Machine Learning
Performance Measures and Statistical Tests

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Program of today and next time

How to do model evaluation and model selection (for classification)

- Different performance measures
  (confusion matrix, ROC-curve and AUC),
- Statistical tests and confidence intervals,
- Test error as an estimator of the true error
  - confidence intervals
  - sample complexity
- Comparison of two/multiple classifiers - Which one is better ?
  Application of statistical tests.
- Model selection
  - using validation sets,
  - using cross-validation.

Performance Measures

Up to now

- 0-1-loss (count of errors),
- convex surrogates of the 0-1-loss $\Rightarrow$ hinge loss, logistic loss, etc.

But

- error count is not always meaningful (unbalanced classes),
- even if we use a convex surrogate for training, evaluation is done using the desired 0-1-loss.

WARNING !

IMPORTANT:	The performance of a learning method has to be evaluated using **independent data** which has **not** been used in the construction of the learning method.

It makes no sense to use the training error because we have optimized it !

Performance Measures II

The basis of all performance measures - the confusion matrix

$$\text{true pos. } tp = \sum_{i=1}^{m} \mathbb{1}_{\hat{f}(X_i)=1} \mathbb{1}_{Y_i=1}, \qquad \text{false neg. } fn = \sum_{i=1}^{m} \mathbb{1}_{\hat{f}(X_i)=-1} \mathbb{1}_{Y_i=1},$$

$$\text{false pos. } fp = \sum_{i=1}^{m} \mathbb{1}_{\hat{f}(X_i)=1} \mathbb{1}_{Y_i=-1}, \qquad \text{true neg. } tn = \sum_{i=1}^{m} \mathbb{1}_{\hat{f}(X_i)=-1} \mathbb{1}_{Y_i=-1}.$$

	positive Prediction	negative Prediction	total cases
positive cases	true positives (tp)	false negatives (fn)	$P = tp + fn$
negative cases	false positives (fp)	true negatives (tn)	$N = fp + tn$
total pred.	$\hat{P} = tp + fp$	$\hat{N} = fn + tn$	$m = N + P = \hat{P} + \hat{N}$

The confusion matrix for a binary classification problem.

Performance Measures III

The basis of all performance measures - the confusion matrix

- all other performance measures can be derived from the confusion matrix
- it makes more sense to report the confusion matrix since then everybody can build its favorite performance measure on its own
- includes all information about class probabilities $\Rightarrow$ important for cost-sensitive learning

Performance Measures IV

The standard performance measures:

Accuracy:	accuracy = (tp+tn)/(tp+fp+fn+tn)= (P*tpr + N*tnr)/(P+N), percentage of examples which are **correctly classified,** the accuracy is an estimator of $\mathrm{P}(f(X) = Y)$
Error:	error = (fp+fn)/(tp+fp+fn+tn) =(fp+fn)/(N+P), percentage of examples which are **wrongly classified,** the error is an estimator of $\mathrm{P}(f(X) \neq Y)$

True/False positive/negative rates

true positive rate: (or **sensitivity**)	tpr $=$ tp/(tp+fn)=tp/P, ratio of **pos. ex. correctly classified as pos.** the tpr is an estimator of $\mathrm{P}(f(X) = 1 \mid Y = 1)$.
false positive rate:	fpr $=$ fp/(fp+tn)=fp/N, ratio of **neg. ex. wrongly classified as pos.** the fpr is an estimator of $\mathrm{P}(f(X) = 1 \mid Y = -1)$.
false negative rate:	fnr $=$ fn/(tp+fn)=fn/P, ratio of **pos. ex. wrongly classified as neg.** the fnr is an estimator of $\mathrm{P}(f(X) = -1 \mid Y = 1)$.
true negative rate: (or **specificity**)	tnr $=$ tn/(fp+tn)=tn/N, ratio of **neg. ex. correctly classified as neg.** the tnr is an estimator of $\mathrm{P}(f(X) = -1 \mid Y = -1)$.

Performance Measures V

Useful measures in case of highly unbalanced classes:

positive predictive value	ppv $=$ tp$/$(tp+fp), ratio of **true pos. ex. classified as pos.,** ppv is an estimator of $\mathrm{P}(Y = 1 \mid f(X) = 1)$.
negative predictive value	npv $=$ tn$/$(tn+fn) ratio of **true neg. ex. classified as neg.,** npv is an estimator of $\mathrm{P}(Y = -1 \mid f(X) = -1)$.

- Measure for how often is the classifier correct when it predicts a certain class.
- In medical applications (diagnosis of diseases), in particular where the class probabilities are highly unbalanced, one uses alternatively to sensitivity and specificity, the **negative and positive predictive value**.

