# Advanced statistics and modelling

5. week

> Parameter inference in statistics Hypothesis testing, MLE, Bootstrap

- Recall: The basic statistical inference problem was the following:
- We have some observed data:  $X_1, X_2, \ldots, X_n \sim F$ .
- Based on the observations we would like to **infer** (or estimate or learn) some parameters (e.g. *p* in a Binomial).
- In data science: based on the observations validate an assumption (hypothesis) on some parameters.
- Statistical decision: calculate the probability, that the observations are consistent with the hypothesis.
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  - assume normal distribution
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- The **critical value** is c if the rejection region can be expressed as  $R = \{x \in \mathcal{X} \mid T(x) > c\}$
- The hypothesis test is to find T and c, which leads the least harmful decision.
  - (e.g. Do I have cancer? or Do I got the most points for home work?)

Hypothesis testing, MLE, Bootstrap

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Possible outcomes:	$H_0$ true	OK	type I error
	$H_1$ true	type II error	OK

• The power function of the test is a  $\Theta \to \mathbb{R}$ 

$$\beta(\theta) = P_{\theta}(X \in R)$$

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#### Note some alternatives in the literature:

- $H_0 \le \theta_0$  for one sided tests (later we see problems with this)
- $1 \beta(\theta) = P_{\theta}(X \in R)$  (though the **power** is the same!)

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Let us define  $T = \overline{X}$  (average of observed values), and find c which rejects  $H_0$  if T > c.

Rejection region:  $R = \{x : T(x) > c\}.$ 

Hypothesis testing, MLE, Bootstrap

The power function:

$$\begin{array}{lcl} \beta(\theta) & = & P_{\mu}(\overline{X} > c) \\ & = & P_{\mu}\left(\frac{\overline{X} - \mu}{\sigma}\sqrt{n} > \sqrt{n}\frac{c - \mu}{\sigma}\right). \end{array}$$

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$$\beta(\theta) = \beta(\mu) = P_{\mu} \left( Z > \sqrt{n} \frac{c - \mu}{\sigma} \right)$$
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Find the level of the test:

$$\alpha = \sup_{\mu \in [-\infty, 0]} \beta(\mu) = \sup_{\mu \in [-\infty, 0]} \left\{ 1 - \Phi\left(\sqrt{n} \frac{c - \mu}{\sigma}\right) \right\}$$
$$= 1 - \Phi\left(\sqrt{n} \frac{c}{\sigma}\right)$$

or vica – verse: at given level find the critical value

$$c = \Phi^{-1}(1-\alpha)\frac{\sigma}{\sqrt{n}}$$

We reject 
$$H_0$$
 if  $T=\overline{X}>c=\Phi^{-1}(1-\alpha)\frac{\sigma}{\sqrt{n}}$ 

Hypothesis testing, MLE, Bootstrap

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Or

$$\frac{\sqrt{n}(\overline{X} - 0)}{\sigma} > z_{\alpha}$$

where  $z_{\alpha}$  is the tabulated critical value of the standard normal distribution.

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Note the substituted value of  $\mu=0$ , which is the  $H_0$  null hypothesis expressed as an equation, instead of an inequality.

Hypothesis testing, MLE Bootstrap

This test is valid for asymptotically normally distributed variables.

- $\bullet$   $\theta$  denotes the real value of the parameter,
- $\hat{\theta}$  an estimated value of the parameter,
- $\hat{se}$  estimated standard error of  $\hat{\theta}$

The formal test:  $H_0: \theta = \hat{\theta}$  and  $H_1: \theta \neq \hat{\theta}$ 

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$$\frac{(\hat{\theta} - \theta)}{\hat{se}} > z_{\alpha}$$
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Note the difference between the one sided and the two sided test: one sided compares with:  $z_{\alpha}$  and no  $|\cdot|$  two sided compares with:  $z_{\alpha/2}$  and takes absolute value

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Hypothesis testing, MLE, Bootstrap

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Hypothesis testing, MLE Bootstrap

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$$P(X \in R) = 1 - P(X \not\in R)$$

where

$$P(X \notin R) = P(\theta_{\star} \text{ close to } \hat{\theta}) = \Phi\left(\frac{\hat{\theta} - \theta_{\star}}{\hat{se}} + z_{\alpha/2}\right) - \Phi\left(\frac{\hat{\theta} - \theta_{\star}}{\hat{se}} - z_{\alpha/2}\right)$$

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The power increases if:

- difference between  $\theta_{\star}$  and  $\theta$  increases (note: we change only  $\theta_{\star}$ )
- sample variance decreases (  $\hat{se} \sim 1/\sqrt{n}$  decreases as n grows)

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$$\theta_{\star} \neq \theta$$
,

the power of the test  $(\beta = P(X \in R))$  will be:

$$\beta = 1 - \Phi\left(\frac{(\hat{\theta} - \theta) - (\theta_{\star} - \theta)}{\hat{se}} + z_{\alpha/2}\right) + \Phi\left(\frac{(\hat{\theta} - \theta) - (\theta_{\star} - \theta)}{\hat{se}} - z_{\alpha/2}\right)$$

which is the probability correctly rejecting a false  $H_0$  under assuming  $\theta_\star$  as the parameter instead  $\theta$ .

