Introduction to Machine Learning
NPFL 054

http://ufal.mff.cuni.cz/course/npfl054

Barbora Hladká
hladka@ufal.mff.cuni.cz

Martin Holub
holub@ufal.mff.cuni.cz

Charles University,
Faculty of Mathematics and Physics,
Institute of Formal and Applied Linguistics

Lecture #5
Details on Decision Tree learning
More on evaluation and statistical tests

I. Details on Decision Tree learning – heuristic algorithms

- How to choose a good node split
- How to stop splitting and prune the tree to avoid overfitting

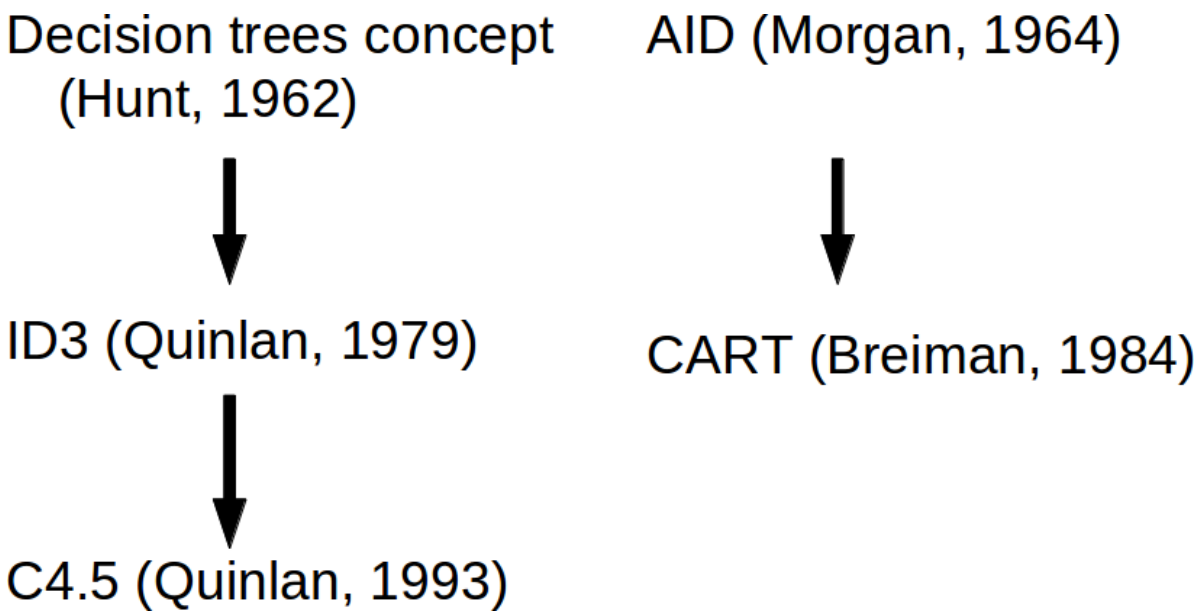
II. Remarks on evaluation

- Sample error and generalization error – a brief recap
- Cross-validation, leave-one-out, bootstrap heuristic

III. Statistical hypothesis testing

- General principles of hypothesis testing
  – classical examples, fair die, classifier accuracy
  – null hypothesis, test statistic, p-values, significance and confidence levels
  – confidence intervals
- Testing the mean of normal population
  – t-test and confidence interval for the mean, paired t-test

Historical excursion



- ID3 $\sim$ Iterative Dichotomiser
- AID $\sim$ Automatic Interaction Detection
- CART $\sim$ Classification and Regression Trees

Probably most well-known is the "C 5.0" algorithm (Quinlan), which has become the industry standard.
Packages in R: `rpart`

Building a classification tree from training data

We work with decisions on the value of only a single feature

- For each categorical feature A_j having values $Values(A_j) = \{b_1, b_2, ..., b_L\}$

$$\text{is } x_j = b_i? \text{ as } i = 1, ..., L$$

- For each categorical feature A_j

$$\text{is } x_j \in \text{a subset} \in 2^{Values(A_j)}?$$

- For each numerical feature A_j

$$\text{is } x_j \leq k?,\ k \in (-\infty, +\infty)$$

Building a classification tree from training data

Which decision is the best?