Performance Measures VI

Measures used in information retrieval (one class problem):

recall:	recall = tp/(tp+fn)=tp/P, (same as true positive rate) ratio of **true pos. ex. correctly classified as pos.** recall is an estimator of $\mathrm{P}(f(X) = 1 \mid Y = 1)$.
precision:	precision = tp/(tp+fp), (same as positive predictive value) ratio of **true pos. examples of all ex. classified as pos.** precision is an estimator of $\mathrm{P}(Y = 1 \mid f(X) = 1)$.

- recall: ratio of the detected relevant documents
- precision: ratio of relevant documents in the result list,

Definition

The **F-score** F is the harmonic mean of precision and recall,

$$F = \frac{2}{\frac{1}{p} + \frac{1}{r}} = \frac{2p\,r}{p + r}.$$

Performance Measures VII

Performance measures:

- different weighting of false positive and false negatives,
- differences most prominent when data is unbalanced,
- solution: assign cost to false positives and false negatives and then optimize this cost.

$\Rightarrow$ In a ROC curve one integrates all possible class probabilities in one plot.

ROC-curve and AUC

Motivation:

- find best threshold for a desired true positive/false positive rate,
- corresponds to a certain ratio of class probabilities,
- ROC= Receiver Operating Characteristic,
- developed in the 2nd world war to access the optimal threshold for radar detection systems,

ROC curve:

- change decision threshold for classifier $f : \mathcal{X} \to \mathbb{R}$,

$$\hat{f}_\theta(x) = \operatorname{sign}(f(x) + \theta),$$

- ROC-curve: plot the true positive rate versus the false positive rate by varying the discrimination threshold θ.
- naive way: compute true positive/false positive rate for all thresholds.

Formal definition:

Definition

Let $tpr(\theta)$ and $fpr(\theta)$ the true and false positive error rate of $\hat{f}_\theta$, then the ROC-function $ROC : [0,1] \to [0,1]$ is defined as

$$\mathrm{ROC}(x) = tpr\Big(fpr^{-1}(x)\Big).$$

Properties:

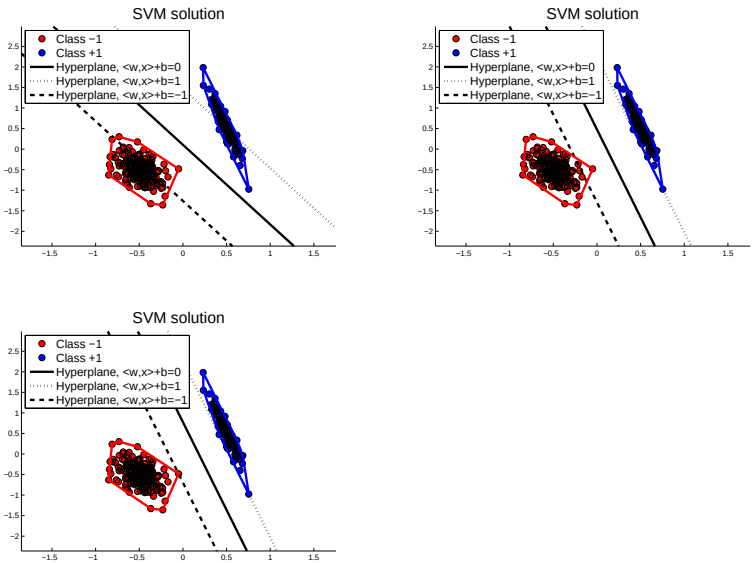
- $\mathrm{ROC}(0) = 0$ and $\mathrm{ROC}(1) = 1$,
- the ROC function is monotonically increasing,
- the ROC function can be multi-valued.

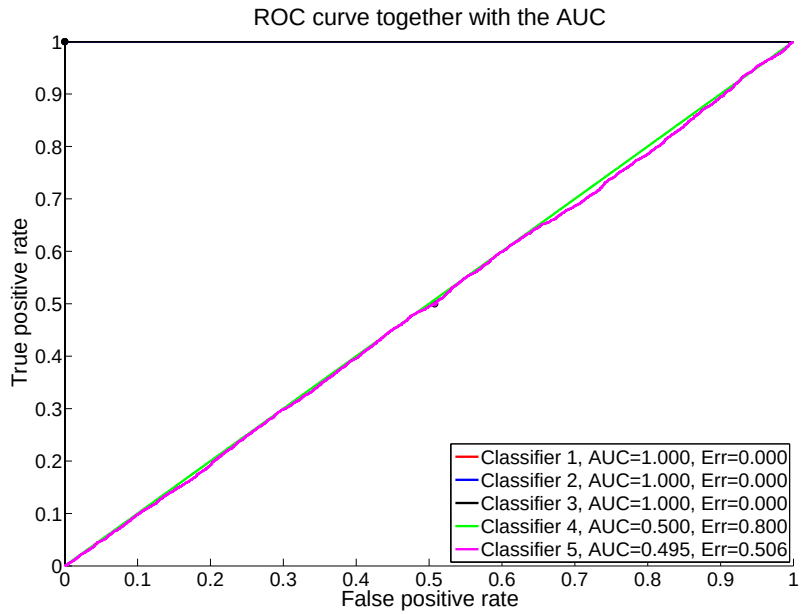
Practical computation:

1. For m test instances there are only $m+1$ possible thresholds.

- sort Y_{test} in **decreasing** order of $f(X_{\text{test}})$, and then start with $(0,0)$,
- for i=1:m
  - if $Y_{test}(i) = 1$, move up by $1/P$,
  - if $Y_{\text{test}}(i) = -1$, move right by $1/N$,
  - ties in $f(X_{\text{test}})$ require special handling.
    - ★ move up by n_+/P, where n_+ is the number of positive test points which have the same output $f(X_{\text{test}})$,
    - ★ move right by n_-/N, where n_- is the number of negative test points which have the same output $f(X_{\text{test}})$.

Ideal ROC-curve:





Left: Three linear soft margin SVM's with $C = 1, 10, 10000$, **Right:** The ROC-curve of the three SVM's (red, blue, black) together with the baseline of the (interpolated) constant classifier (green) and a random classifier (magenta). We have perfect separation of the classes - ideal ROC curve. What is the ROC curve of the constant classifier ?

Linear Interpolation of points on the ROC-curve:

- two different thresholds θ_1, θ_2,
- tpr_1, tpr_2 and fpr_1, fpr_2 are the true and false positive error rates associated to the thresholds θ_1, θ_2,
- Then the linearly interpolated true/false positive error rates

$$tpr(\lambda) = \lambda\, tpr_1 + (1-\lambda)\, tpr_2, \qquad fpr(\lambda) = \lambda\, fpr_1 + (1-\lambda)\, fpr_2,$$

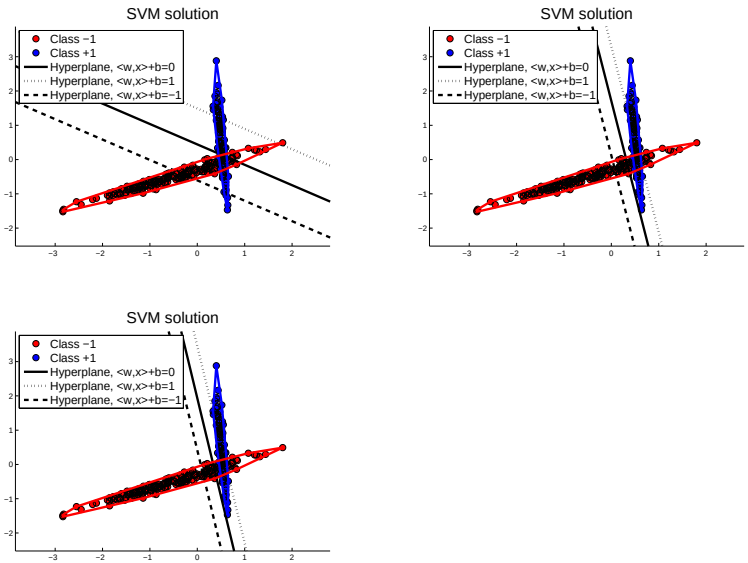
can be generated by combining $\hat{f}_{\theta_1}$ and $\hat{f}_{\theta_2}$ using a weighted coin flip,

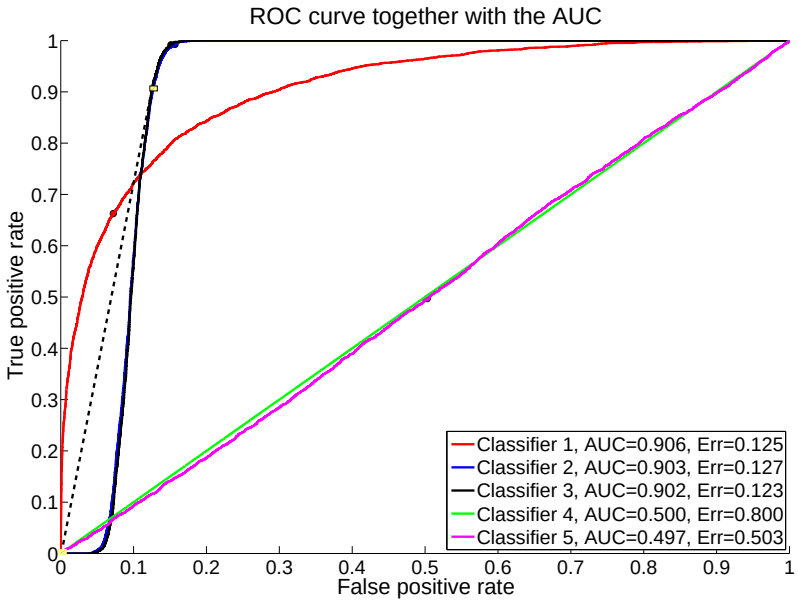
$$\forall\, \lambda \in [0,1], \qquad \hat{f}_{\lambda\theta_1+(1-\lambda)\theta_2}(x) = \begin{cases} \hat{f}_{\theta_1}(x) & \text{with probability } \lambda, \\ \hat{f}_{\theta_2}(x) & \text{with probability } 1-\lambda. \end{cases}$$

Combination of classifier

- given a set of classifiers and their ROC-curves construct the convex hull of the ROC curves by combining different classifiers.

