Part V :

Statistics

Point estimates, bias & variance, consistency

Standard setup in parametric statistics

We assume that data is generated by a particular family of distributions, for example

$$\mathcal{F} = \left\{ N(\mu, \sigma^2) \;\middle|\; \underbrace{\mu \in \mathbb{R},\ \sigma^2 > 0}_{\Theta} \right\} .$$

The family $\mathcal{F}$ is called the <u>statistical model.</u>

More generally,

$$\mathcal{F} = \{ f_{\underset{\substack{\uparrow \\ \text{one particular} \\ \text{parameter}}}{\theta}} \mid \theta \in \underset{\substack{\uparrow \\ \text{space of all possible parameters}}}{\Theta} \}$$

We are given a sample $X_1, \dots, X_n \sim f_\theta$ (typically, iid) but the true, underlying θ is unknown.

Conventions

Parameter space Θ ("capital theta")

True (unknown) parameter θ ("lower case theta")

P_θ, E_θ, ... refers to the probability, expectation under the distribution f_θ

Estimates typically get a "hat": $\hat{\theta}$, $\hat{\mu}$, ...

Point estimation

The goal of point estimation is to estimate θ.

Def Given a statistical model $\mathcal{F} = \{ f_\theta \mid \theta \in \Theta \}$, and a sample $X_1, \dots, X_n \sim F \in \mathcal{F}$. A point estimator $\hat{\theta}_n$ of parameter θ is a function

$$\hat{\theta}_n := g(X_1, \dots, X_n)$$

Bias of an estimator

Def The bias of such an estimator is defined as

$$\text{bias}(\hat{\theta}_n) := \underbrace{E_\theta}_{\text{expectation wrt the distribution } f_\theta \text{ (the true one!)}}\big(\underbrace{\hat{\theta}_n}_{\text{estimate}}\big) - \underbrace{\theta}_{\text{true para}}$$

Intuition: repeat the procedure very often (infinitely often) and average over the estimate $\hat{\theta}_n$.

An estimate is unbiased if its bias is zero.

Variance and standard error

Def The variance of an estimator is defined as $\mathrm{Var}_\theta(\hat{\theta}_n)$. The corresponding standard deviation is called the standard error se. Typically, se is unknown, but it can be estimated: $\widehat{se}$.

Example

$$X_1, \dots, X_n \sim \overset{\{0,1\}}{\overset{\shortparallel}{\text{Bernoulli}}}(p), \quad \text{parameter } \overbrace{p}^{\theta} \in \overbrace{[0,1]}^{\Theta},$$

$\hat{p}_n := \frac{1}{n} \sum_{i=1}^{n} X_i$ an estimate of p.

$$E_p(\hat{p}_n) = E_p\left(\frac{1}{n} \sum_{i=1}^{n} X_i\right) = \frac{1}{n} \sum_{i=1}^{n} \overbrace{E_p(X_i)}^{p} = p.$$

Thus, $\hat{p}_n$ is unbiased because

$$E_p(\hat{p}_n) - p = p - p = 0.$$

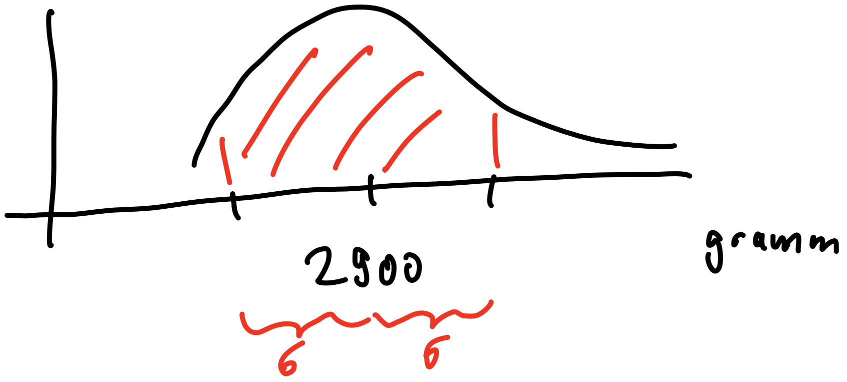
The standard error of this estimate is

$$se = \sqrt{\mathrm{Var}_p(\hat{p}_n)} = \sqrt{\frac{1}{n} \mathrm{Var}_p(X_1)} = \sqrt{\frac{p(1-p)}{n}}$$

We can for example estimate it by

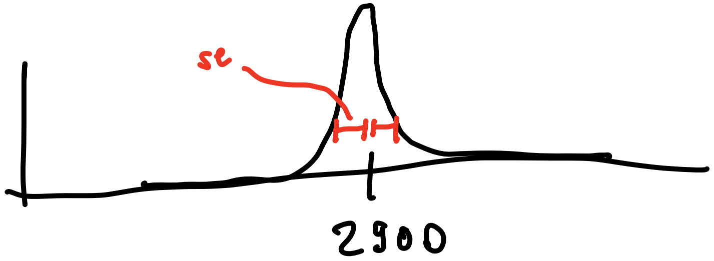
$$\hat{se} = \sqrt{\frac{\hat{p}_n(1-\hat{p}_n)}{n}}.$$

Example: weight of baby



Distribution of individual data pts: $\mu = 2900$

$\sigma = 500$



distribution of the estimate $\hat{\mu}_n$

Mean squared error

__Def__ The mean squared error (MSE) of an estimate is the quantity

$$\mathrm{MSE}(\hat{\theta}, \theta) = E_\theta\left((\hat{\theta}_n - \underbrace{\theta}_{\text{deterministic}})^2 \right)$$

Bias - Variance decomposition

Theorem : bias - variance - decomposition

$$\underbrace{MSE(\hat{\theta}_n, \theta)}_{\text{how good is our estimate}} = bias^2(\hat{\theta}_n) + Var_\theta(\hat{\theta}_n)$$

Proof $E_\theta\left((\hat{\theta}_n - \theta)^2\right) =$

$$= E_\theta\left(\left(\overbrace{\hat{\theta}_n - E\hat{\theta}_n}^{a} + \overbrace{E\hat{\theta}_n - \theta}^{b}\right)^2\right)$$

$$= E_\theta\left(\overbrace{(\hat{\theta}_n - E\hat{\theta}_n)^2}^{a^2}\right) + 2E_\theta\left(\overbrace{(\hat{\theta}_n - E\hat{\theta}_n)}^{a}\underbrace{\overbrace{(E\hat{\theta}_n - \theta)}^{b}}_{\text{deterministic}}\right) + E_\theta\left(\overbrace{(E\hat{\theta}_n - \theta)^2}^{b^2}\right)$$

$$\underbrace{2(E\hat{\theta}_n - \theta)\cdot \underbrace{E_\theta(\hat{\theta}_n - E\hat{\theta}_n)}_{= E_\theta(\hat{\theta}_n) - E_\theta\hat{\theta}_n = 0}}_{= 0}$$

$$= \underbrace{E_\theta\left((\hat{\theta}_n - E\hat{\theta}_n)^2\right)}_{Var(\hat{\theta}_n)} + \underbrace{\cancel{E}\left(\left(\underbrace{E\hat{\theta}_n - \theta}_{\text{deterministic}}\right)^2\right)}_{\substack{= (E\hat{\theta}_n - \theta)^2 \\ = (bias(\hat{\theta}_n))^2}}$$

∎

Example

$$\mathcal{F} = \{ N(\mu, \sigma^2) \mid \mu \in \mathbb{R}, \ \sigma > 0 \}$$

Sample : $X_1, \dots, X_n \sim N(\mu, \sigma^2)$ with unknown μ, σ^2, iid

$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i$ is an unbiased estimate of μ.

$$\hat{\sigma}_1^2 := \frac{1}{n} \sum_{i=1}^{n} (X_i - \hat{\mu})^2$$ "first estimate"

$$\hat{\sigma}_2^2 := \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \hat{\mu})^2$$ "second estimate"

$E(\hat{\sigma}_1^2) = \frac{n-1}{n} \sigma^2$ so the bias is $\frac{1}{n} \sigma^2$

$E(\hat{\sigma}_2^2) = \sigma^2$ unbiased!

$$\mathrm{Var}(\hat{\sigma}_1^2) = \frac{2(n-1)\sigma^4}{n^2}$$

$$\mathrm{Var}(\hat{\sigma}_2^2) = \frac{2\sigma^4}{n-1}$$

$$MSE(\hat{\sigma}_1^2) = \text{bias}^2 + \text{var} = \ldots = \left(\frac{2n-1}{n^2}\right) \sigma^4$$

$$MSE(\hat{\sigma}_2^2) = \ldots = \frac{2}{n-1} \sigma^4$$

$$\Rightarrow MSE(\hat{\sigma}_1^2) < MSE(\hat{\sigma}_2^2)$$

Consistent estimator

Def A point estimator $\hat{\theta}_n$ of θ is **consistent** (strongly consistent) if

$\hat{\theta}_n \to \theta$ in probability (a.s.)

as $n \to \infty$

Theorem If an estimate satisfies bias $\to 0$ and se $\to 0$ as $n \to \infty$, the the estimate is consistent.

Confidence sets

Confidence sets

__Def__ A (1-α)-confidence interval for a parameter $\theta \in \mathbb{R}$ is an interval $C_n = (a_n, b_n)$ where $a_n = a(X_1, \dots, X_n)$, $b_n = b(X_1, \dots, X_n)$ are functions of the sample $X_1, \dots, X_n$ such that

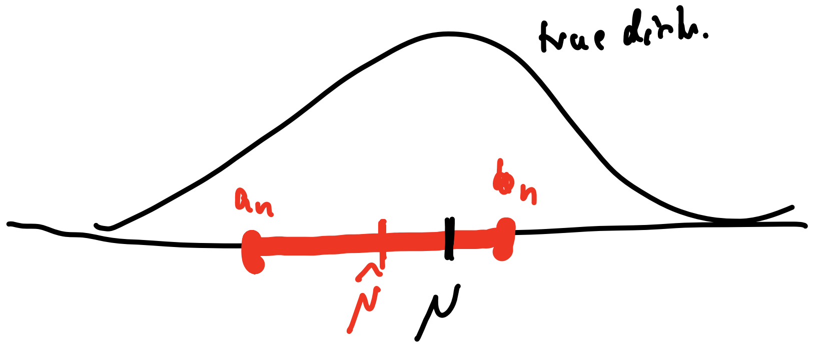
$$P_{\theta}(\underbrace{\theta}_{\text{deterministic}} \in \underbrace{C_n}_{\text{random}}) \geq \underbrace{1-\alpha} \quad \text{for all } \theta \in \Theta .$$

true (unknown) parameters $\rightarrow \theta$

$(1-\alpha)$ is called the coverage of the confidence interval.

