypothesis
testing, MLE,
Bootstrap

How can we find $T = T(t_1, t_2, \dots)$ functions?

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Parameter inference

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

How can we find $T = T(t_1, t_2, \dots)$ functions?

E.g. by estimating the parameters t_1, t_2, \dots

Two methods:

- moments (MME)
- max. likelihood (MLE)

Method of moments (MME)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Given a measured dataset, any moments of the distribution can be approximated:

$$\alpha_k = \int x^k dF = \frac{1}{n} \sum x_i^k$$

Method of moments (MME)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Given a measured dataset, any moments of the distribution can be approximated:

$$\alpha_k = \int x^k dF = \frac{1}{n} \sum x_i^k$$

If the distribution F depends on the parameter t , the left hand side provides a formula for t based on the m -th moment.

$$\alpha_m(t) = \frac{1}{n} \sum x_i^m$$

Method of moments (MME)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Expressing t at the left and substituting the data values at the right, one gets an approximation for the parameter t .

Method of moments (MME)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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In case of more parameters, use so many moments as many unknown parameters.

Method of moments (MME)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Some properties of the method:

- An estimate for \hat{t} exists with $\mathbb{P} = 1$

Method of moments (MME)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- An estimate for \hat{t} exists with $\mathbb{P} = 1$
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Method of moments (MME)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Some properties of the method:

- An estimate for \hat{t} exists with $\mathbb{P} = 1$
- The estimate is consistent: $\hat{t} \rightarrow t$
- The estimate is asymptotically normal: $\sqrt{n}(\hat{t} - t) \rightarrow N(0, \sigma^2)$
(allows Wald test)

Maximum Likelihood Estimate (MLE)

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

We measure n values: X_1, X_2, \dots, X_n

These are IID random variables with PDF $f(X_i, \theta)$

- The **likelihood function** is $\mathcal{L}(\theta) = \prod_i f(X_i, \theta)$
- The **log-likelihood function** is $\ell(\theta) = \sum_i \log f(X_i, \theta)$
- The **Maximum Likelihood Estimator** is $\hat{\theta}$ that maximizes \mathcal{L}

Properties of MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- The $\mathcal{L}(\theta) \in [0, \infty)$: it is the join density of data, but not a probability:
 $\int d\theta \mathcal{L}(\theta) \neq 1$
- consistent: $\hat{\theta} \rightarrow \theta$
- equivariant: if $\hat{\theta}$ MLE of θ then $g(\hat{\theta})$ MLE of $g(\theta)$
- asymptotically normal: $\sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, \hat{s}e)$
- asymptotically optimal: MLE has smallest variance for large samples

Working with sheets

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- Open weblink
 - Open file: sh1 in your browser
- create an empty sheet under your google drive
- Copy and paste data from first sheet to your sheet
- Now you are ready to work with your sheet: add some formulas, data etc

Note: if your browser is set to a default language other than English, you will see translated version of functions and menus of the instructing screen.

Do not worry, in most cases you can give function names in English in this case as well.

Method of moments, MME 1.

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- Find the appropriate distribution of inter arrival times!
 - Which distribution?
 - Express the first moment with the parameter of the distribution!
- Check the fitted parameter: compare distribution from data and fitted PDF! (Use QQ-plot!)
- Calculate the residuals as well!

Note:

$$F(x) = 1 - e^{-\lambda x}$$

$$f(x) = \lambda e^{-\lambda x}$$

$$\langle x \rangle = 1/\lambda$$

Method of Moments, MME 2.

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

- Set up a dataset with uniformly distributed random numbers! You can choose to copy numbers from your "master" sheet, or from the "sh1" file (sheet: Fit_Uniform), or generate your self with the function "rand()".
- Try to estimate the parameters of the uniform distribution for your dataset!
 - Note: you have to find two parameters now, so you need to calculate two moments.

How are the parameters, the moments and the QQ-plot changing?

Method of Moments, MME 2.

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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 - Hint: $\langle \text{Uniform}(a, b) \rangle = \frac{a+b}{2}$ and $\sigma^2(\text{Uniform}(a, b)) = \frac{(b-a)^2}{12}$
- Prepare a QQ-plot for testing the fitted values!
 - Fit the best line on the QQ-plot!

How are the parameters, the moments and the QQ-plot changing?

Method of Moments, MME 2.

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

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- Prepare a QQ-plot for testing the fitted values!
 - Fit the best line on the QQ-plot!
- Experiment with the parameters: try to
 - shift the raw dataset,

How are the parameters, the moments and the QQ-plot changing?

Method of Moments, MME 2.