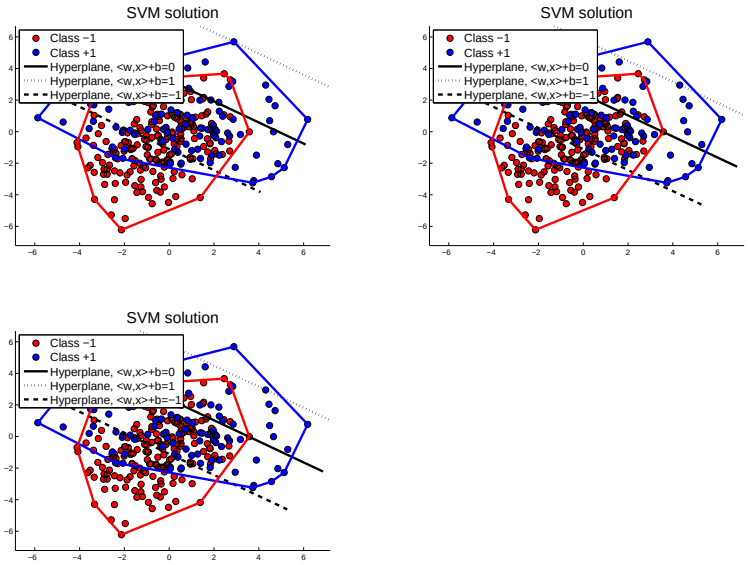
Reasonable ROC-curve:

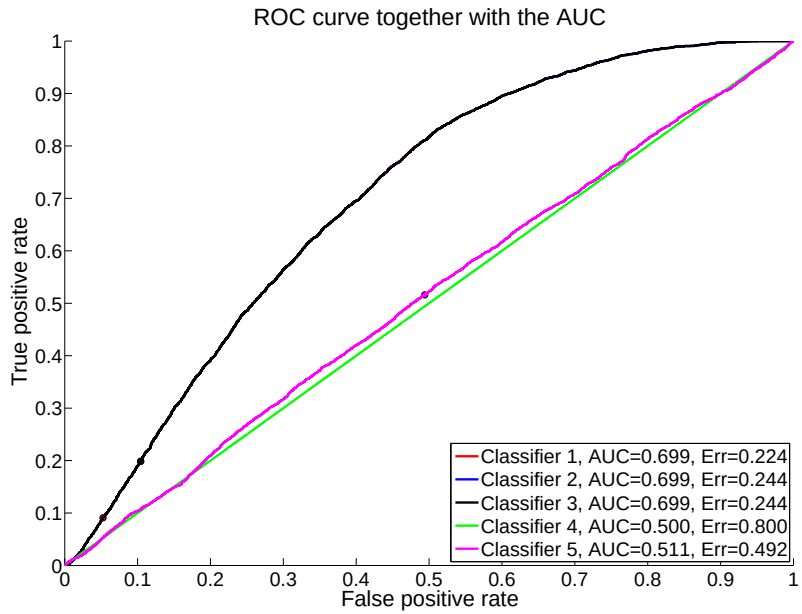




Problem is not separable anymore - ROC-curves come closer to the random baseline For small false positive error rates two of the SVM's perform worse than random. Combination of classifiers - indicated by the dotted line in the ROC plot and the yellow rectangles indicate the classifiers which are combined.

Bad ROC-curve:





A very difficult problem, where the classes are largely overlapping. The ROC-curves of the three SVM's are still above random.

ROC-curve and AUC IV

How to compare different ROC curves ?

- A ROC curve can only be said to be better than another curve if the curve always lies above the second one,
- alternative: summarize the curve with a single number,
- measure the **Area under the Curve (AUC)**,

Interpretation of the AUC:

The AUC measures basically the **quality of the ranking** of a classifier.

- all positive ex. are ranked higher than all negative ones $\Longrightarrow$ AUC$= 1$,
- all negative ex. are ranked higher than all positive ones $\Longrightarrow$ AUC$= 0$,
- If the ordering is random, then the expectation of the AUC is 0.5.

Definition

Let $f : \mathcal{X} \to \mathbb{R}$ be the original classifier and denote by $X_1^+, \ldots, X_P^+$ and $X_1^-, \ldots, X_N^-$ the set of points from positive and negative class in the test set (drawn i.i.d.). Then the **AUC** is defined as,

$$\text{AUC} = \frac{1}{NP} \sum_{j=1}^{N} \sum_{i=1}^{P} \mathbb{1}_{f(X_i^+) > f(X_j^-)}.$$

(equivalent to the 2-sample Mann-Whitney U-test or Wilcoxon rank sum test).