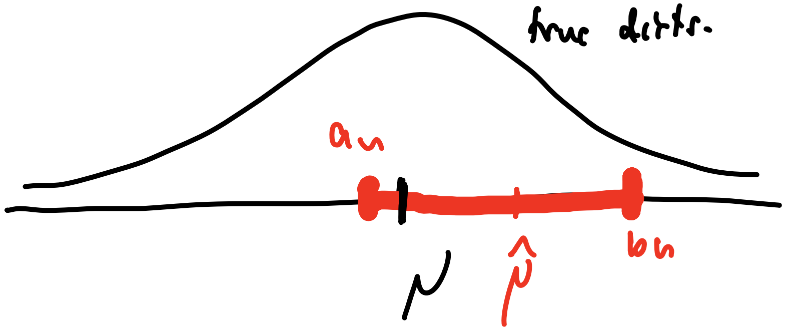
Illustration

First experiment
$x_1, \dots, x_n \rightsquigarrow \hat{\mu}$



First confidence set:

Second experiment
$x_1, \dots x_n \rightsquigarrow \hat{\mu}$



Second confidence set

... in $(1-\alpha)$ of the repetitions, the true μ is inside the red interval.

Example

Coin flips, with $P(X=1) = p$, $P(X=0) = 1-p$, $p \in [0,1]$ unknown. Want to estimate it.

$\rightsquigarrow$ observe $X_1, \dots, X_n \sim f_p$

$\hat{p}_n := \frac{1}{n} \sum_{i=1}^{n} X_i$. Choose a confidence level α,

now want to define $C_n = (a_n, b_n)$. To this end, define

$$\varepsilon_n^2 := \frac{\log(2/\alpha)}{2n}.$$

<u>Proposition:</u> $C_n := \left(\hat{p}_n - \varepsilon_n , \hat{p}_n + \varepsilon_n \right)$ is a CI with coverage $1-\alpha$.

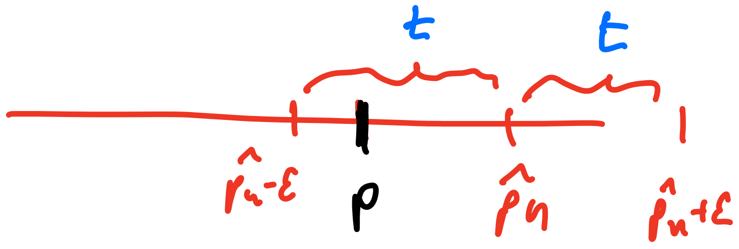
Proof (example)

<u>Proof</u>: By Hoeffding inequality, for any t we have

$$P(|\hat{p}_n - p| > t) \le \underbrace{2\exp(-2nt^2)}_{\alpha}$$

Set $\alpha := 2\exp(-2nt^2)$

and solve for t:



$$\log\left(\frac{\alpha}{2}\right) = -2nt^2 \Rightarrow t^2 = \frac{-\log(\alpha/2)}{2n} = \frac{\log(2/\alpha)}{2n}$$

Chose $\varepsilon_n = t$. ∎

Maximum likelihood estimator

Motivating example

$\mathcal{F} = \{ A \mid A$ symmetric, $n \times n$ matrix, $a_{ij} \in \{0,1\} \}$

adjacency matrices of graphs

Observe k random walks from the graph of length 10.

Goal: reconstruct (estimate) A

Idea: among all adjacency matrices $A \in \mathcal{F}$, select the one that has the highest likelihood to have produced the random walks you have observed.

$\rightsquigarrow$ Maximum likelihood approach

Likelihood

<u>More formally</u> :   Parametric family $\mathcal{F} = \{ f_\theta \mid \theta \in \Theta \}$,

observe iid points $x_1, \dots, x_n \sim f_\theta \in \mathcal{F}$.

The likelihood of the data given a parameter θ_0 is

$$p_{\theta_0}(x_1, \dots, x_n) = p(x_1, \dots, x_n \mid \theta_0)$$

notation!

$$= \prod_{i=1}^{n} p(x_i \mid \theta_0)$$

Maximum likelihood

To estimate the true parameter θ, we now select $\hat{\theta}$ such that this likelihood is maximized:

$$\hat{\theta} := \underset{\theta \in \Theta}{\arg\max}\; P(X_1, \dots, X_n \mid \theta) \overset{\text{ind.}}{=} \underset{\theta}{\arg\max} \prod_{i=1}^{n} P(X_i \mid \theta)$$

This is equivalent to the problem

$$\hat{\theta} = \arg\max \log \left(\prod_{i=1}^{n} P(X_i \mid \theta) \right) = \arg\max \sum_{i=1}^{n} \underbrace{\log \underbrace{P(X_i \mid \theta)}_{\in [0,1]}}_{< 0}$$

which is equivalent to minimizing the negative log-likelihood:

$$\hat{\theta} = \underset{\theta}{\arg\min} \sum_{i=1}^{n} \underbrace{- \log P(X_i \mid \theta)}_{> 0}$$

= maximum-likelihood estimator **MLE**

Solving max. likelihood problems

Sometimes this optimization problem is easy:

- it might be able to solve it analytically (rare)
- if you are lucky it is convex
- Most typically, it is not convex.

Example for an analytic solution

Model: $X \sim \text{Poisson}(\lambda)$, this means that

$$P(X=x) = \frac{\lambda^x e^{-\lambda}}{x!}, \quad \text{it has } E(X) = \lambda$$
$$Var(X) = \lambda.$$

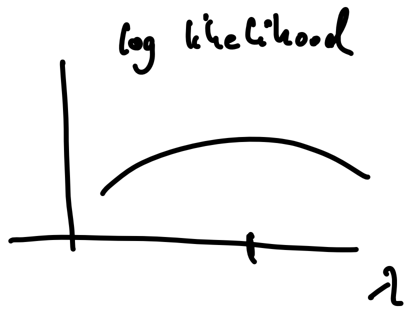
Observe $X_1, \dots, X_n \sim \text{Poisson}(\lambda)$

Want to construct the ML-estimator.

Compute the likelihood:

$$\mathcal{L}(\lambda) = P(x_1, \dots, x_n \mid \lambda) = \prod_{i=1}^{n} \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}$$

Example (continued)



$$\log(\dots) = \sum_{i=1}^{n} \log\left(\frac{\lambda^{x_i} e^{-\lambda}}{x_i!}\right)$$

$$= \underbrace{\sum_{i=1}^{n} \left(x_i \log \lambda - \lambda - \log(x_i!)\right)}_{f(\lambda)}$$

Now want to optimize for λ. Take the derivative (wrt λ):

$$f'(\lambda) = \sum_{i=1}^{n} \left(\frac{x_i}{\lambda} - 1 \right) = \frac{1}{\lambda} \left(\sum_{i=1}^{n} x_i \right) - n \overset{!}{=} 0$$

$$\Rightarrow \underline{\lambda = \frac{1}{n} \sum_{i=1}^{n} x_i}$$

So $\hat{\lambda} := \frac{1}{n} \sum_{i=1}^{n} x_i$ is the ML estimate of λ. ■

MLE properties

From the theory side, MLE often (but not always) has nice properties:

(1) If the model $\mathcal{F}$ consists of "nice" functions, then the MLE based on an iid sample is consistent.

(2) If $\mathcal{F}$ consists of "nice" functions, the MLE estimate $\hat{\theta}_{MLE}$ is asymptotically normal:

$$\frac{\hat{\theta}_{MLE} - \theta}{se} \xrightarrow{\text{in distr.}} N(0,1) \quad \text{and}$$

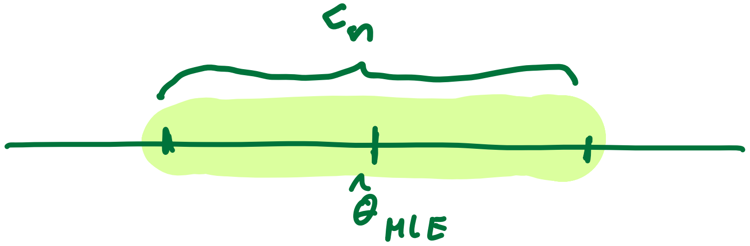
$$\frac{\hat{\theta}_{MLE} - \theta}{\hat{se}} \xrightarrow{\text{in distr.}} N(0,1)$$

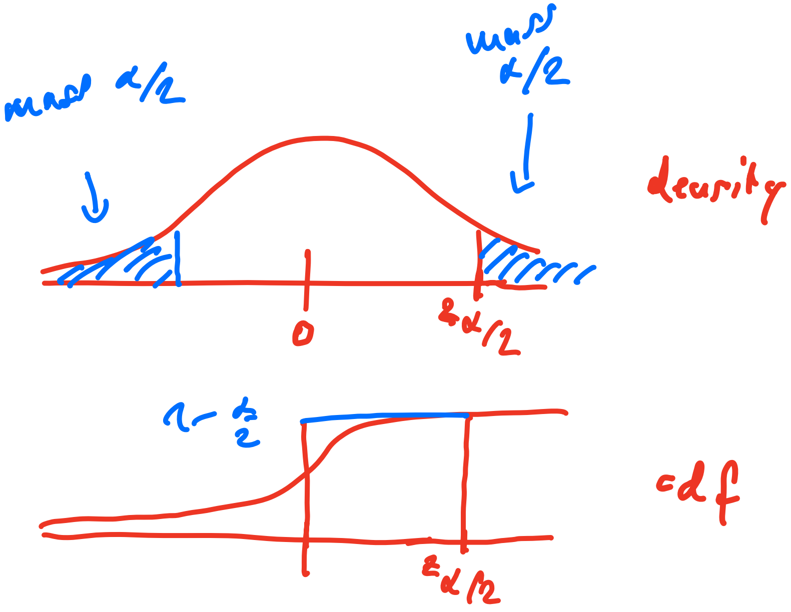
(5) This can be used to construct (approximate) confidence intervals:

$$C_n := \Big(\hat{\theta}_{MLE} - \underbrace{z_{\alpha/2} \; \hat{se}}_{-\varepsilon} \; , \; \hat{\theta}_{MLE} + \underbrace{z_{\alpha/2} \cdot \hat{se}}_{+\varepsilon} \Big)$$

where $z_{\alpha/2} := \underset{\uparrow}{\Phi}^{-1}\left(1 - \frac{\alpha}{2}\right)$

cdf of $N(0,1)$





C_n is an "approximate CI" in the sense that

$$P_\theta(\theta \in C_n) \longrightarrow 1-\alpha \quad \text{as } n \to \infty.$$

Sufficiency & Identifiability

Sufficiency

Intuition: given sample $X_1, \dots, X_n \sim f_\theta \in \mathcal{F}$

we typically convert the (large) sample to a statistic

$T(X_1, \dots, X_n)$ (in the extreme case, one number). ?