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

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- Prepare a QQ-plot for testing the fitted values!
 - Fit the best line on the QQ-plot!
- Experiment with the parameters: try to
 - shift the raw dataset,
 - rescale the dataset,

How are the parameters, the moments and the QQ-plot changing?

Method of Moments, MME 2.

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

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 - Fit the best line on the QQ-plot!
- Experiment with the parameters: try to
 - shift the raw dataset,
 - rescale the dataset,
 - insert outliers into the data

How are the parameters, the moments and the QQ-plot changing?

Method of Moments, MME 2.

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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 - Fit the best line on the QQ-plot!
- Experiment with the parameters: try to
 - shift the raw dataset,
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How are the parameters, the moments and the QQ-plot changing?

Note: in real scenarios you will meet similar biased or transformed data usually.

Method of Moments, MME 3

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- We have a dataset with counts of incoming calls at the secretary of the dean for each working hours in a week. Assuming constant calling rate, try to fit an appropriate distribution for the number of calls!
Which distribution would you try first?

Method of Moments, MME 3

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- We have a dataset with counts of incoming calls at the secretary of the dean for each working hours in a week. Assuming constant calling rate, try to fit an appropriate distribution for the number of calls!
Which distribution would you try first?
- Calls can be modeled by a stationary Poisson process. How many parameters do you need to fit?

Method of Moments, MME 3

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Which distribution would you try first?
- Calls can be modeled by a stationary Poisson process. How many parameters do you need to fit?
- Prepare a QQ-plot for testing the fitted values! Take into account, that you work with a discrete distribution!

Poisson:

$$P(k) = \frac{\lambda^k}{k!} e^{-\lambda}$$

Method of Moments, MME 3

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Which distribution would you try first?

- Calls can be modeled by a stationary Poisson process. How many parameters do you need to fit?
- Prepare a QQ-plot for testing the fitted values! Take into account, that you work with a discrete distribution!
- Fit the best line on the QQ-plot! Check the slope and the abscissa of the line! Correspond these numbers to your expectations?

Poisson:

$$P(k) = \frac{\lambda^k}{k!} e^{-\lambda}$$

Method of Moments, MME 3

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- We have a dataset with counts of incoming calls at the secretary of the dean for each working hours in a week. Assuming constant calling rate, try to fit an appropriate distribution for the number of calls!
Which distribution would you try first?
- Calls can be modeled by a stationary Poisson process. How many parameters do you need to fit?
- Prepare a QQ-plot for testing the fitted values! Take into account, that you work with a discrete distribution!
- Fit the best line on the QQ-plot! Check the slope and the abscissa of the line! Correspond these numbers to your expectations?
- Plot the residuals and plot the cumulative distribution functions! Can you retain the Poissonian assumption?

Poisson:

$$P(k) = \frac{\lambda^k}{k!} e^{-\lambda}$$

Method of Moments, MME 3

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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Which distribution would you try first?
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- Prepare a QQ-plot for testing the fitted values! Take into account, that you work with a discrete distribution!
- Fit the best line on the QQ-plot! Check the slope and the abscissa of the line! Correspond these numbers to your expectations?
- Plot the residuals and plot the cumulative distribution functions! Can you retain the Poissonian assumption?

Conclusions: QQ-plot indicates, that this is the good distribution family. But further parameters are to be fitted: inhomogeneous Poisson process could be better.

Poisson:

$$P(k) = \frac{\lambda^k}{k!} e^{-\lambda}$$

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

- Find the MLE for the uniform distribution using the data from the MME example!

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- Find the MLE for the uniform distribution using the data from the MME example!
- Recall: PDF of uniform

$$f(x) = \frac{1}{b-a} \quad x \in [a, b]$$

- Can you solve it? How do you interpret the result?

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
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- Find the MLE for the uniform distribution using the data from the MME example!

- Recall: PDF of uniform

$$f(x) = \frac{1}{b-a} \quad x \in [a, b]$$

- MLE:

$$\mathcal{L}(a, b) = \prod_i f(x_i; a, b) = \frac{1}{(b-a)^n}$$

where x_i are fixed numbers from the n data.

- Can you solve it? How do you interpret the result?

Maximum Likelihood Estimation, MLE

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

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- MLE:

$$\mathcal{L}(a, b) = \prod_i f(x_i; a, b) = \frac{1}{(b-a)^n}$$

where x_i are fixed numbers from the n data.

- \mathcal{L} seems to be good behaving function, find the maximum with usual analysis:

$$\partial_a \mathcal{L} = 0$$

$$\partial_b \mathcal{L} = 0$$

- Can you solve it? How do you interpret the result?