Proposition

Let X^+ *be distributed as* $\mathrm{P}(X|Y=1)$ *and* X^- *as* $\mathrm{P}(X|Y=-1)$*, then*

$$\mathbb{E}[\,\mathrm{AUC}] = \mathrm{P}\big(f(X^+) > f(X^-)\big).$$

Proof: Decompose test sample X_{test} into the samples $X_1^+, \ldots, X_p^+$ and $X_1^-, \ldots, X_{m-p}^-$ from positive and negative class. Note, that

$$\mathbb{E}_{\{(X_1,Y_1),(X_2,Y_2),\ldots,(X_m,Y_m)\}}[\,\mathrm{AUC}] = \mathbb{E}_p[\mathbb{E}_{\{(X_1^+,\ldots,X_p^+),(X_1^-,\ldots,X_{m-p}^-)\}}[\,\mathrm{AUC}\,|\,p]],$$

where $p \sim \mathrm{Bin}(m, \mathrm{P}(Y=1))$ and X_i^+ and X_j^- are i.i.d. samples from $\mathrm{P}(X|Y=1)$ and $\mathrm{P}(X|Y=-1)$. Thus,

$$\mathbb{E}[\,\mathrm{AUC}] = \mathbb{E}_p[\frac{1}{(m-p)p}\sum_{i=1}^{p}\sum_{j=1}^{m-p}\mathbb{E}_{X_i^+,X_j^-}\mathbb{1}_{f(X_i^+)>f(X_j^-)}\,|\,p]$$

$$= \mathbb{E}_p[\frac{1}{(m-p)p}(m-p)p\,\mathrm{P}\big(f(X^+) > f(X^-)\big)\,|\,p] = \mathrm{P}\big(f(X^+) > f(X^-)\big),$$

where we have used that the pairs X_i^+ and X_j^- are i.i.d.

Multiclass performance measures

- generalization of binary measures to the multi-class case can be difficult.
- **Class balanced error:** Let X_j^k denote the samples from class k and let N_k be the cardinality of class k in the test set, then

$$\text{error}_{\text{balanced}} = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{N_k} \sum_{j=1}^{N_k} \mathbb{1}_{f(X_j^k) \neq k}.$$

	prediction class 1	...	prediction class K	total cases
pred. class 1	$\lvert\{f(X_i) = 1, Y_i = 1\}\rvert$	...	$\lvert\{f(X_i) = K, Y_i = 1\}\rvert$	$\lvert\{Y_i = 1\}\rvert$
$\vdots$	$\vdots$		$\vdots$	$\vdots$
pred. class K	$\lvert\{f(X_i) = 1, Y_i = K\}\rvert$	...	$\lvert\{f(X_i) = K, Y_i = K\}\rvert$	$\lvert\{Y_i = K\}\rvert$
total pred.	$\lvert\{f(X_i) = 1\}\rvert$	...	$\lvert\{f(X_i) = K\}\rvert$	

Table : The confusion matrix for a multi-class problem.

Golden rule for your machine learning problem

Golden rule for solving problems:

Think about what is the correct performance measure/cost matrix for your problem and then optimize that and not something else !

Relation between test and true error

Test error = True error ?

Given the test error of the classifier on m test samples.

Questions:

- Can we make any assertions if the true error is close to the test error ?
- For a given confidence level and sample size can we give a confidence interval for the true error given the error on an independent test set ?
- For a given confidence interval and confidence level how many test samples do we need ?
- Can we test if the classifier is significantly better than random guessing ?

Statistical Test

What is a statistical test ?

- try to falsify a given null hypothesis H_0 (e.g. SVM and LDA perform equally on data set XYZ),
- define a region of rejection which if H_0 is true has probability (less than) α (where α is the significance level),
- compute a test statistic T (e.g. difference of the test errors of SVM and LDA),
- we reject the null hypothesis if T attains a value in the region of rejection otherwise we keep the null hypothesis,
  - If we reject the null hypothesis, we say that the difference between SVM and LDA is **statistically different,**
  - In the other case we can make no statement about the relation between SVM and LDA,

Formal definition of a statistical test

1. Let Θ be a set of values, then the null hypothesis H_0 is an assertion that $\theta \in \Theta_0 \subset \Theta$ whereas the alternative hypothesis H_1 is that $\theta \in \Theta \backslash \Theta_0$,
2. A significance level α is chosen (common values are 0.05 or 0.01),
3. A test statistic $T : \mathbb{R}^n \to \mathbb{R}^d$ and a region of rejection B_n is chosen, such that if the null hypothesis is true

$$\forall\, \theta \in \Theta_0, \quad \mathrm{P}_\theta\Big(T(X_n) \in B_n\Big) \leq \alpha,$$

   where X_n is a set of n sample points,
4. An experiment is done which gives X_n,
5. H_0 is rejected (one assumes that H_1 holds) if $T(X_n) \in B_n$.