Question: can we recover the true parameter θ from this statistic

If yes we would like to call the statistics $T(X_1, \dots, X_n)$

"sufficient".

Sufficiency

Which properties would we need to assert sufficiency?

- when we observe two samples $x_1, \dots, x_n$ and $x_1', \dots, x_n'$, and $T(x_1, \dots, x_n) = T(x_1', \dots, x')$, then we would infer the same θ.
- When we know $T(x_1, \dots, x_n)$, then we would need some way to compare the likelihood of the data.

Formal definition is technical, skipped.

Identifiability

Sometimes families of distributions can be described in different ways with different sets of parameters.

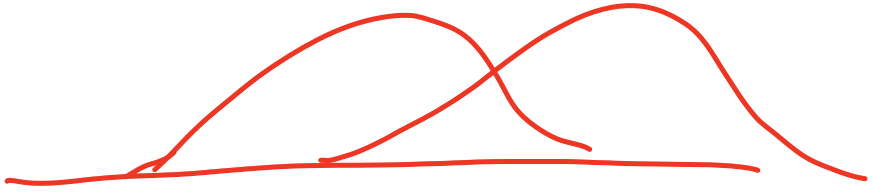
Def A parameter θ for a family $\mathcal{F} = \{ f_\theta \mid \theta \in \Theta \}$ is identifiable if distinct values of θ correspond to distinct pdfs in $\mathcal{F}$:

$$\theta \neq \theta' \Rightarrow f_\theta \neq f_{\theta'}$$

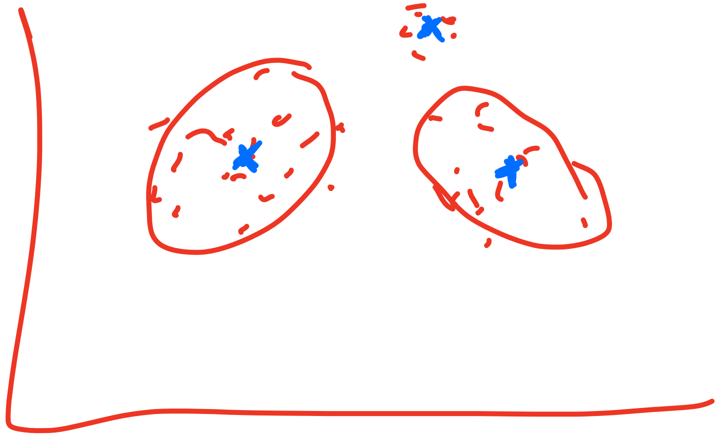
Example (identifiability)

Example: Mixture distributions

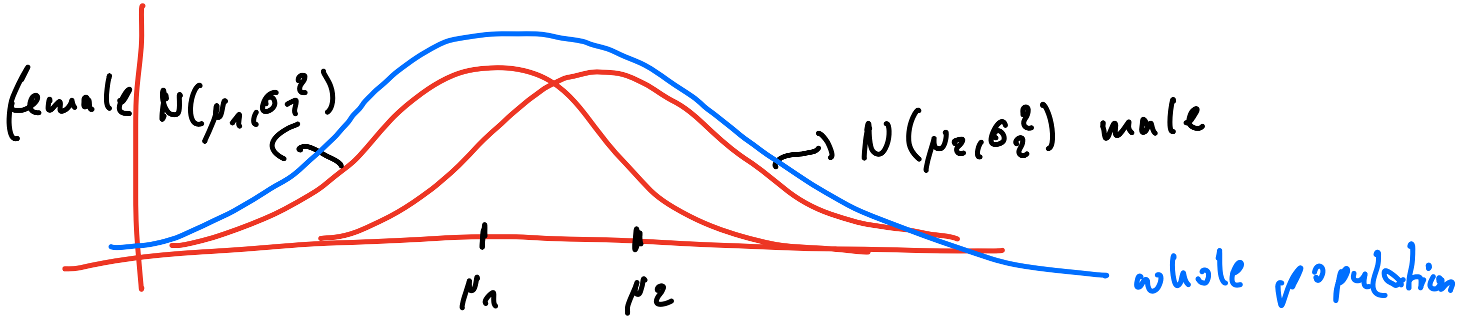
$$\mathcal{F} = \left\{ \sum \alpha_i \, N(\mu_i, \sigma_i^2) \right\} \quad \text{with} \quad \sum \alpha_i = 1$$



Example 1-d



Example 2-d



You observe samples from the whole population.

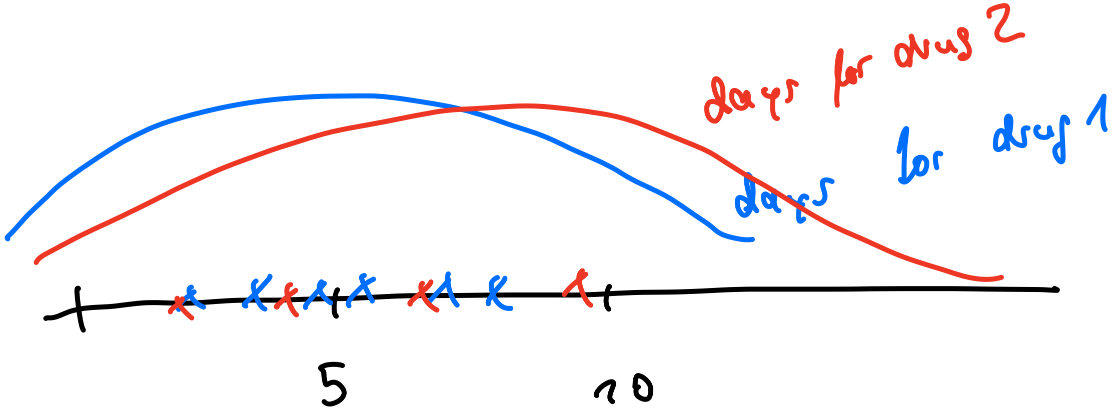
$$0.5\, N(\mu_1, \sigma_1^2) + 0.5\, N(\mu_2, \sigma_2^2)$$

It is impossible without further knowledge to identify the original distribution parameters just from observing the full distribution (you don't know who was female and who not)

Hypothesis testing

Motivation

Example: Two drugs D_1, D_2, we measure number of days to recovery for both drugs: $x_1, \dots, x_n$ treated with D_1
$x_1', \dots, x_n'$ D_2

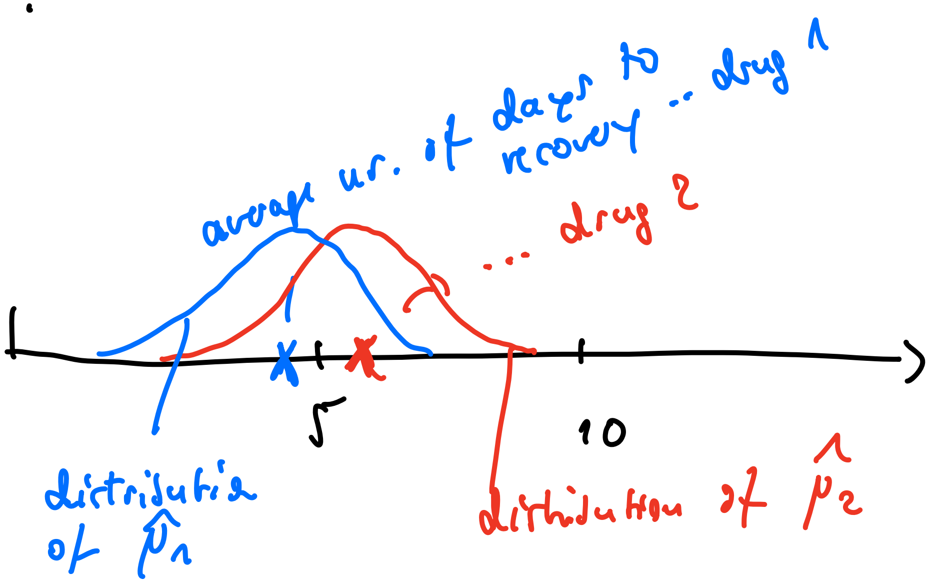


Question: is Drug 1 better than Drug 2 ?

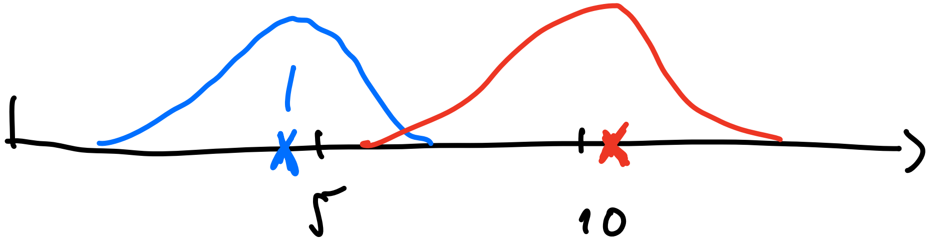
General idea

... will be: consider the distributions of the estimates $\hat{\mu}_1, \hat{\mu}_2$.

If they are "far apart", we would say that they are different...



average nr. of days to recovery ... drug 1
... drug 2
5
10
distribution of $\hat{\mu}_1$
distribution of $\hat{\mu}_2$



But how do we know what "far apart" is?

Example Want to test whether a coin is fair.