- Focus on the distribution of target class values in the associated subset of training examples.
- Then select the decision that splits training data into subsets as pure as possible.

Building a classification tree from training data

Which decision is the best?

We say a data set is **pure** (or **homogenous**) if it contains only a single class. If a data set contains several classes, then the data set is **impure** (or **heterogenous**).

Example:

$\oplus$: 5, $\ominus$: 5		$\oplus$: 9, $\ominus$: 1
heterogenous high degree of impurity		almost homogenous low degree of impurity

Building a classification tree from training data

Which decision is the best?

1. **Define** a candidate set S of splits at each node using possible decisions. $s \in S$ splits t into two subsets t_1 and t_2.
2. **Define** the node proportions $p(y_j|t), j = 1, \ldots, k$, to be the proportion of instances $\langle \mathbf{x}, y_j \rangle$ in t.
3. **Define** an **impurity measure** $i(t)$, i.e. **splitting criterion**, as a non-negative function Φ of the $p(y_1|t), p(y_2|t), \ldots, p(y_k|t)$,

$$i(t) = \Phi(p(y_1|t), p(y_2|t), \ldots, p(y_k|t)), \tag{1}$$

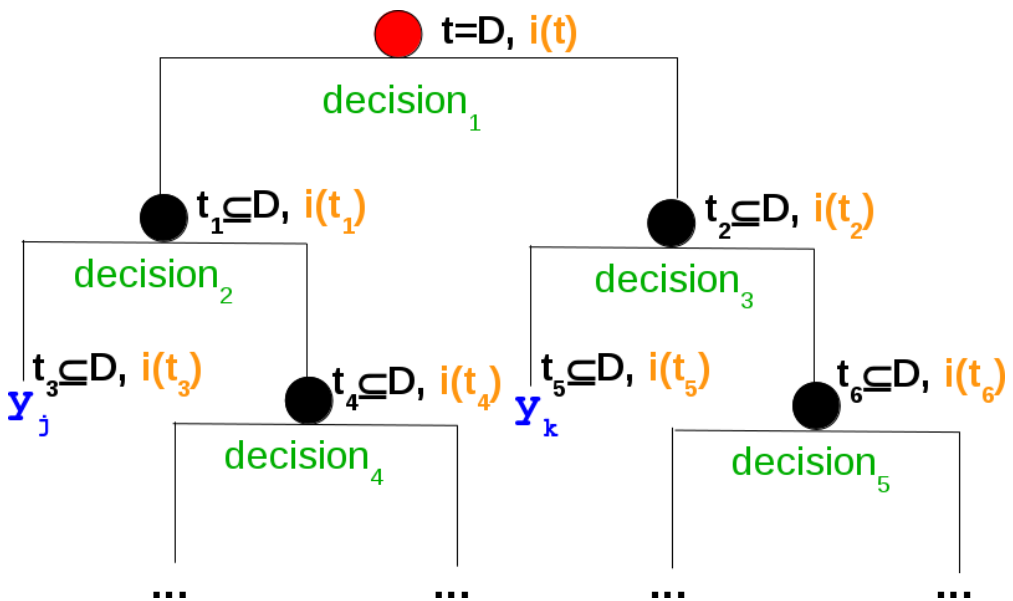
such that

- $\Phi(\frac{1}{k}, \frac{1}{k}, ..., \frac{1}{k}) = max$, i.e. the node impurity is largest when all examples are equally mixed together in it.
- $\Phi(1, 0, ..., 0) = 0, \Phi(0, 1, ..., 0) = 0, ..., \Phi(0, 0, ..., 1) = 0$, i.e. the node impurity is smallest when the node contains instances of only one class

Building a classification tree from training data

Which decision is the best?