Test can be **parametric** or **nonparametric**. If $\Theta = \mathbb{R}$, $H_0 : \theta \gtreqless \theta_0$ is a **one-sided test** and $H_0 : \theta = \theta_0$ is a **two-sided test**.

Statistical Test III

Confusion matrix of a statistical test:

decision\ reality	H_0 is correct	H_1 is correct
H_0 is not rejected	correct decision	type II error with prob. $1-\beta(\theta)$
H_0 is rejected	type I error (prob. $\leq \alpha$)	correct decision

Definition

Let P_θ be the probability measure with parameter θ, then the **power function** of a test is

$$\beta(\theta) = \mathrm{P}_\theta(T(X_n) \in B_n).$$

The rejection region B_n has been chosen such that,

$$\beta(\theta) \leq \alpha, \text{ for all } \theta \in \Theta_0.$$

The **type II error** is $1-\beta(\theta)$ for $\theta \in \Theta \backslash \Theta_0 \Longrightarrow$ **Goal:** high power

p-Value

Definition

Suppose that for every $\alpha \in (0,1)$ we have a test of size α with a corresponding rejection region $B_n(\alpha)$. Then, the **p-value** is defined as

$$\text{p-value} = \inf\{\alpha \mid T(X_n) \in B_n(\alpha)\}.$$

The p-value is thus **the smallest significance level α at which the null-hypothesis would be rejected.**

If we have

- a test statistic of the form $T : \mathbb{R}^n \to [0, \infty)$,
- and the rejection region is given as $[c(\alpha), \infty)$ for $c : (0,1) \to \mathbb{R}$.

and the computed test statistic has value t_{obs}, then

$$\text{p-value} = \mathrm{P}_{\theta_0}\Big(T(X_n) \geq t_{\text{obs}}\Big).$$

Example - Gauss test

- **Parametric test:** Gaussians $\mathcal{N}(\mu, \sigma^2)$ on $\mathbb{R}$ of fixed variance.
- **Null hypothesis:** $\mu = \mu_0$ and significance level α,
- The **test statistic**, is

$$T(X) = \sqrt{n} \frac{\frac{1}{n} \sum_{i=1}^{n} X_i - \mu_0}{\sigma}.$$

- Reject the null hypothesis if $|T(X)| > q_{1-\frac{\alpha}{2}}$, where q_γ is the γ-Quantile of $\mathcal{N}(0,1)$. Under the null hypothesis, $T(X) \sim \mathcal{N}(0,1)$, and thus

$$\mathrm{P}\Big(|T(X)| > q_{1-\frac{\alpha}{2}}\Big) = \alpha.$$

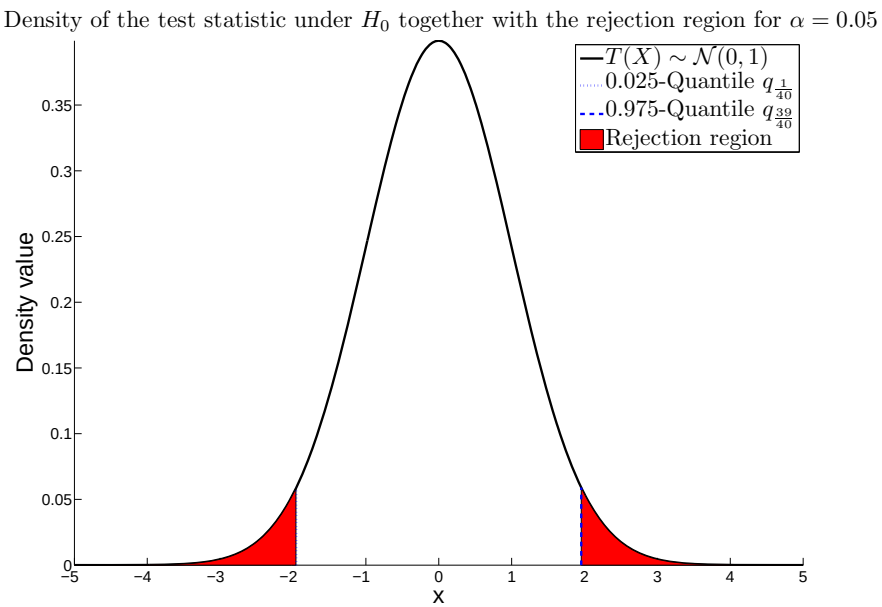
- **Power function:** $T(X) \sim \mathcal{N}(\sqrt{n}\frac{\mu-\mu_0}{\sigma}, 1)$, with