Null hypothesis: H_0 : coin is fair

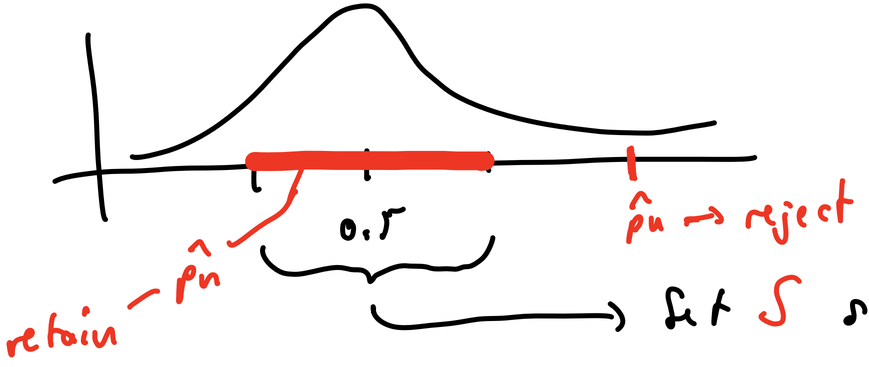
Alternative hypothesis: H_1 : coin is unfair

Sample many coin flips and estimate $\hat{p}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$.

We want to reject H_0 if $\hat{p}_n$ is "far away" from 0.5.

Question: "far away"?

Look at the distribution of $\hat{p}$ under the null hypothesis:



→ Set S such that

$$P_p(\hat{p}_n \in S) \geq 95\%$$

More formal setup

Statistical model $\mathcal{F} = \{ f_\theta \mid \theta \in \Theta \}$. Assume that

$\Theta_0 \subset \Theta$, $\Theta_1 \subset \Theta$, $\Theta_0 \cap \Theta_1 = \emptyset$.

Want to test

$$\underbrace{H_0 : \theta \in \Theta_0}_{\text{null hyp.}} \qquad \text{against} \qquad \underbrace{H_1 : \theta \in \Theta_1}_{\text{alternative hyp.}} .$$

Sample data from the unknown f_θ, compute a test statistic $T(x_1, \dots, x_n)$. Now we construct a rejection region R_n

such that $\quad T(x_1,\dots,x_n) \in R_n \Rightarrow$ reject H_0

$\qquad\qquad\quad T(x_1,\dots,x_n) \in R_n \Rightarrow$ retain H_0

Typical hypotheses are of the form

- $H_0 : \theta = \theta_0$ vs $H_1 : \theta \neq \theta_0$

- $H_0 : \theta < \theta_0$ vs $H_1 : \theta \geq \theta_0$

Two types of error can occur:

	Test retains H_0	Test rejects H_0
H_0 true	☺	Type I error
H_1 true	Type II error	☺

Power of a test, β

<u>Def</u> The <u>power function</u> of a test with rejection region R is the function

$$\beta(\theta) := P_\theta(T(x) \in R)$$

- If $\theta \in \Theta_0$ then $T(x)$ should not end up in R. For such θ, $\beta(\theta) = P(\text{Type I error})$. Ideally, $\beta(\theta)$ should be small.
- If $\theta \in \Theta_1$ then we hope that $T(x) \in R$. So

$$\beta(\theta) = 1 - P(\text{Type II error}).$$

Ideally, $\beta(\theta)$ is large.

Level of a test, α

Def We say that a test is of level α if

$$\sup_{\theta \in \Theta_0} \beta(\theta) \leq \alpha$$

Intuition: worst case guarantee: no matter which $\theta \in \Theta_0$ we pick, the type I error is not larger than α.

(Intuition to remember: $\alpha \hat{=}$ type I error)

Standard approach for testing

Standard procedure: We fix the level α of a test in advance, for example 0.05 or 0.01.

Then we can also look at the type II error. For example among several tests of level α, you might now choose the one that has the smallest type-II-error.

Notation used often in literature:

$$\alpha = P(\text{type I error}) \qquad \alpha = \text{level of the test}$$

$$\beta = P(\text{type II error}) \qquad 1-\beta = \text{power of a test}$$

Remark: the power of a test is typically evaluated when we test against a concrete hypothesis $\theta_1 \in \Theta_1$. We say "the power of the test against alternative $\theta_1 \in \Theta_1$".

Uniformly most powerful test

Def Let $\mathcal{J}$ be a set of tests of level α for testing

$H_0 : \theta \in \Theta_0$ vs $H_1 : \theta \notin \Theta_0$.

A test in $\mathcal{J}$ with power function $\beta(\theta)$ is uniformly most powerful (UMP) if

$$\beta(\theta) \geq \beta'(\theta) \quad \text{for all } \theta \in \Theta_0^c$$

and for all β' that are power functions for other tests in $\mathcal{J}$.

Remark: In practice it is often impossible to find an UMP test.

Neyman - Pearson - lemma
&
# likelihood ratio tests

Neyman-Pearson

Theorem Suppose we test $H_0 : \theta = \theta_0$ against $H_1 : \theta = \theta_1$.

Consider

$$T = \frac{\mathcal{L}(\theta_1)}{\mathcal{L}(\theta_0)} = \frac{\prod_{i=1}^{n} f(x_i \mid \theta_1)}{\prod_{i=1}^{n} f(x_i \mid \theta_0)} \Bigg\} \text{ likelihood ratio.}$$

Assume we reject H_0 if $T > k$ (for some k).

If we choose k such that $P_{\theta_0}(T > k) = \alpha$,

then this is the most powerful level-α-test.

More general likelihood-ratio-test :

parameter space Θ, $\Theta_0 \subset \Theta$, $\Theta_1 = \Theta_0^c$. Then we consider the test statistic

$$\tilde{T} = \frac{\sup_{\theta \in \Theta_0} \mathcal{L}(\theta)}{\sup_{\theta \in \Theta_1} \mathcal{L}(\theta)} \quad \text{or even simpler} \quad T = \frac{\sup_{\theta \in \Theta_0} \mathcal{L}(\theta)}{\sup_{\theta \in \Theta} \mathcal{L}(\theta)}$$

and we determine a parameter λ such that the rejection region is of the form $R = \{ T \leq \lambda \}$.

In practice the difficulties are

- compute the suprema (in practice)
- fix R, fix λ (in theory)

p-values

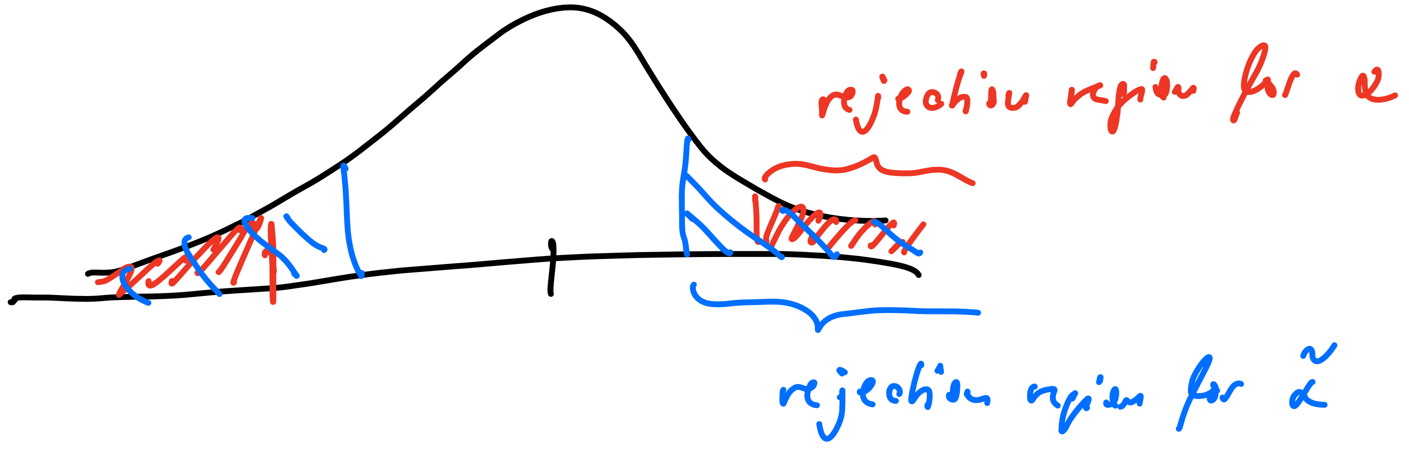
p - values

Consider a test at level α, and denote its rejection region as R_α.

Recall: $\alpha = P(\text{Type-I-error})$.

The smaller α, the more difficult does it get to reject H_0.

(we often even have that $\alpha < \tilde{\alpha} \Rightarrow R_\alpha \subset R_{\tilde{\alpha}}$)


rejection region for α
rejection region for $\tilde{\alpha}$

p - value

Def The p-value is defined as

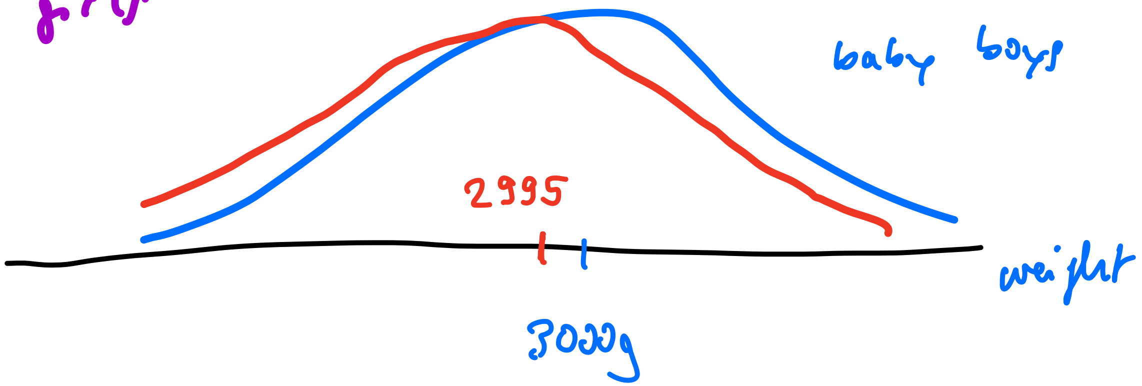
$$p = \inf \{ \alpha \mid T(X_1,\dots,X_n) \in R_\alpha \}$$

i.e the smallest α for which the level-α-test would reject the null hypothesis.