4. **Define** the **goodness of split** s to be the decrease in impurity
   $\Delta i(s,t) = i(t) - (p_1 * i(t_1) + p_2 * i(t_2))$,
   where p_i is the proportion of instances in t that go to t_i.
5. **Find** split s^* with the largest decrease in impurity:
   $\Delta i(s^*,t) = max_{s \in S} \Delta i(s,t)$.
6. **Use** splitting criterion $i(t)$ to compute $\Delta i(s,t)$ and get s^*.



Building a classification tree from training data

Which decision is the best?

Splitting criteria – examples that are really used

- Misclassification Error – $i(t)_{ME}$
- Information Gain – $i(t)_{IG}$
- Gini Index – $i(t)_{GI}$

Building a classification tree from training data
Which decision is the best?

Splitting criteria — Misclassification Error $i(t)_{ME}$

$$i(t)_{ME} = 1 - max_{j=1,\ldots,k}\, p(y_j|t) \tag{2}$$

Example:

	$\oplus$: 0, $\ominus$: 6	$\oplus$: 1, $\ominus$: 5	$\oplus$: 2, $\ominus$: 4	$\oplus$: 3, $\ominus$: 3
$i(t)_{ME}$	$1 - \frac{6}{6} = 0$	$1 - \frac{5}{6} = 0.17$	$1 - \frac{4}{6} = 0.33$	$1 - \frac{3}{6} = 0.5$

Building a classification tree from training data
Which decision is the best?

Splitting criteria — Information Gain $i(t)_{IG}$

$$i(t)_{IG} = -\sum_{j=1}^{k} p(y_j|t) * \log p(y_j|t). \tag{3}$$

Recall the notion of entropy $H(t)$, $i(t)_{IG} = H(t)$.

$$Gain(s,t) = \Delta i(s,t)_{IG} \tag{4}$$

Building a classification tree from training data
Which decision is the best?

Splitting criteria — Gini Index $i(t)_{GI}$

$$i(t)_{GI} = 1 - \sum_{j=1}^{k} p^2(y_j|t) = \sum_{j=1}^{k} p(y_j|t)(1 - p(y_j|t)). \quad (5)$$

Interpretation

Use the rule that assigns an instance selected at random from the node to class i with probability $p(i|t)$. The estimated probability that the item is actually in class j is $p(j|t)$. The estimated probability of misclassification is the Gini index. In other words, Gini can be interpreted as expected error rate.