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- Because $f(x) = 0$ if $x \notin [a, b]$, we have

$$a \leq x_1 \leq x_2 \leq \dots \leq x_n \leq b$$

where data (x_i) are in increasing order.

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

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testing

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- \mathcal{L} is not differentiable in x_1 and x_n !

Maximum Likelihood Estimation, MLE

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

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- \mathcal{L} is not differentiable in x_1 and x_n !

- MLE:

$$(a, b) = (\min(x), \max(x))$$

But: this is a biased estimation.

(Recall: what is a biased estimation?)

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- MLE:

$$(a, b) = (\min(x), \max(x))$$

But: this is a biased estimation.

(Recall: what is a biased estimation?)

- Try to correct the results to have an unbiased estimation with estimation values:

$$(a, b) = (\langle \min(x) \rangle, \langle \max(x) \rangle)$$

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

- Calculate $\langle \max(x) \rangle$ from the CDF!

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- Calculate $\langle \max(x) \rangle$ from the CDF!
- Utilize the independence of data points!

Maximum Likelihood Estimation, MLE

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

- Calculate $\langle \max(x) \rangle$ from the CDF!
- Utilize the independence of data points!

$$\begin{aligned} F_{\max}(y) &= \mathbb{P}((x_1 < y) \cap (x_2 < y) \cap \dots \cap (x_n < y)) \\ &= \prod_i F(y) = F^n(y) = \frac{(y-a)^n}{(b-a)^n} \end{aligned}$$

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- Expectation value for $\max(x)$:

$$\langle \max(x) \rangle = \int_a^b dy \, y n \frac{(y-a)^{n-1}}{(b-a)^n} = \frac{n}{n+1} (b-a) + a$$

Maximum Likelihood Estimation, MLE

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- From this we have an estimate for b , assuming a is known:

$$b = \frac{n+1}{n} (\max(x) - a) + a$$

Maximum Likelihood Estimation, MLE

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

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- From this we have an estimate for b , assuming a is known:

$$b = \frac{n+1}{n}(\max(x) - a) + a$$

- Because we do not know a at the beginning, we use the MLE value for a . Then (using a similar formula for the minimum), the estimated b will be used for a . Iterate this procedure until convergence!

Bootstrap

**Hypothesis
testing, MLE,
Bootstrap**

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

**Bootstrap
example**

Independence
testing

- Calculate the 95% confidence interval for the median of experimental data! Apply bootstrap method with percentile calculation!

Bootstrap

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

- Calculate the 95% confidence interval for the median of experimental data! Apply bootstrap method with percentile calculation!
- Create a sample with replacement, and calculate the median for the sample! Repeat 2000 times!

Bootstrap

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- Calculate the 95% confidence interval for the median of experimental data! Apply bootstrap method with percentile calculation!
- Create a sample with replacement, and calculate the median for the sample! Repeat 2000 times!
- Create PDF for the median values from the bootstrapped sample, calculate the percentile values. Remind: confidence intervals are two sided by default.

Multiple testing

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

● Problem:

- We have 25 disease indicators for a child. We want to conduct an experiment, where we need a healthy subject, none of the indicators are allowed to show a disease. Our lab is able to test **each indicator** at 0.95 confidence against the disease. We found some indicators, where the test for being healthy was rejected. Should we discard this subject, if our threshold is 95% confidence level for conducting the experiment?

Multiple testing

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- Solution:

Multiple testing

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- Solution:

- Bonferroni method

Multiple testing

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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● Solution:

- Bonferroni method
- Benjamini-Hochberg method

Multiple testing

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

**Bootstrap
example**

Independence
testing

Multiple testing: Bonferroni correction

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

- How to set the confidence level for **each test** if we want to ensure the probability of false rejection of **any** null hypothesis is less than α ?

Multiple testing: Bonferroni correction

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

- How to set the confidence level for **each test** if we want to ensure the probability of false rejection of **any** null hypothesis is less than α ?
- We have m separate hypothesis tests

$$H_0^i \leftrightarrow H_1^i \text{ with } p\text{-value } P_i$$

Multiple testing: Bonferroni correction

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

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$$H_0^i \leftrightarrow H_1^i \text{ with } p\text{-value } P_i$$

- Bonferroni correction:

$$\text{reject } H_0^i \text{ if } P_i < \alpha/m$$

Multiple testing: Bonferroni correction

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

Independence testing

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- Bonferroni correction:

$$\text{reject } H_0^i \text{ if } P_i < \alpha/m$$

Proof: $\mathbb{P}(\text{any test } A_i \text{ falsely rejected})$

$$= \mathbb{P}(\cup_i^m A_i) \leq \sum_i^m \mathbb{P}(A_i) = \sum_i^m \alpha/m = \alpha$$

Multiple testing: Bonferroni correction

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- This correction is very conservative.

