

# Advanced Topics in Software Engineering: Statistical Inference

#### Prof. Michele Loreti

## Advanced Topics in Software Engineering Corso di Laurea in Informatica (L31) Scuola di Scienze e Tecnologie



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In our context  $X_i$  will be the outcome of a simulation!

Statistical models...



## A statistical model is a set of distributions $\mathfrak{F}.$

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A nonparametric model is a set  $\mathfrak F$  that cannot be parametrised by a finite number of parameters

$$\mathfrak{F} = \left\{ F \middle| F \text{ is a CDF} \right\}$$

Parametric models...



**Example.** Parametric model for data coming from a *Normal distribution*:

$$\mathfrak{F} = \left\{ f(x:\mu,\sigma) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2} \Big| \mu \in \mathbb{R}, \sigma > 0 \right\}$$

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In general a parametric model takes the form:

$$\mathfrak{F} = \left\{ f(x; heta) \middle| heta \in \Theta 
ight\}$$

where:

- $\theta$  is an unknown parameter (or vector of parameters);
- $\Theta$  is the parameter space.

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 $(X_1, Y_1), (X_2, Y_2) \dots (X_n, Y_n)$ 

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Y is called outcome/response variable/dependent variable.

The regression function is the function

$$r(x) = E(Y|X = x)$$

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Let us assume that  $r \in \mathfrak{F}$ ...

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The goal of predicting Y for a new patients based on their X values is called prediction.

If Y is *discrete* the prediction is called classification.

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Corner Stones of Inference...



#### Point Estimation

Confidence Sets

## Hypothesis Testing

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369 / 450



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The quantity of interest can be...

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The quantity of interest can be...

- a parameter in a parametric model;
- a CDF *F*;
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• . . .

By convention we denote a point to estimate of  $\theta$  by  $\hat{\theta}$ ...

- $\theta$  is a fixed, unknown quantity;
- $\hat{\theta}$  is a random variable.



Let  $X_1, \ldots, X_n$  be *n* IID data points from some distribution *F*. A point estimator  $\hat{\theta}_n$  of a parameter  $\theta$  is some function of  $X_1, \ldots, X_n$ :

$$\widehat{\theta}_n = g(X_1, \ldots, X_n)$$



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$$\mathsf{bias}(\widehat{\theta}_n) = E(\widehat{\theta}_n) - \theta$$



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A model is **unbiased** if  $E(\hat{\theta}_n) = \theta$ .



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$$\mathsf{bias}(\widehat{ heta}_n) = E(\widehat{ heta}_n) - heta$$

A model is unbiased if  $E(\hat{\theta}_n) = \theta$ .

A point estimator  $\hat{\theta}_n$  is consistent if  $\hat{\theta}_n \xrightarrow{P} \theta$ .

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## The distribution $\hat{\theta}_n$ is called the sampling distribution.

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The standard deviation of  $\hat{\theta}_n$  is called the standard error, denoted by se:

$$\mathsf{se} = \mathsf{se}(\widehat{ heta}_n) = \sqrt{\mathcal{V}[\widehat{ heta}_n]}$$



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Often it is not possible to compute the standard error but usually we can estimate it. The estimated standard error is denoted by  $\hat{se}$ .

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The quality of a point estimate is sometimes assessed by the mean squared error (MSE):

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If bias  $\rightarrow 0$  and se  $\rightarrow 0$  as  $n \rightarrow \infty$  then  $\hat{\theta}_n$  is consistent, that is  $\hat{\theta}_n \xrightarrow{P} \theta$ 

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## An estimator is asymptotically Normal if

$$\frac{\widehat{\theta}_n - \theta}{\mathsf{se}} \rightsquigarrow N(0, 1)$$



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## Mean is asymptotically Normal!

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## **Confidence Sets**



A  $1 - \alpha$  confidence interval for a parameter  $\theta$  is an interval  $C_n = (a, b)$  where

$$a = g_a(X_1, \ldots, X_n)$$
  $b = g_b(X_1, \ldots, X_n)$ 

are functions such that:

$$Pr(\theta \in C_n) \geq 1 - \alpha$$

for all  $\theta \in \Theta$ .