Building a classification tree from training data

Which decision is the best?
Splitting criteria – a comparison example

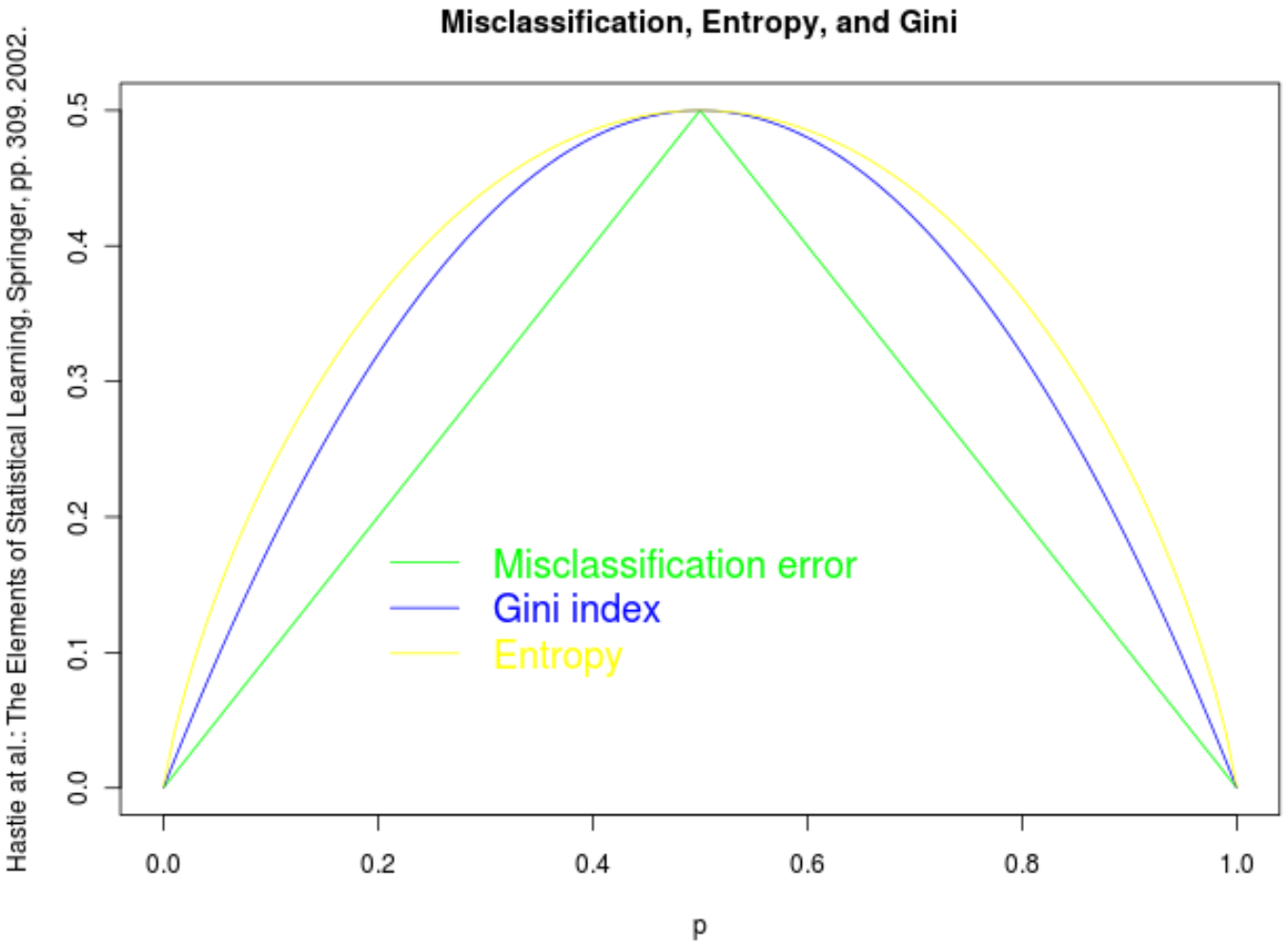
	$\oplus$: 0 $\ominus$: 6	$\oplus$: 1 $\ominus$: 5	$\oplus$: 2 $\oplus$: 4	$\oplus$: 3 $\oplus$: 3
Gini	0	0.278	0.444	0.5
Entropy	0	0.65	0.92	1.0
ME	0	0.17	0.333	0.5

For two classes ($k = 2$), if p is the proportion of the class "1", the measures are:

- Misclassification error: $1 - max(p, 1 - p)$
- Entropy: $-p * \log p - (1 - p) * \log(1 - p)$
- Gini: $2p * (1 - p)$

Building a classification tree from training data

Which decision is the best?
Splitting criteria



Building a *regression* tree from training data

Again, we work with decisions on the value of only a single feature

Which decision is the best?

Splitting criterion – usually used

- Squared Error – $i(t)_{SE}$

$$i(t)_{SE} = \frac{1}{|t|} \sum_{\mathbf{x}_i \in t} (y_i - y^t)^2,$$

where $y^t = \frac{1}{|t|} \sum_{\mathbf{x}_i \in t} y_i$.

Building decision tree from training data
When to stop the splitting process?

The recursive binary splitting is stopped when a stopping criterion is fulfilled. Then a leaf node is created with an output value.

Stopping criteria, e.g.

- the leaf node is associated with less than five training instances
- the maximum tree depth has been reached
- the best splitting criteria is not greater than a certain threshold

Building a decision tree from training data
How to avoid overfitting?

Overfitting can be avoided by

- applying a stopping criterion that prevents some sets of training instances from being subdivided,
- removing some of the structure of the decision tree after it has been produced.

Preferred strategy
Grow a large tree T_0, stop the splitting process when only some minimum node size (say 5) is reached. Then prune T_0 using some pruning criteria.