Intuition: smaller p-values are "better", more evidence for rejecting the null (less error).

Example baby boys and girls

sample distribution

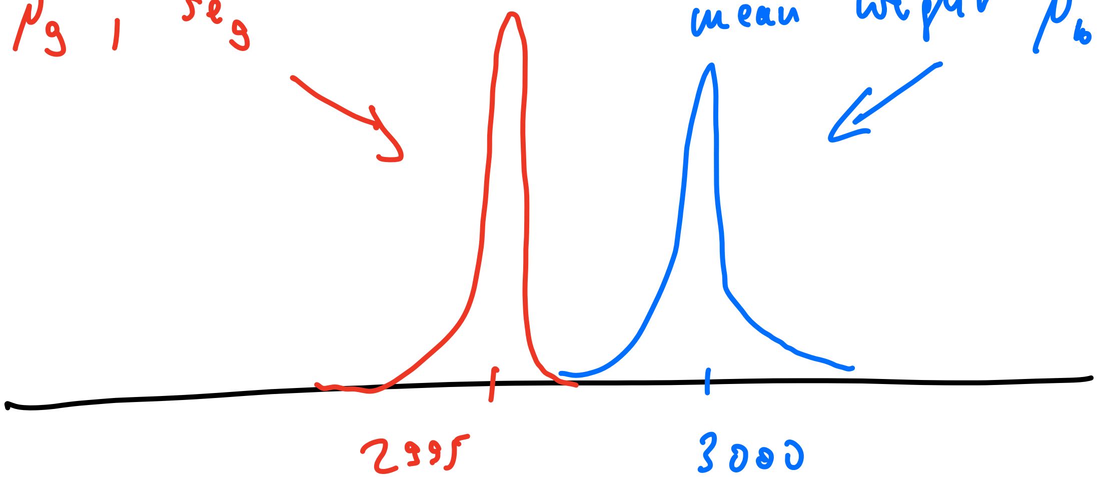


distribution of test statistics

Sample many baby girls, many baby boys

$\hat{\mu}_g$, $\hat{se}_g$

mean weight $\hat{\mu}_b$, & $\hat{se}_b$



For n large test will find a statistically significant difference. ~> small p

Multiple testing

Motivation

Example: gene expression data

	patients with cancer ($n = 20$)	control group ($n = 20$)
gene 1		
gene 2		
.		
gene 17	0.5 0.2 0.9 0.8 0.5	0.01 0.05 0.1 0.02
gene 105		
gene $\underbrace{1000}_{=:m}$		

α % of the test will "ring a bell"

Assume we run, for each gene, a test of level α

$P($ Test i makes type-I-error $) = 5\%$. Now we have m tests.

$$P(\text{at least one of the tests makes a type-I-error}) =$$

$$= P(t_1 \text{ makes error } \underline{\text{or}}\ t_2 \text{ error } \underline{\text{or}} \ldots \underline{\text{or}}\ t_m \text{ makes error})$$

$$= 1 - P(\text{no error in } t_1 \ \underline{\text{and}} \text{ no error in } t_2 \ \underline{\text{and}} \ldots) \overset{\text{assume independence}}{=}$$

$$= 1 - \prod_{i=1}^{m} P(\text{no error in } t_i) = \underbrace{1 - (0.95)^m}_{*} \xrightarrow[m\to\infty]{} 1$$

$m = 1 \Rightarrow * = 0.05$

$m = 10 \Rightarrow * = 0.40$

$m = 50 \Rightarrow * = 0.92$

Many "wrong" tests!

Family-wise error rate (FWER)

Definition: Consider a family of m tests. The family-wise error rate (FWER) is the probability that at least one type-I-error occurs in the family:

$$
\begin{aligned}
\text{FWER} = P(\, & t_1 \text{ makes type-I-error } \underline{\text{or}} \\
& t_2 \ \ldots \\
& \ldots \\
& t_m \text{ makes type-I-error } \quad).
\end{aligned}
$$

Bonferoni correction

Assume we run m tests, and we want to achieve a FWER α (e.g. $\alpha = 0.05$). Then we run the individual tests with level $\frac{\alpha}{m} =: \alpha_{single}$. Then:

$$\text{FWER} = P(\text{at least one type-I-error}) =$$

$$= P(t_1 \text{ error } \underline{\text{or}} \ t_2 \ \dots \ ) \leq$$

$$\leq \sum_{i=1}^{m} \underbrace{P(t_i \text{ makes error})}_{\alpha_{single}} = m \cdot \alpha_{single} = m \cdot \frac{\alpha}{m} = \alpha .$$

Bonferroni, discussion

Bonferroni controls the FWER.

Advantage: simple, correct

Disadvantage: too conservative, low power (high type-II-error)

the test barely discovers anything!

False discovery rate, FDR

Def. Assume we have a family of m tests. We call

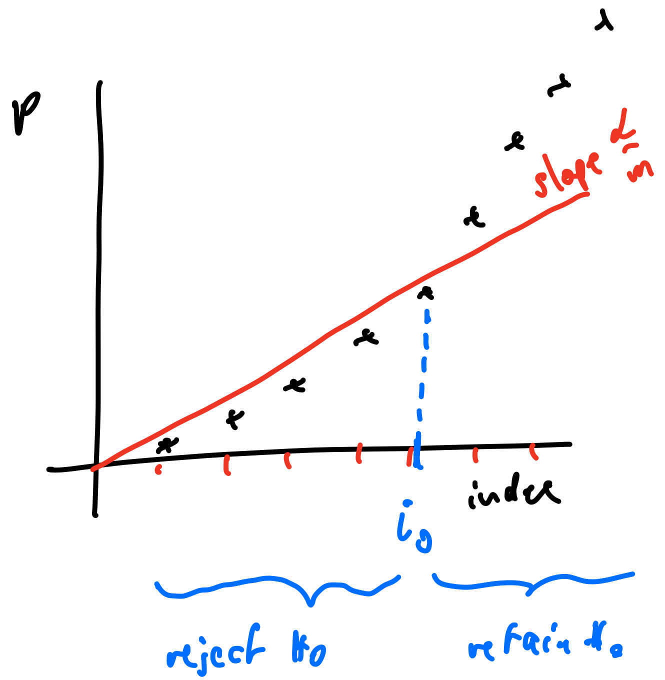
$$E\left(\frac{\#\text{ false rejections}}{\#\text{ all rejections}}\right) =: FDR$$

the false discovery rate.

Benjamini/Hochberg: Controling FDR

Benjamini/Hochberg (1998) approach:

- Fix FDR α in advance.
- Run the m individual tests and evaluate their p-values.
- Sort p-values increasingly: $p_{(1)} \leq p_{(2)} \leq p_{(3)} \leq \dots \leq p_{(m)}$
- Define thresholds $l_i := i \cdot \frac{\alpha}{m}$
- Find the largest index i_0 such that $p_{(i_0)} \leq l_{i_0}$. (below the red line)
- Reject the hypotheses for $i = 1, \dots, i_0$, retain all the others.



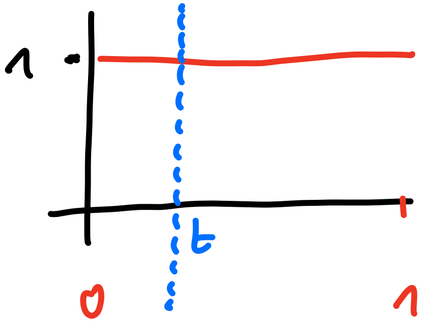
Theorem (Benjamini-Hochberg)

<u>Theorem</u> : If the Benjamini-Hochberg procedure is applied (and the tests are independent), then regardless of how many null hypotheses are true and regardless of the distribution of p-values when the null is false, we obtain $\text{FDR} \leq \alpha$.

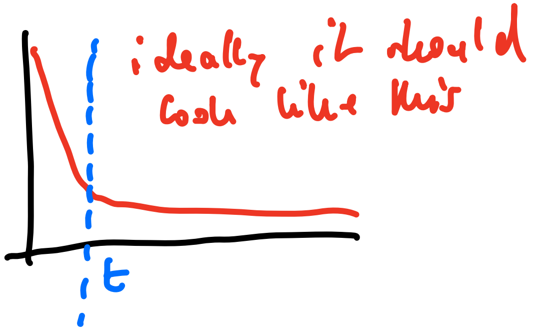
(Remark: similar approach also works without independence assumption, many modifications exist.)

Intuition

- Under the null hypothesis, the p-values always have a uniform distribution on $[0, 1]$.

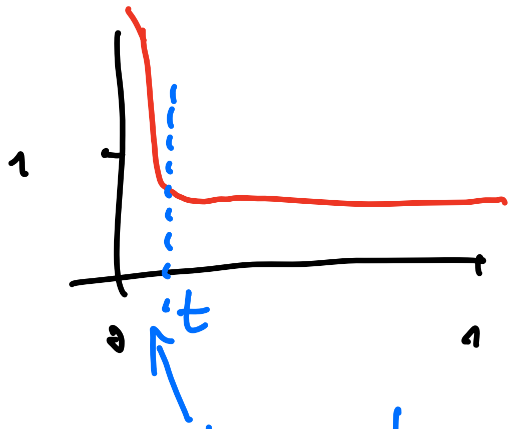


density of p-values under H_0



density of p-values under H_1

If we have some H_0 and some H_1 being true ~~an~~ then the density would maybe look like that:

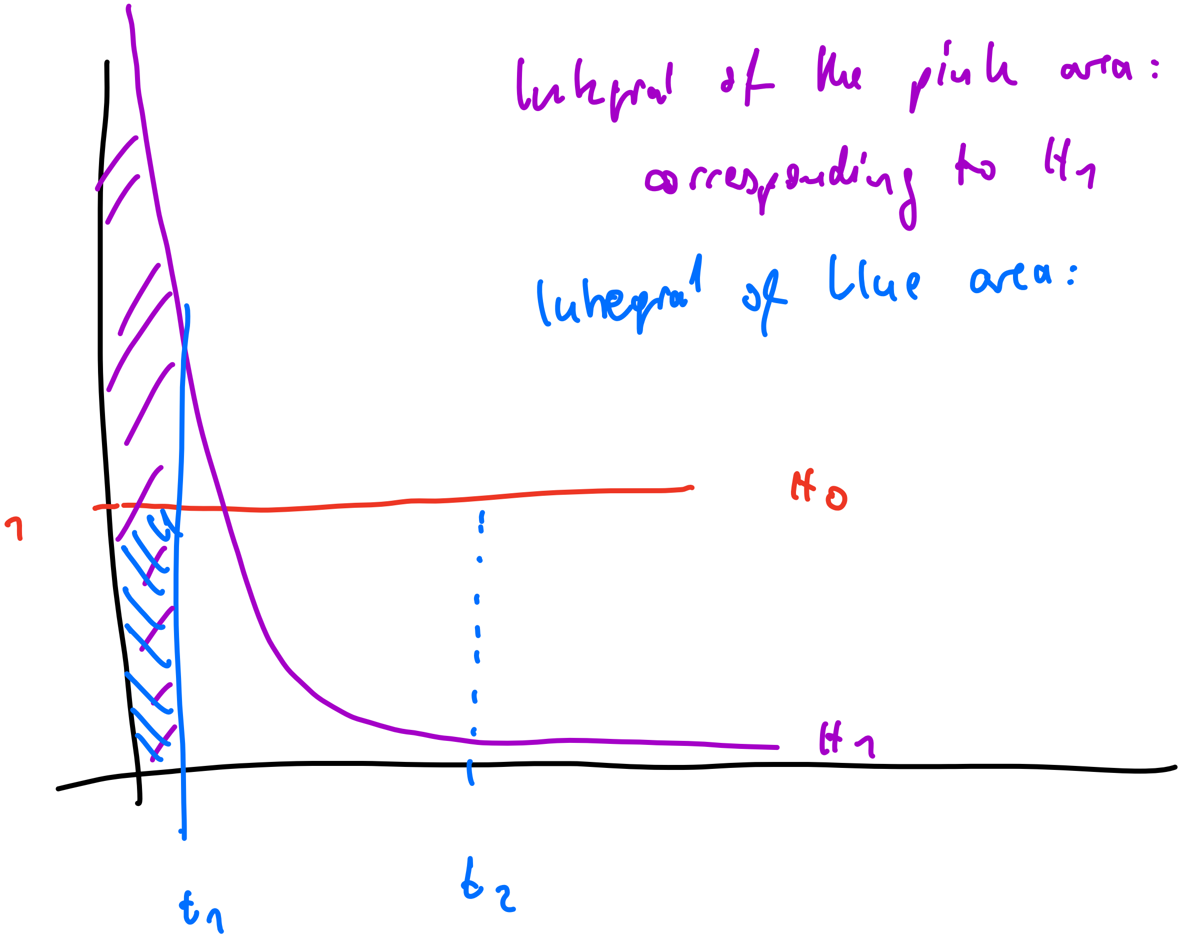


here we have (hopefully) many of the H_1 s but we also have some H_0 s.

Goal: set threshold t such that FDR satisfies what we want.

Integral of the pink area: Expected number of pvalues corresponding to H_1 that are below t_1

Integral of blue area: ... H_0



By moving t from 0 to 1 we control the FDR:

For t_1, the FDR is small

t_2 large

General Remarks

- BH tends to have more power than Bonferroni
- BH controls FDR, not FWER (overall type-I-error)!
- BH works best in sparse regime where only few tests reject the null
- BH gives guarantees on FDR, but in general does not minimize it.
- When all the H_0 are true, BH $\approx$ Bonferroni.

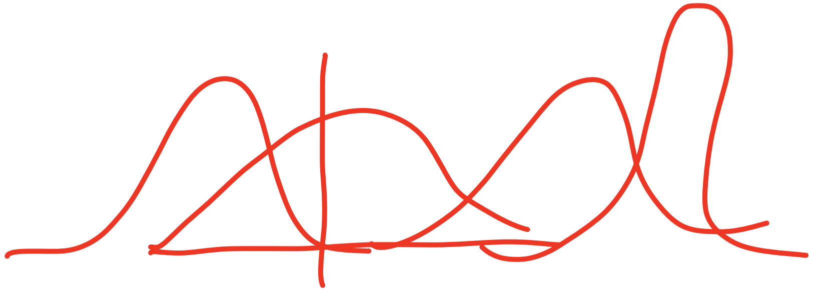
Non-parametric

tests

Non-parametric tests

Standard (parametric scenario):

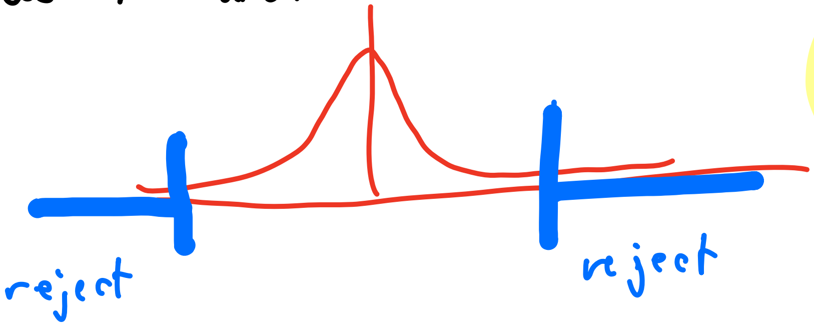
- Statistical model $\mathcal{F} = \{ f_\theta \mid \theta \in \Theta \}$



distribution of the samples

- Observe data, compute a test statistics T_n, for example the mean $\bar{X}$

- Need to know the distribution of the test statistics T_n under the null distribution:



distribution of T_n under the null hyp.

Goodness-of-fit test (gof)

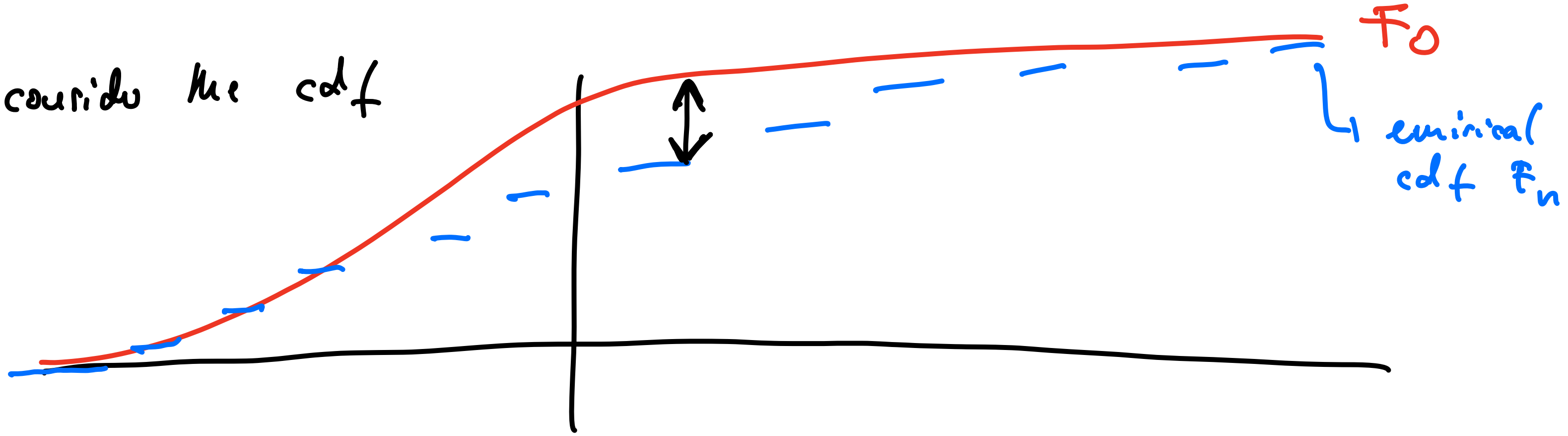
Goodness-of-fit tests: Goal is to test whether a data set comes from a particular distribution F_0

$$H_0: \quad \underset{\uparrow \text{ true distribution that generated the data}}{F(x)} = F_0(x)$$

$$H_1: \quad F(x) \neq F_0(x)$$

Kolmogorov-Smirnov test for g.o.f

We consider the cdf



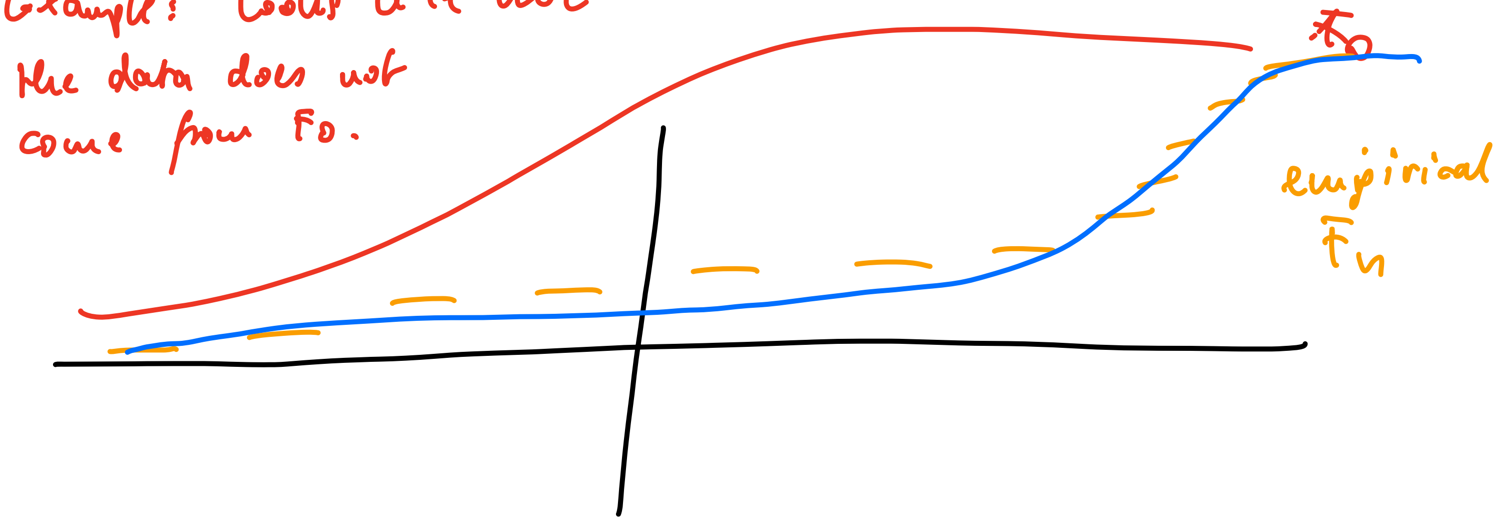
F_0 = cdf of the given distribution

F_n = cdf of the data

$$D_n := \sup_{x \in \mathbb{R}} \left| F_n(x) - F_0(x) \right|$$

By the Glivenko-Cantelli theorem we know that under the null hypothesis, $F_n \to F_0$ uniformly. a.s.