#### Confidence Sets Example



Consider flipping a coin for which the probability of *heads* is p. Let  $X_i$  denote the outcome of a single toss (0 or 1). Hence,  $p = Pr(X_i = 1) = E[X_i].$ 

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The  $1 - \alpha$  confidence interval for p can be computed as:

$$C_n = (\hat{p}_n - \epsilon_n, \hat{p}_n + \epsilon_n)$$
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This because  $X_1, \ldots, X_n$  have a Bernulli distribution with parameter p and that for any  $\epsilon > 0$ :

$$Pr(|\overline{X}_n - p| > \epsilon) \le 2e^{-2n\epsilon^2}$$



Suppose that  $\hat{\theta}_n \approx N(\theta, \text{se}^2)$ . Let  $\Phi$  be the CDF of a standard Normal and let  $z_{\alpha/2} = \Phi^{-1}(1 - (\alpha/2))$ , that is (where  $Z \sim N(0, 1)$ ):

$${\it Pr}({\it Z}>{\it z}_{lpha/2})\geq lpha/2$$
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Let

$$C_n = (\hat{\theta}_n - z_{\alpha/2}\hat{s}\hat{e}, \hat{\theta}_n + z_{\alpha/2}\hat{s}\hat{e})$$



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Then

$$Pr(\theta \in C_n) \to 1 - \alpha$$

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For  $1 - \alpha = 0.95$  (95% confidence interval)  $\alpha = 0.05$ ,  $z_{\alpha/2} = 1.96 \approx 2$ .

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## Normal-based Confidence Interval Example



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We know by the Central Limit Theorem that  $\hat{p}_n \approx N(p, \hat{se}^2)$  where:

$$\widehat{p}_n = \frac{1}{n} \sum_{i=1}^n X_i$$
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An approximate  $1 - \alpha$  confidence interval is:

$$\widehat{p}_n \pm z_{lpha/2} \sqrt{rac{\widehat{p}_n(1-\widehat{p}_n)}{n}}$$



## From theory to practice...



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379 / 450



### Let $X_1, \ldots, X_n \sim F$ be IID where F is a CDF on the real line.



Let  $X_1, \ldots, X_n \sim F$  be IID where F is a CDF on the real line.

We can estimate F via the empirical distribution function  $\hat{F}_n$  defined as follows:

$$\widehat{F}_n(x) = \frac{\sum_{i=1}^n I(X_i \le x)}{n}$$

where

$$I(X_i \le x) = \begin{cases} 1 & X_i \le x \\ 0 & X_i > x \end{cases}$$



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For  $T(\hat{F}_n)$  we can compute a Normal-based interval by assuming:

$$T(\widehat{F}_n) \approx N(T(F), \widehat{se})$$



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Warning: calculating se is not easy in the general case!

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#### Plug-in estimator Examples



### Let $X_1, \ldots, X_n \sim F$ be IID where F is an unknown CDF:

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382 / 450

#### Plug-in estimator Examples



Let  $X_1, \ldots, X_n \sim F$  be IID where F is an unknown CDF:

Mean:

$$\overline{X}_n = \frac{1}{n} \sum_{i}^{n} X_i$$

#### Plug-in estimator Examples



Let  $X_1, \ldots, X_n \sim F$  be IID where F is an unknown CDF:

#### Mean:

$$\overline{X}_n = \frac{1}{n} \sum_{i}^{n} X_i$$

#### Variance:

$$\widehat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \overline{X}_n)^2 \qquad S_n^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \overline{X}_n)^2$$

The two are equivalent for large values of n.

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## From theory to practice...



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383 / 450





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Suppose we want to know  $V_F(T_n)$ , the variance of  $T_n$ . This value depends on the unknown distribution function F.



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Suppose we want to know  $V_F(T_n)$ , the variance of  $T_n$ . This value depends on the unknown distribution function F.

The idea of bootstrap method is to approximate F with  $\hat{F}_n$ .

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Suppose we draw an IID sample  $Y_1, \ldots, Yd_B$  from a distribution G. By the law of large numbers we have that when  $B \to \infty$ :

$$\overline{Y}_n = \frac{1}{B} \sum_{j=1}^{B} Y_j \xrightarrow{P} E[Y]$$



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We can use sample mean  $\overline{Y}_n$  to approximate E[Y]. In a simulation we can make B as large as we like.