Decision trees learning parameters

2 phases of decision tree learning:

- growing
- pruning

Learning parameters are used to control these two phases:

- when to stop growing
- how much to prune the tree

... to avoid overfitting and improve performance

Example heuristic — implementation in R
Learning parameters in `rpart()`

`rpart.control`

minsplit

- the minimum number of observations that must exist in a node in order for a split to be attempted

cp

- complexity parameter, influences the depth of the tree

... and others, see `?rpart.control`

T: try to set different `cp` and `minsplit` values in the M1 model learning and observe the resulting tree

cp parameter

Any split that does not decrease the **relative training error** by a factor of cp is not attempted

$\Rightarrow$ That means, the learning algorithm measures for each split how it improves the tree relative error and if the improvement is too small, the split will not be performed.

Relative error is the error relative to the misclassification error (without any splitting relative error is 100%)

How to choose the optimal cp value?

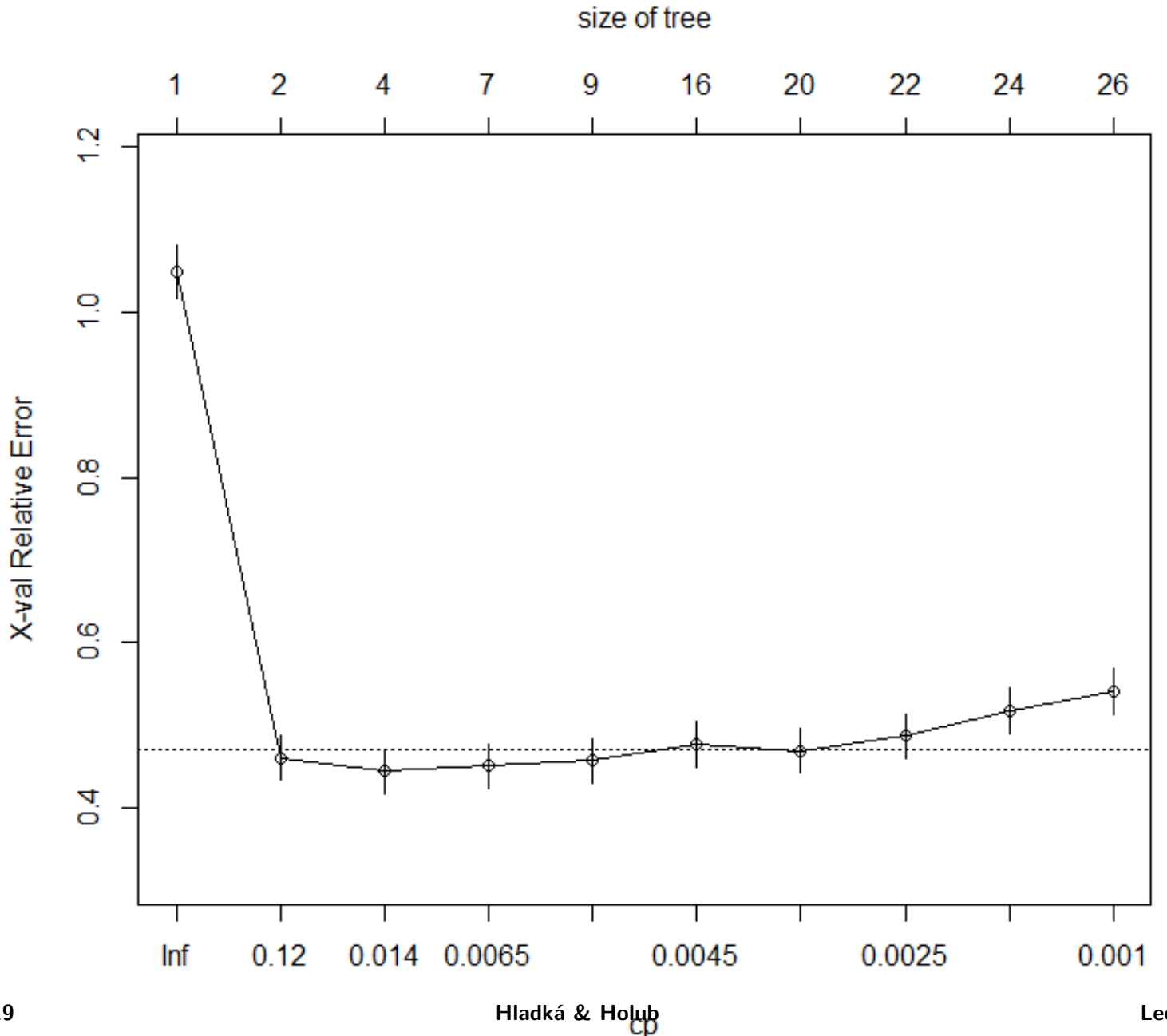
```
> m = rpart(profits ~ category + sales + assets + marketvalue,
            data=F[data.train, 1:8], cp=0.001)
> m$cptable
            CP nsplit rel error    xerror       xstd
1  0.543259557      0 1.0000000 1.0482897 0.03178559
2  0.027162978      1 0.4567404 0.4607646 0.02673551
3  0.007042254      3 0.4024145 0.4446680 0.02640028
4  0.006036217      6 0.3762575 0.4507042 0.02652763
5  0.005030181      8 0.3641851 0.4567404 0.02665301
6  0.004024145     15 0.3279678 0.4768612 0.02705703
7  0.003018109     19 0.3118712 0.4688129 0.02689795
8  0.002012072     21 0.3058350 0.4869215 0.02725122
9  0.001006036     23 0.3018109 0.5171026 0.02780383
10 0.001000000     25 0.2997988 0.5412475 0.02821490
```