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{x^2}{2}} dx,$$

$$\beta(\mu) = \mathrm{P}_\mu\Big(|T(X)| > q_{1-\frac{\alpha}{2}}\Big)$$

$$= 1 - \Phi\Big(q_{1-\frac{\alpha}{2}} - \sqrt{n}\frac{\mu-\mu_0}{\sigma}\Big) + \Phi\Big(-q_{1-\frac{\alpha}{2}} - \sqrt{n}\frac{\mu-\mu_0}{\sigma}\Big).$$

Example - Gauss test II



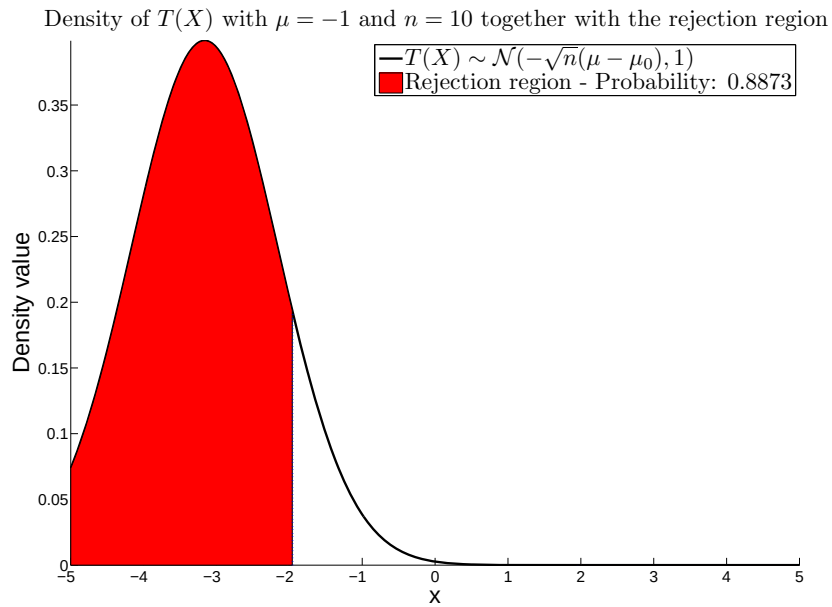


Figure : Left: The distribution of the test-statistic under the null hypothesis together with the rejection region for the significance level $\alpha = 0.05$. Right: The computation of the power of the test for $\mu = -1$ and $n = 10$.

Example - Gauss Test III

Numerical example:

- 10 samples from Gaussians with $\sigma = 2$.
- Test $H_0 : \mu = 0$ with $\alpha = 0.05 \Longrightarrow$ acceptance region: $[q_{0.025}, q_{0.975}] = [-1.96, 1.96]$.

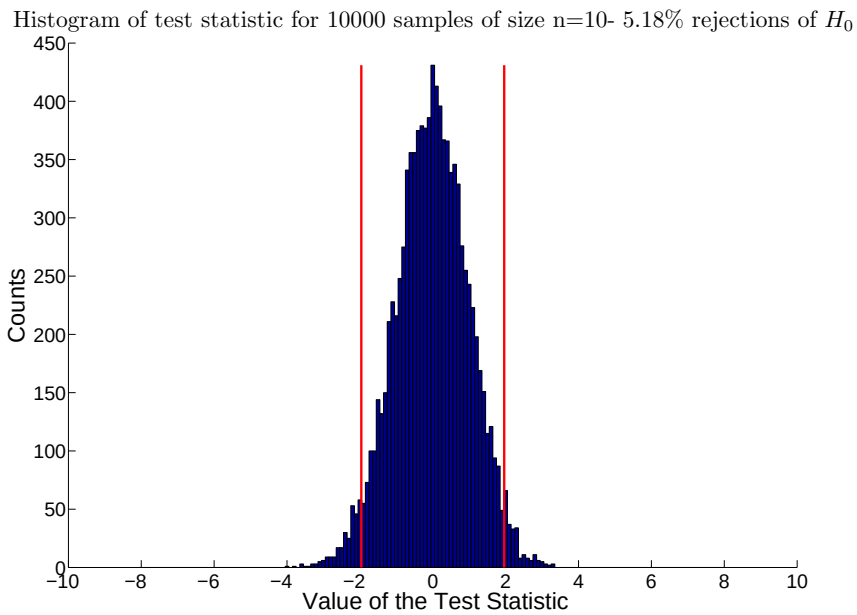
	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}
Sample 1	-2.80	-0.62	-0.37	-0.58	0.58	-0.66	0.38	-4.40	-2.04	-2.31
Sample 2	0.59	-2.67	1.43	3.25	-1.38	1.72	2.51	-3.19	-2.88	1.14