It is possible to compute the distribution of D_n, and it is independent of F_0, it just depends on n. From this we can compute rejection thresholds and design a test.


Example: looks like here the data does not come from F_0.

two sample test

Two sample test: $X_1, \dots, X_n \sim F_1$ a first sample distributed according to F_1,

$Y_1, \dots, Y_m \sim F_2$ a second sample distributed acc. to F_2.

Question: $F_1 = F_2$?

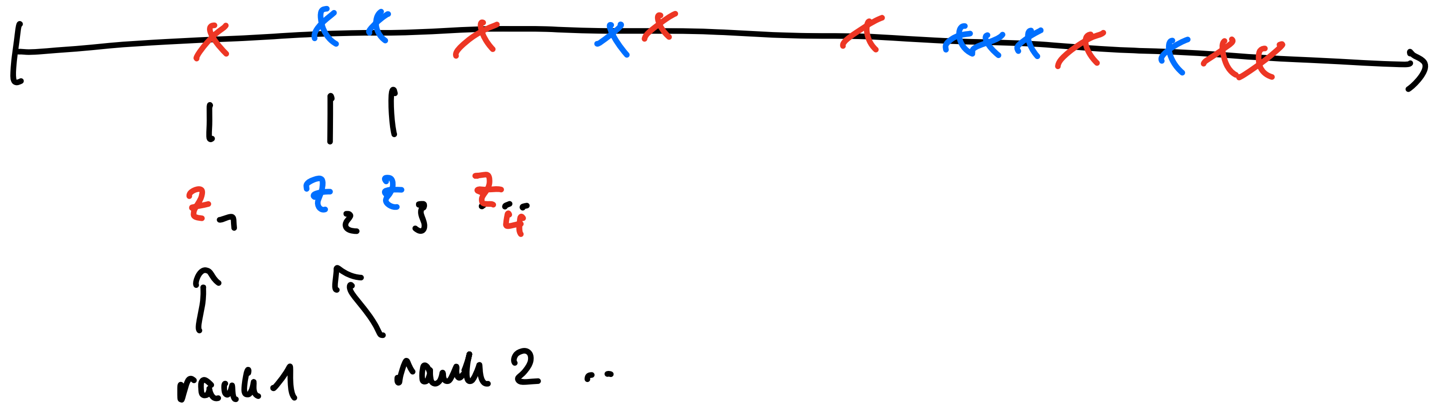
$H_0: \quad F_1 = F_2 \quad , \quad H_1: \quad F_1 \neq F_2$

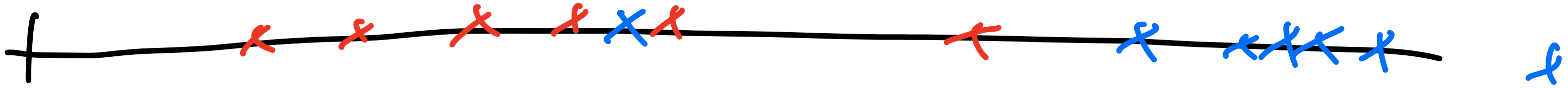
Wilcoxon - Mann - Whitney test (based on ranks)

<u>Test</u>:

- "Pool the sample" : $\underline{x_1, \dots, x_n}, \underline{y_1, \dots, y_m} \in \mathbb{R}$

- Sort the pooled sample in increasing order and retrieve the rank of all points ⇝ rank(x_i)
  rank(y_i)





- Compute the rank sums for both groups:

red group: $$W_{red} = \sum_{i \in \text{red population}} \text{rank}(X_i)$$

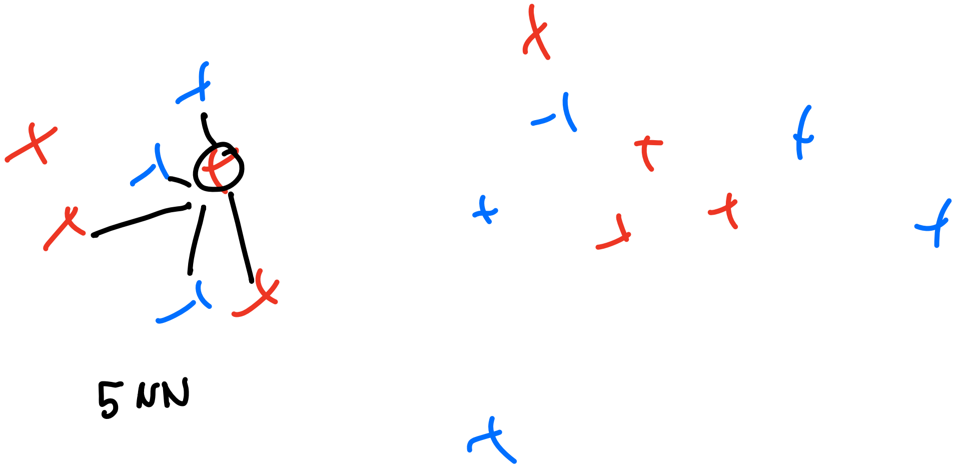
$$W_{blue} = \sum_{i \in \text{blue pop.}} \text{rank}(Y_i)$$

- If $|W_{red} - W_{blue}|$ is small, we retain H_0,

if large, reject H_0.

Extension to a multivariate setting using k nearest neighbors

- Two samples, we pool them:



- For each point, we look at the colors of the k nearest neighbors:

- Under the null hypothesis we expect that the number of red neighbors ≈ number of blue neighbors.

Permutation (randomization) tests

- Sample $X_1, \dots, X_n$ group A $\rightsquigarrow$ mean $\bar{X}$ \

  $Y_1, \dots, Y_n$ group B mean $\bar{Y}$ — $\bigcirc\!\!\!\!?$

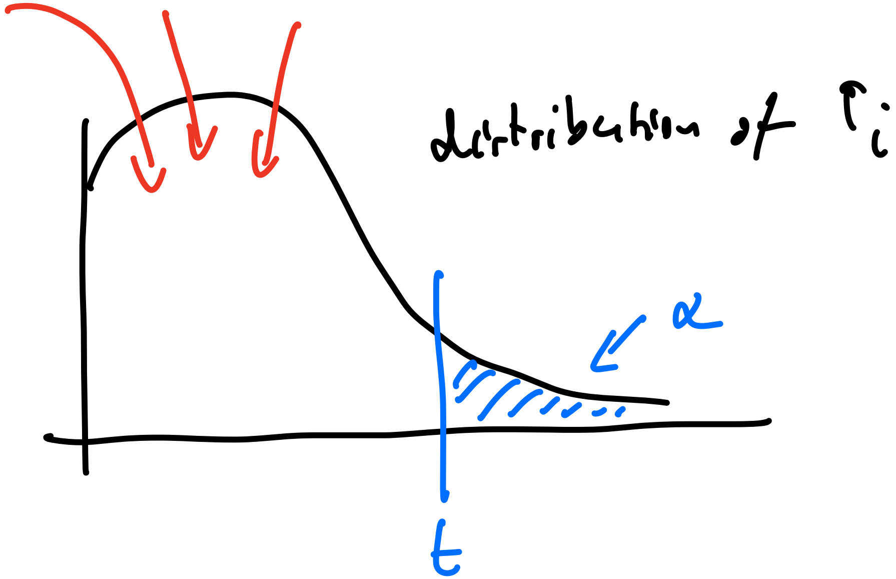
- Compute observed statistics $T_{\text{observed}} = \text{mean(red)} - \text{mean(blue)}$

- Pool the sample

- For $k = 1, \dots, 10^3$: shuffle the group membership ("colors")

- Compute the difference $T_k = \text{mean}(\text{red}) - \text{mean}(\text{blue})$

~) $T_1, T_2, \dots, T_{1000}$



- Find α-quantile to determine rejection threshold.

- Check whether the observed T_{observed} on the true data is $\leq t$.

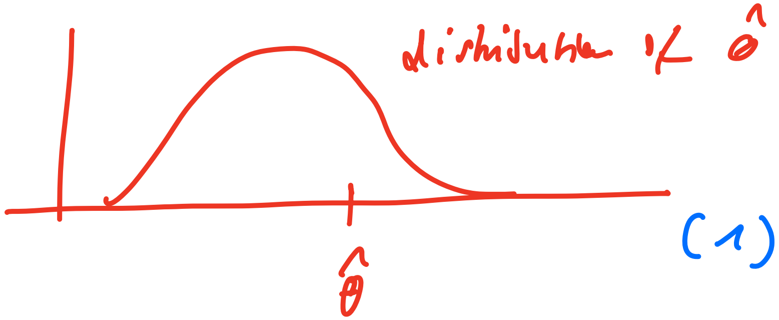
Bootstrap tests

Motivation

Motivation: $X_1, \dots, X_n \sim F$, no knowledge on F want to estimate a parameter $\theta = t(F)$. You generate an estimate $\hat{\theta}$ based on $X_1, \dots, X_n$, want to know how reliable $\hat{\theta}$ is.

The first thing to look at is the standard error se,

- If we have assumptions on F, we can analytically compute the distribution of $\hat{\theta}$, the $\hat{se}$, ... (this is rare!)



(1)

- We could also try to obtain many samples

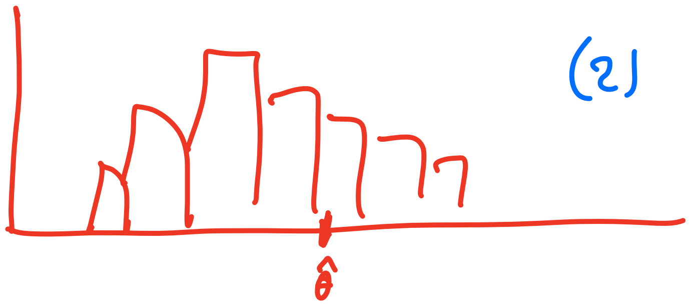
  - $x_1^{(1)}, \dots, x_n^{(1)}$
  - $x_1^{(2)} \dots x_n^{(2)}$

  $\vdots$

  $x_1^{(m)} \dots x_n^{(m)}$

and then estimate the distribution of $\hat{\theta}$:

Problem: need too many samples.