- The power increases if:
  - difference between  $\theta_{\star}$  and  $\theta$  increases (note: we change only  $\theta_{\star}$ )
  - sample variance decreases (  $\hat{se} \sim 1/\sqrt{n}$  decreases as n grows)

Wald test is equivalent with a confidence interval:

$$C = (\hat{\theta} - z_{\alpha/2}\hat{se}, \hat{\theta} + z_{\alpha/2}\hat{se},)$$

 $H_0: \hat{\theta} = \theta_{\star}$  rejected at level  $\alpha$  if and only if  $\theta_{\star} \not\in C$ 

<u>\_</u>

Hypothesis testing, MLE, Bootstrap

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Note2: *X* and *Y* independent, two different samples

Note3: if X and Y measured together (**paired samples**), then  $\delta = \overline{D}$  and  $\hat{se}^2 = \overline{(D-\overline{D})^2}/\sqrt{n}$ , where  $D_i = X_i - Y_i$  for each case i

- If a test rejects at level  $\alpha$ , then it rejects for all  $\alpha' > \alpha$ .
- The rejection region R depends on the  $\alpha$  level (smaller  $\alpha$  results smaller R).
- The **p-value** of a test is the smallest  $\alpha$  where the test rejects.

$$p$$
-value = inf  $\{\alpha \mid \exists X \in R_{\alpha}\}$ 

Recall: X is a random variable taking values from the observed values  $\mathcal{X}$  Note: the p-value is a measure **against**  $H_0$ , and different from  $\mathbb{P}(H_0|data)$  (which is the probability of  $H_0$  being true with the condition of observed data.) The latter will be discussed under Bayesian inference later.

Hypothesis testing, MLE, Bootstrap

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Hypothesis testing, MLE Bootstrap

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- Large p-value can result when:
  - Ho is true
- H1 is true and the test has low power

#### Let's calculate the p-value:

$$\operatorname{reject} H_0: T(X) > c_\alpha \Leftrightarrow \operatorname{p-value} = \sup_{\theta \in \Theta_0, \xi \in \mathcal{X}} \mathbb{P}_{\theta}(T(\xi) \geq T(X))$$

which is the probability of observing a test statistics as extreme or more extreme that was actually observed.

Hypothesis testing, MLE, Bootstrap

- Why prefer the null hypothesis  $H_0: \theta = \theta_0$  against  $H_0: \theta \leq \theta_0$ ?
  - In practice, the probability is calculated at a given value of the parameter  $\theta$ , which is set according to the null hypothesis.
  - If the distribution of T(X) is continuous, and  $H_0: \theta = \theta_0$ , then the p-value has a uniform distribution on [0,1]

The test is **statistically significant** if  $\alpha > p$ -value.

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Note: a test can be statistically significant, but practically not significant, if the confidence interval is very small.

#### Calculating c and T in general

Hypothesis testing, MLE, Bootstrap

The Ward test assumes normal distributions:  $N(\mu,\sigma^2)$  needs the expected value and the variance of the quantity. How to calculate  $\overline{()}$ ,  $\hat{se}$  and how to derive T(x) functions in general? Some methods:

- Bootstrap
- Method of Moments
- Maximum Likelihood Estimation

# Bootstrap

Hypothesis testing, MLE, Bootstrap

Theory behind this method:

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

For each function *h* with a finite mean

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

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

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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  $\langle . \rangle_B$ The standard error is just another function:  $se^2 = \langle (. - \langle . \rangle_B)^2 \rangle_B$ 

#### Bootstrap

Hypothesis testing, MLE Bootstrap

#### 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 apporixmated, 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  $T(X) = \sum_{i=1}^{n} X_i/n$  is the average, using all values of the sample.

Hypothesis testing, MLE, Bootstrap

Hypothesis testing, MLE Bootstrap

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

• Normal method:  $\hat{T} \pm z_{\alpha/2} \hat{s} e_{bootstrap}$ , so

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

Hypothesis testing, MLE Bootstrap

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- Pivotal method: C=(a,b)  $a=\hat{T}-H^{-1}(1-\alpha/2) \text{ and } b=\hat{T}+H^{-1}(\alpha/2)$  where  $H(r)=\mathbb{P}_F(\hat{T}-T\leq r)$

Hypothesis testing, MLE Bootstrap

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

Hypothesis testing, MLE Bootstrap

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- Percentile interval:  $(T_{\alpha/2}^*, T_{1-\alpha/2}^*)$

#### Parameter inference

Hypothesis testing, MLE, Bootstrap

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

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Hypothesis testing, MLE, Bootstrap

How can we find  $T = T(t_1, t_2,...)$  functions? E.g. by estimating the parameters  $t_1, t_2,...$ Two methods:

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

Hypothesis testing, MLE, Bootstrap

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

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

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

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- The estimate is asymptically normal:  $\sqrt{n}(\hat{t}-t) \rightarrow N(0,\sigma^2)$  (allows Ward test)

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#### Maximum Likelihood Estimate (MLE)

Hypothesis testing, MLE Bootstrap

> 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

- 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  $\theta$  then  $g(\hat{\theta})$  MLE of  $g(\theta)$
- asymptotically normal:  $\sqrt{n}(\hat{\theta} \theta) \rightarrow N(0, \hat{se})$
- asymptotically optimal: MLE has smallest variance for large samples