More generally, if h us a function with finite mean then when  $B 
ightarrow \infty$  then:

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More generally, if h us a function with finite mean then when  $B \to \infty$  then:

$$\overline{Y}_n = \frac{1}{B} \sum_{j=1}^B Y_j \xrightarrow{P} E[Y]$$

In particular:

$$\frac{1}{B}\sum_{j=1}^{B}(Y_j-\overline{Y})^2 = \frac{1}{B}\sum_{j=1}^{B}Y_j^2 - \left(\frac{1}{B}\sum_{j=1}^{B}Y_j\right)^2 \xrightarrow{P} V[Y]$$

## Bootstrap Variance Estimation

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We can approximate  $V_{\widehat{F}_n}[T_n]$  by simulation.

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387 / 450

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#### **Boostrap Variance Estimation**

- 1. Draw  $X_1, \ldots, X_n$  from F
- 2. For i = 0 to m do: Sample  $X_{i_1}^*, \dots, X_{i_n}^*$  from  $\widehat{F}_n$ Let  $T_i^* = g(X_{i_1}^*, \dots, X_{i_n}^*)$ 3. Let

$$v_{boot} = \frac{1}{m} \sum_{i=1}^{m} \left( T_i^* - \frac{1}{m} \sum_{j=1}^{m} T_j^* \right)$$







#### Warning: We are using two approximations:

$$V_F[T_n] \approx V_{\widehat{F}_n}[T_n] \approx v_{boot}$$

## From Theory to Practice



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389 / 450



# **Normal Interval:** let $\hat{se}_{boot}$ be the bootstrap estimate of the standard error

$$T_n \pm z_{\alpha/2} \widehat{se}_{boot}$$



# **Normal Interval:** let $\hat{se}_{boot}$ be the bootstrap estimate of the standard error

$$T_n \pm z_{\alpha/2} \widehat{se}_{boot}$$

#### The interval is not accurate unless $T_n$ is close to Normal.

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Let  $\theta = T(F)$  and  $\widehat{\theta_n} = T(\widehat{F}_n)$ . The pivot  $R_n = \widehat{\theta}_n - \theta$ .



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$$\theta = T(F)$$
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Let  $\widehat{\theta}_{n,1}^*,\ldots, \widehat{\theta}_{n,m}^*$  denote the bootstrap replications of  $\widehat{\theta}_n$ .



Let 
$$\theta = T(F)$$
 and  $\widehat{\theta_n} = T(\widehat{F}_n)$ . The pivot  $R_n = \widehat{\theta}_n - \theta$ .

Let  $\widehat{\theta}_{n,1}^*,\ldots, \widehat{\theta}_{n,m}^*$  denote the bootstrap replications of  $\widehat{\theta}_n$ .

Let H(r) denote the CDF of the pivot:

 $H(r) = Pr_F(R_n \leq r)$ 

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We can consider  $C_n^* = (a, b)$  where

$$a = \widehat{\theta}_n - H^{-1}\left(1 - \frac{\alpha}{2}\right)$$
 and  $b = \widehat{\theta}_n - H^{-1}\left(\frac{\alpha}{2}\right)$ 



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$$Pr(a \leq \theta \leq b)$$



We can consider  $C_n^* = (a, b)$  where

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$$Pr(a \le \theta \le b) = Pr(a - \widehat{\theta}_n \le \theta - \widehat{\theta}_n \le b - \widehat{\theta}_n)$$



We can consider  $C_n^* = (a, b)$  where

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 and  $b = \widehat{\theta}_n - H^{-1}\left(\frac{\alpha}{2}\right)$ 

$$\begin{aligned} \Pr(\mathsf{a} \leq \theta \leq \mathsf{b}) &= \Pr(\mathsf{a} - \widehat{\theta}_n \leq \theta - \widehat{\theta}_n \leq \mathsf{b} - \widehat{\theta}_n) \\ &= \Pr(\widehat{\theta}_n - \mathsf{b} \leq \mathsf{R}_n \leq \widehat{\theta}_n - \mathsf{a}) \end{aligned}$$