(2)

Then we could maybe build a hist on this.

Idea of the bootstrap

- Given the sample $X_1, \dots, X_n$ ⤳ estimate $\hat{\theta}_{orig}$
- Draw a subsample of $X_1 \dots X_n$, compute $\hat{\theta}^*$, repeat very often

histogram of θ^* based on resampled data

"Hope: histogram $\overset{(3)}{}$ of $\hat{\theta}^*$ is "close" to histogram of $\hat{\theta}$ (2), which is close to (1)

Example: estimate the standard errors of an estimate $\hat{\theta}$

Algorithm in pseudo code

```
Input: $x_1, \dots, x_n$        number of original sample points
For $b = 1, \dots, B$           number of bootstrap replications
    • Sample $x_1^*, \dots, x_{\underline{\underline{n}}}^*$ uniformly with replacement
      from $x_1, \dots, x_n$
    • Estimate the parameter $\hat{\theta}_b^*$
                                gives us $\hat{\theta}_1^*, \dots, \hat{\theta}_B^*$
```

Estimate the standard error $\hat{se}$ of the original estimate $\hat{\theta}$ by the standard dev. of the bootstrap replicates:

$$\hat{se}_B := \left(\frac{1}{B-1} \sum_{b=1}^{B} \left(\hat{\theta}_b^* - \underbrace{\left(\frac{1}{B} \sum_{i=1}^{B} \hat{\theta}_i^* \right)}_{\text{mean of replicates}} \right)^2 \right)^{1/2}$$

Does it always work?

Consistency result for bootstrap

Theorem (Consistency of the estimate of the standard error)

- Assume that $X_1, \dots, X_n \sim F$, iid, and $E(\|X_1\|^2) < \infty$.
- Let $\hat{\theta}_n = g(X_1, \dots, X_n)$ be the parameter that we estimate. Assume that g is continuously differentiable in a neighborhood of $\mu = EX_1$, with a non-zero gradient.

Then the bootstrap estimate of the standard error is strongly consistent.

Example where it goes wrong

$X_1, \dots, X_n \sim$ Uniform $[0, \theta]$. , where $\theta \in [0, 1]$. unknown.

Want to estimate θ. The ML estimate of θ is simply the largest number we observe:

$$\hat{\theta} = \max_{i=1\dots n} X_i \, .$$

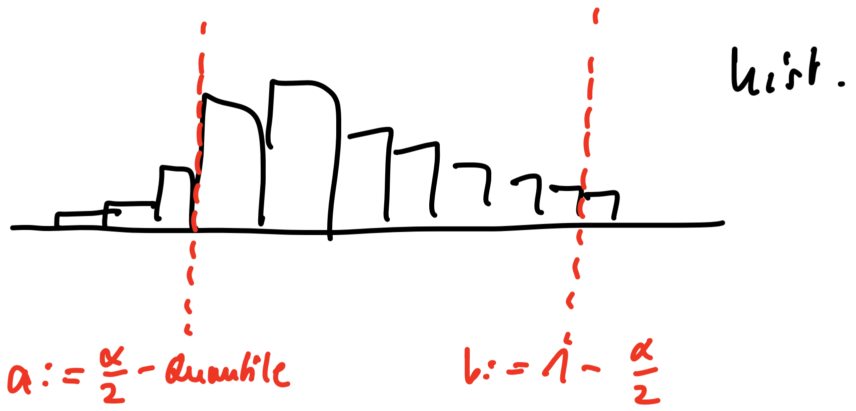
Estimating the $\hat{se}$ by bootstrap is going to fail.

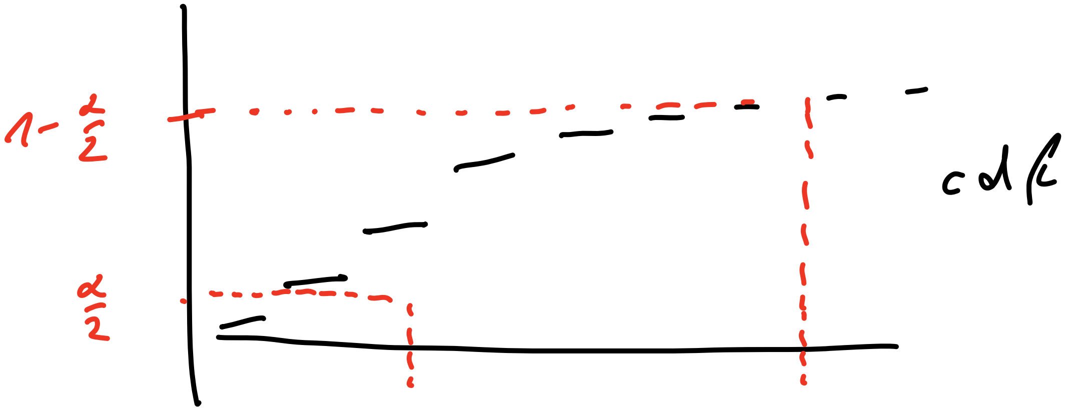
Estimating tails or extreme values by bootstrap is problematic.

Confidence sets by bootstrap

Bootstrap-percentile-method:

- Given sample $X_1, \dots, X_n$, estimate $\hat\theta$
- Generate bootstrap replicates $\hat\theta_1^*, \dots, \hat\theta_B^*$
- look at the histogram of the $\hat\theta_b^*$





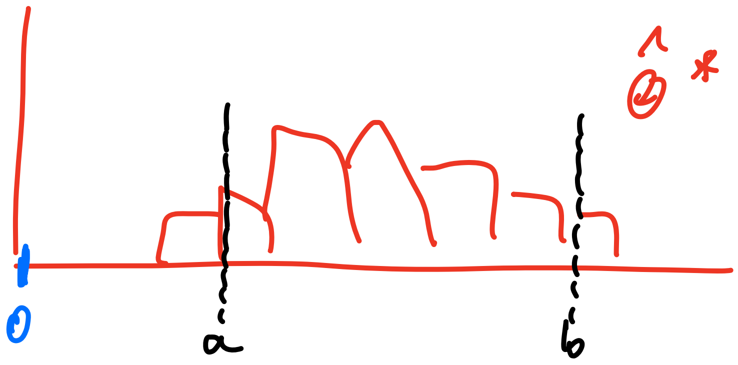
- $CI = [a, b]$

It has coverage $1-\alpha$ because

$$P_\theta(\hat{\theta} \in CI) \geq 1-\alpha$$

(approximately, because n, B finite)

Subsequently you can construct bootstrap tests in the obvious way



$H_0: \hat{\theta}_n = \theta$ vs $H_1: \hat{\theta} \neq \theta$

Bayesian statistics

Frequentist vs. Bayesian statistics

Frequentist statistics:

- probability = limiting frequency
- parameters θ are constants, we cannot assign probabilities to them
- statistics behaves well when repeated often

Bayesian statistics

- probability = degree of belief
- parameters do have probabilities
- have a prior belief about the world, update it based on observed data.

Bayesian statistics : the model

Assume a statistical model $\{f_\theta \mid \theta \in \Theta\}$, as in frequentist approach.

It encodes our prior assumptions on the data-generating process in general.

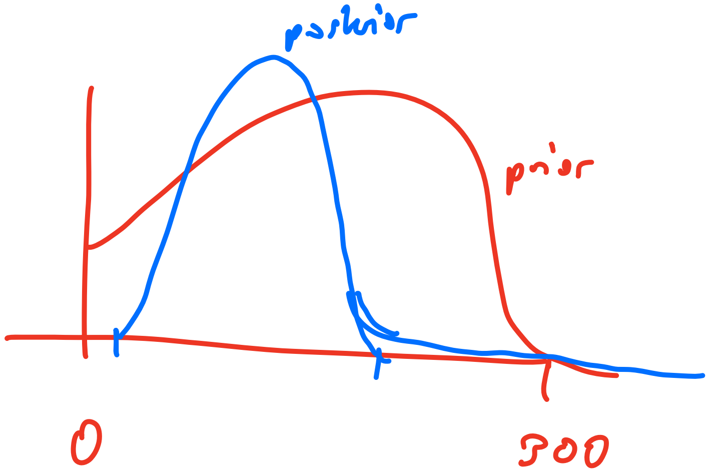
Θ unknown, want to estimate it.

Bayesian approach: prior distribution

We assume that we have a prior belief about the parameters θ:

$f(\theta)$ prior distribution

the parameter, not the data



Bayesian statistics: the likelihood

Observe data $X_1, \dots, X_n$ iid from some of the f_θ (θ unknown).

We call $\underset{\text{density}}{f}(\underset{\text{data}}{x} \mid \underset{\text{parameter}}{\theta})$ the likelihood of the data given the parameter θ

(In frequentist world, we could now use MLE to select the para that maximizes the likelihood)

Bayesian statistics: posterior

Now we update our belief ; we compute the posterior using Bayes rule: $f(\theta | x_1 \dots x_n)$

$$\overbrace{f(\theta | x_1 \dots x_n)}^{\text{posterior}} = \frac{\overbrace{f(x_1 \dots x_n | \theta)}^{\text{likelihood}} \cdot \overbrace{f(\theta)}^{\text{prior}}}{\underbrace{\int f(x_1 \dots x_n | \theta)\, f(\theta)\, d\theta}_{\substack{\text{normalizing constant} \\ \text{(does not depend on } \theta \text{ any more)}}}}$$

The posterior is a distribution.

Statistics derived from posterior

- Now you can make statements based on the posterior.
  - If you want to return one "best guess" for θ, you could use
    - max of posterior (MAP)
    - mean of posterior
  - You can construct confidence intervals: find a, b such that

$$P(\theta \in [a, b]) = 95\%.$$

Discussion

Advantages:

- easy to interpret
- natural way to incorporate prior knowledge

Disadvantages

- analytic solutions are rare, typically you have to solve computationally hard problems
- need to choose a prior