rel error relative error on training data

xerror relative error in x-fold **cross-validation**

xstd standard deviation of `xerror` on x validation folds

How to choose the optimal cp value?



Summary of examination requirements

- Decision Trees – splitting criteria: typical heuristics
- Decision Trees – pruning and overfitting: the complexity parameter
- Decision Trees – practical use of the `rpart()` package

Fundamentals of classifier evaluation

Definition (Empirical and sample error)

Given a sample set S, the **empirical error** (aka *observed error*) of classifier $\hat{f}$ is the observed number of errors that $\hat{f}$ does on S.

The **sample error** of hypothesis $\hat{f}$ with respect to target function f and data sample S is the proportion of examples that $\hat{f}$ misclassifies

$$\text{error}_S = \frac{1}{n} \sum_{x \in S} \delta(f(x) \neq \hat{f}(x))$$

where

- $n = |S|$ is the sample size
- $f(x)$ is the true classification of example x
- $\hat{f}(x)$ is the predicted class of example x
- $\delta(f(x) \neq \hat{f}(x))$ is 1 if $f(x) \neq \hat{f}(x)$, and 0 otherwise.

Sample error and generalization error

Definition (Generalization error)

The **generalization error** (aka *true error*) of hypothesis $\hat{f}$ with respect to target function f and distribution $\mathcal{D}$ is the probability that $\hat{f}$ will misclassify an instance drawn randomly according to $\mathcal{D}$.

$$\text{error}_{\mathcal{D}} = \Pr_{x \in \mathcal{D}} \left\{ \delta(f(x) \neq \hat{f}(x) \right\}$$