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$$\begin{aligned} \Pr(a \le \theta \le b) &= \Pr(a - \widehat{\theta}_n \le \theta - \widehat{\theta}_n \le b - \widehat{\theta}_n) \\ &= \Pr(\widehat{\theta}_n - b \le R_n \le \widehat{\theta}_n - a) \\ &= H(\widehat{\theta} - a) - H(\widehat{\theta} - b) \\ &= H(H^{-1}(1 - \frac{\alpha}{2})) - H(H^{-1}(\frac{\alpha}{2})) \end{aligned}$$



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$$Pr(a \le \theta \le b) = Pr(a - \hat{\theta}_n \le \theta - \hat{\theta}_n \le b - \hat{\theta}_n)$$
  
$$= Pr(\hat{\theta}_n - b \le R_n \le \hat{\theta}_n - a)$$
  
$$= H(\hat{\theta} - a) - H(\hat{\theta} - b)$$
  
$$= H(H^{-1}(1 - \frac{\alpha}{2})) - H(H^{-1}(\frac{\alpha}{2}))$$
  
$$= 1 - \frac{\alpha}{2} - \frac{\alpha}{2} = 1 - \alpha$$



We can consider  $C_n^* = (a, b)$  where

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We have that (a and b are random variables):

$$Pr(a \le \theta \le b) = Pr(a - \hat{\theta}_n \le \theta - \hat{\theta}_n \le b - \hat{\theta}_n)$$
  
$$= Pr(\hat{\theta}_n - b \le R_n \le \hat{\theta}_n - a)$$
  
$$= H(\hat{\theta} - a) - H(\hat{\theta} - b)$$
  
$$= H(H^{-1}(1 - \frac{\alpha}{2})) - H(H^{-1}(\frac{\alpha}{2}))$$
  
$$= 1 - \frac{\alpha}{2} - \frac{\alpha}{2} = 1 - \alpha$$

**Good news:**  $C_n^*$  is an exact  $1 - \alpha$  interval for  $\theta$ !

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We can consider  $C_n^* = (a, b)$  where

$$a = \widehat{\theta}_n - H^{-1}\left(1 - \frac{\alpha}{2}\right)$$
 and  $b = \widehat{\theta}_n - H^{-1}\left(\frac{\alpha}{2}\right)$ 

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**Good news:**  $C_n^*$  is an exact  $1 - \alpha$  interval for  $\theta$ ! **Bad news:** *H* is unknown!

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We can form a bootstrap estimate of H:

$$\widehat{H}(r) = \frac{1}{m} \sum_{j=1}^{m} I(R_{n,j}^* \leq r)$$

where  $R_{n,j}^* = \hat{\theta}_{n,j}^* - \hat{\theta}_n$ . We let  $r_{\beta}^*$  and  $\theta_{\beta}^*$  denote the  $\beta$  sample quantiles of  $(R_{n,1}^*, \ldots, R_{n,m}^*)$  and  $(\theta_{n,1}^*, \ldots, \theta_{n,m}^*)$ .



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An approximate  $1 - \alpha$  confidence interval  $C_n = (\widehat{a}, \widehat{b})$  is:

$$\widehat{a} = \widehat{\theta}_n - \widehat{H}^{-1}(1 - \frac{\alpha}{2}) = \widehat{\theta}_n - r_{1-\frac{\alpha}{2}}^* = 2\widehat{\theta}_n - \theta_{1-\frac{\alpha}{2}}^*$$

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**Bootstrap pivotal confidence interval**  $C_n$  is typically pointwise, asymptotic confidence interval.

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#### Bootstrap percentile interval is defined as

$$C_n = \left(\theta_{\frac{\alpha}{2}}^*, \theta_{1-\frac{\alpha}{2}}^*\right)$$

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394 / 450

# From Theory to Practice



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In our bike sharing system we have to choose among two different allocation policy P1 and P2 in terms of balanced use of resources.



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We can consider two hypothesis:

- The Null Hypothesis, *P*1 is worst than *P*2;
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- The Null Hypothesis, P1 is worst than P2;
- The Alternative Hypothesis, P1 is not worst than P2.

If we observe that performance in  $M_{P1}$  is much better than that observed in  $M_{P2}$  we reject the null hypothesis in favour of alternative hypothesis.