Multiple testing: Bonferroni correction

Hypothesis testing, MLE, Bootstrap

Introduction

Bootstrap theory

Method of moments theory

Maximum Likelihood Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap example

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- This correction is very conservative.
- The power of this correction is quite low.

Multiple testing: B-H correction

Hypothesis
testing, MLE,
Bootstrap

Benjamini-Hochberg correction

- Allow some more false rejection, but control the False Discovery Rate (FDR):

$$FDR = \left\langle \frac{\text{number of false rejections}}{\text{number of all rejections}} \right\rangle \leq \alpha$$

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Multiple testing: B-H correction

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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$$FDR = \left\langle \frac{\text{number of false rejections}}{\text{number of all rejections}} \right\rangle \leq \alpha$$

- The correction procedure:
 - * order the tests by increasing p-values: $P_i \leq P_j$ for $i < j$

Multiple testing: B-H correction

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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- The correction procedure:
 - * order the tests by increasing p-values: $P_i \leq P_j$ for $i < j$
 - * set temporary threshold $t_i = i \frac{1}{C_m} \frac{\alpha}{m}$ for all tests, where $C_m = \sum_{i=1}^m 1/i$

Multiple testing: B-H correction

Hypothesis
testing, MLE,
Bootstrap

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 - * Starting from the largest P_i and going down, find the first $P_j < t_j$

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Multiple testing: B-H correction

Hypothesis
testing, MLE,
Bootstrap

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 - * Starting from the largest P_i and going down, find the first $P_j < t_j$
 - * reject all H_0 with lower p-value.

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Multiple testing: B-H correction

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

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 - * Starting from the largest P_i and going down, find the first $P_j < t_j$
 - * reject all H_0 with lower p-value.
- The B-H correction is more popular in case of testing a large number of hypotheses.

Multiple testing: B-H correction

Hypothesis
testing, MLE,
Bootstrap

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Benjamini-Hochberg correction

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- The correction procedure:
 - * order the tests by increasing p-values: $P_i \leq P_j$ for $i < j$
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 - * Starting from the largest P_i and going down, find the first $P_j < t_j$
 - * reject all H_0 with lower p-value.
- The B-H correction is more popular in case of testing a large number of hypotheses.
- The correction factor for independent tests is smaller: $C_m \leq 1$

Independence

Hypothesis
testing, MLE,
Bootstrap

Main concept:

- two by two table of outcomes

.	$a = 0$	$a = 1$.
$b = 0$	p_{00}	p_{01}	$p_{0.}$
$b = 1$	p_{10}	p_{11}	$p_{1.}$
.	$p_{.0}$	$p_{.1}$	$p_{..} = 1$

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Independence

Hypothesis
testing, MLE,
Bootstrap

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$b = 1$	p_{10}	p_{11}	$p_{1.}$
.	$p_{.0}$	$p_{.1}$	$p_{..} = 1$

- Odds ratio:

$$OR = \frac{p_{00}p_{11}}{p_{01}p_{10}}$$

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Independence

Hypothesis
testing, MLE,
Bootstrap

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- two by two table of outcomes

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$b = 0$	p_{00}	p_{01}	$p_{0.}$
$b = 1$	p_{10}	p_{11}	$p_{1.}$
.	$p_{.0}$	$p_{.1}$	$p_{..} = 1$

- Odds ratio:

$$OR = \frac{p_{00}p_{11}}{p_{01}p_{10}}$$

- a and b are independent iff:

$$OR = 1$$

or equivalently

$$p_{ij} = p_{i.}p_{.j}$$

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing

Independence

Hypothesis
testing, MLE,
Bootstrap

Main concept:

- two by two table of outcomes

.	$a = 0$	$a = 1$.
$b = 0$	p_{00}	p_{01}	$p_{0.}$
$b = 1$	p_{10}	p_{11}	$p_{1.}$
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- Odds ratio:

$$OR = \frac{p_{00}p_{11}}{p_{01}p_{10}}$$

- a and b are independent iff:

$$OR = 1$$

or equivalently

$$p_{ij} = p_{i.}p_{.j}$$

- Main tests:

- χ^2 sheet: "chi2"
- Fisher-exact, sheet: "fish"

Introduction

Bootstrap theory

Method of
moments theory

Maximum
Likelihood
Estimate theory

Technical

MME

MME2

MME3

MLE

Bootstrap
example

Independence
testing