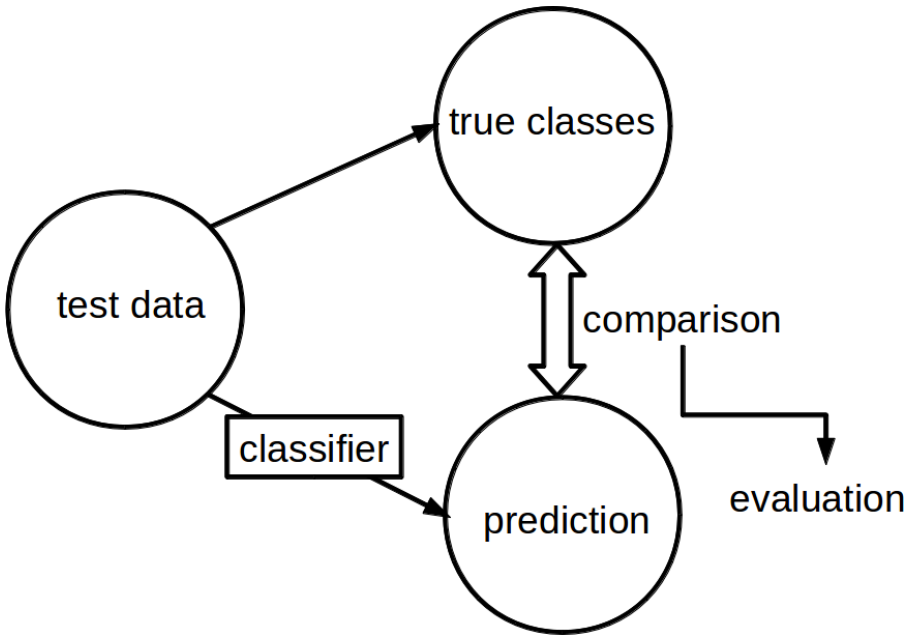
Generalization error – how to estimate?
Typically, the generalization error is not an observable quantity because the distribution $\mathcal{D}$ is usually unknown.

$\longrightarrow$ **The question is**

How well does error_S estimate $\text{error}_{\mathcal{D}}$?

Classifier evaluation

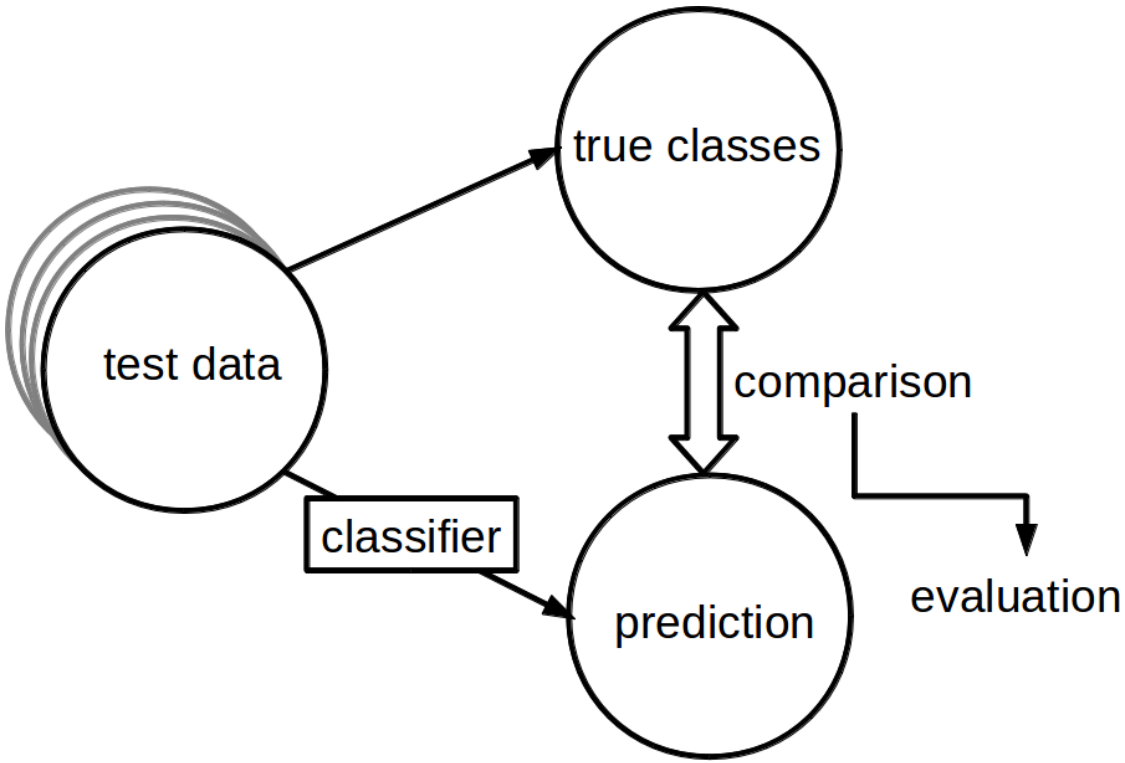
The evaluation process



Is it enough to test your classifier on one test set?
You can get a good/bad result by chance!