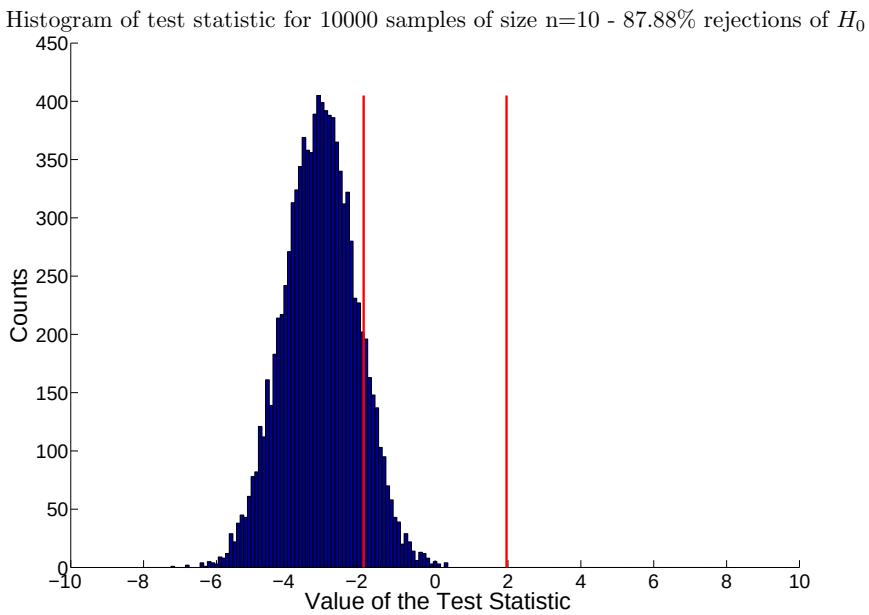
- test statistic for sample 1 is $T = -2.03$
  $\Longrightarrow$ reject null hypothesis (true: $\mu = -1$),
- test statistic for sample 2 is $T = 0.08$
  we do not reject the null hypothesis (true: $\mu = 0$).

Example - Gauss Test IV

Numerical test for α and power

- we draw 10000 samples of size 10 from the same distributions and plot histograms of the value of the test statistic
- rejections: 5.2% for the true parameter and 87.9% for the distribution with true parameter -1.





Confidence regions

Confidence regions

- Hypothesis tests are directly connected to confidence sets of estimated quantities.
- tests make sense if one wants to check some hypothesis about the data.

Definition

A **confidence interval** for a parameter $\theta \in \mathbb{R}$ is an interval $C_n = (a, b)$, where the interval borders $a = a(X_n)$ and $b = b(X_n)$ are functions of the data, such that

$$\mathrm{P}_\theta(\theta \in C_n) \geq 1 - \alpha, \quad \text{for all } \theta \in \Theta \subseteq \mathbb{R}.$$

The value $1 - \alpha$ is called the **coverage** of the confidence interval. If $\theta \in \mathbb{R}^d$ a **confidence set** (usually an ellipsoid) is a set $C_n \in \mathbb{R}^d$, which depends on the data X_n, such that

$$\mathrm{P}_\theta(\theta \in C_n) \geq 1 - \alpha, \quad \text{for all } \theta \in \Theta \subseteq \mathbb{R}^d.$$

Confidence regions II

Remark:

- the confidence set C_n is random and θ is fixed,
- it is common to use 95% intervals, that is $\alpha = 0.05$,
- there are two ways of interpreting in probabilistic terms a confidence interval.
  1. If one repeats the **same** experiment over and over again the true parameter θ will be contained in the interval in 95% of the cases. This interpretation is valid but practically usually difficult to realize, since one does an experiment once.
  2. One does k **different** experiments with data from different sources and constructs for each case a confidence interval. Then, in the limit $k \to \infty$, 95% of the constructed k confidence intervals will contain the true parameter.

Confidence regions III

- normal distributions $\mathcal{N}(\mu, \sigma^2)$ with fixed variance σ^2
- i.i.d. samples X_i from $\mathcal{N}(\mu_0, \sigma^2)$, where μ_0 denotes the true parameter.
- the empirical mean, $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} X_i$ has distribution given by $\mathcal{N}(\mu_0, \frac{\sigma^2}{n}) \Longrightarrow \sqrt{n}\frac{\hat{\mu}-\mu_0}{\sigma} \sim \mathcal{N}(0,1)$.

Thus, for every true mean $\mu \in \mathbb{R}$ and every $\alpha \in (0,1)$, we have

$$\mathrm{P}_\mu\left(\left|\sqrt{n}\frac{\hat{\mu}-\mu}{\sigma}\right| \leq q_{1-\frac{\alpha}{2}}\right) = 1-\alpha,$$

where q_γ is the γ-quantile of $\mathcal{N}(0,1)$. Thus,

$$a(X_n) = \hat{\mu} - \frac{\sigma}{\sqrt{n}} q_{1-\frac{\alpha}{2}}, \qquad b(X_n) = \hat{\mu} + \frac{\sigma}{\sqrt{n}} q_{1-\frac{\alpha}{2}},$$

are the boundaries of the confidence interval $[a(X_n), b(X_n)]$ for the parameter μ.