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Suppose that we partition the parameter space  $\Theta$  in two disjoint sets  $\Theta_0$  and  $\Theta_1$  and that we wish to test:

 $H_0: \theta \in \Theta_0$  versus  $H_1: \theta \in \Theta_1$ 



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We call:

- H<sub>0</sub> the null hypothesis;
- $H_1$  the alternative hypothesis.



Let X be a random variable and let  $\mathcal{X}$  be the range of X. We test a hypothesis by finding an appropriate subset of outcomes  $R \subseteq \mathcal{X}$  called the rejection region.



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The problem in hypothesis testing is to find an appropriate test statistic T and an appropriate cutoff value c.

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**Type I error:** we reject  $H_0$  when  $H_0$  is true.

**Type II error:** we reject  $H_1$  when  $H_1$  is true.

Possible outcomes of hypothesis testing are:

	Retain Null	Reject Null
$H_0$ is true	OK	Type I error
$H_1$ is true	Type II error	OK

Hypothesis testing... Power function, size and level of a test



#### The power function of a test with rejection region R is defined by

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

Hypothesis testing... Power function, size and level of a test



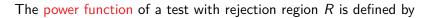
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Hypothesis testing... Power function, size and level of a test



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A test is said to have a level  $\alpha$  if its size is less than or equal to  $\alpha$ .





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$$H_0: \theta \leq \theta_0$$
 versus  $H_0: \theta > \theta_0$ 

or

$$H_0: \theta \ge \theta_0$$
 versus  $H_0: \theta < \theta_0$ 

is called one-sided test.

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Let  $\theta$  be a scalar parameter, let  $\hat{\theta}$  be an estimate of  $\theta$  and let  $\hat{se}$  be the estimated standard error of  $\hat{\theta}$ .



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The size  $\alpha$  Wald test is: reject  $H_0$  when  $|W| > z_{\alpha/2}$  where:

$$W = rac{\widehat{ heta} - heta}{\widehat{ ext{se}}}$$

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The Wald test has asymptotically size  $\alpha$ :

$$\Pr_{\theta_0}(|Z| > z_{\alpha/2}) \to \alpha$$

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as  $n \to \infty$ .

Suppose that  $\theta$  is  $\theta_{\star} \neq \theta_0$ . The power  $\beta(\theta_{\star})$  (that is the probability of correctly rejecting the null hypothesis) is (approximatively):

$$1 - \Phi\left(\frac{\theta_0 - \theta_\star}{\widehat{se}} + z_{\alpha/2}\right) + \Phi\left(\frac{\theta_0 - \theta_\star}{\widehat{se}} - z_{\alpha/2}\right)$$

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# Compute $z_{\alpha/2}$



- 1. Divide  $\alpha$  by two;
- 2. Subtract what you obtain from .5;
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# Compute $z_{\alpha/2}$

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- 1. Divide  $\alpha$  by two;
- 2. Subtract what you obtain from .5;
- 3. Find the value in the z table.

Easy approach, use table for recurrent values of  $\alpha$ :

Confidence Level	$\alpha$	$\alpha/2$	$z_{\alpha/2}$
90%	0.1	0.05	1.645
95%	0.05	0.025	1.96
98%	0.02	0.01	2.326
99%	0.01	0.005	2.576

Wald test... Comparing two means...



Let  $X_1, \ldots, X_m$  and  $Y_1, \ldots, Yd'_n$  be two independent samples from populations with means  $\mu_1$  and  $\mu_2$ , respectively.

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Let's test for null hypothesis that  $\mu_1 = \mu_2$ , that we can write as:

 $H_0: \delta = 0$  versus  $H_1: \delta \neq 0$ 

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The size  $\alpha$  Wald test reject  $H_0$  when  $|W| > z_{\alpha/2}$ 

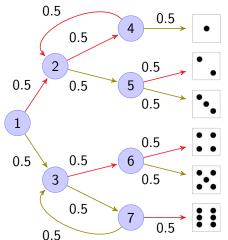
$$W = \frac{\widehat{\delta} - 0}{\widehat{se}} = \frac{\overline{X} - \overline{Y}}{\widehat{se} = \sqrt{\frac{s_1^2}{m} + \frac{s_2^2}{n}}}$$

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### Wald Test in Action...



We can use Wald test to check correctness of Knut-Yao Algorithm:





#### To be continued...

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407 / 450