The ideal evaluation

The more test data, the more confident evaluation . . .

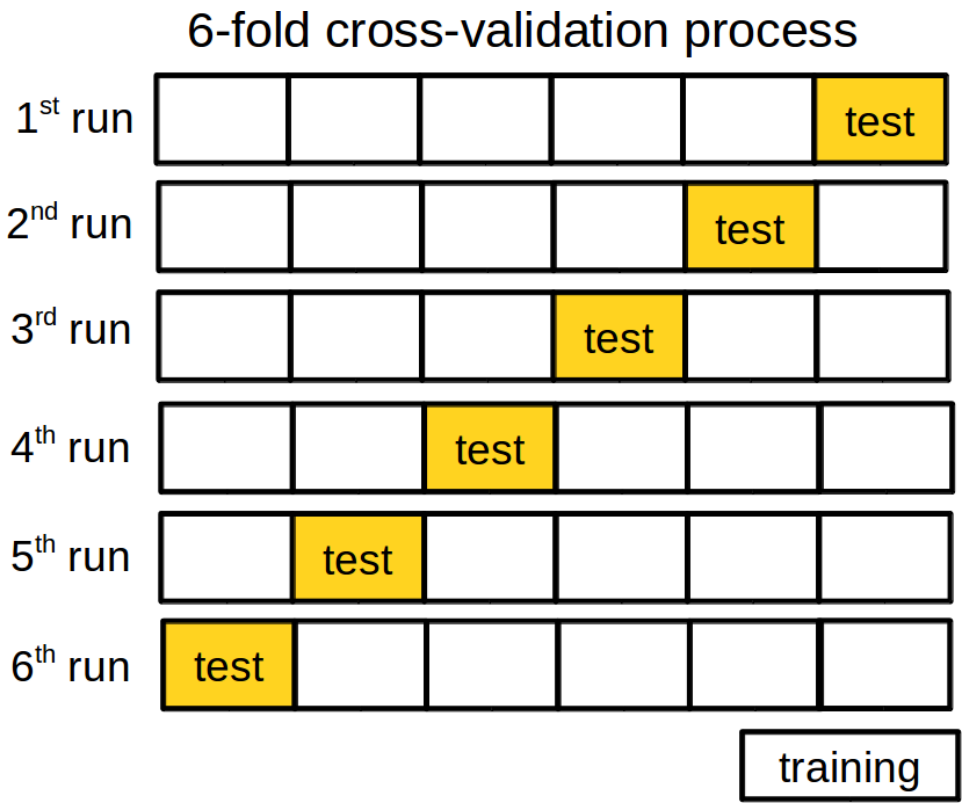


k-fold cross-validation

Development working data is partitioned into k subsets of equal (or approximately equal) size. Then you do k iterations.

In the i-th step of the iteration, the i-th subset is used as a test set, while the remaining parts form a training set.

Example



Using k-fold cross-validation: Which k is the best?

The goal: get a good estimate of generalization error

$\Rightarrow$ low bias: not to underestimate, nor overestimate

$\Rightarrow$ low variance: low sensitivity to the data sample

Small k (k close to 2)

$\longrightarrow$ small training sets, error rate tends to be overestimated

Large k (up to the data set size)

$\longrightarrow$ could be computationally demanding = main practical problem

$\longrightarrow$ small test sets, training sets are almost identical

$\longrightarrow$ low bias, but high variance

Heuristic recommendation: cca $5 \leq k \leq 10$

$\longrightarrow$ moderate bias, moderate variance, moderate computational cost

$\longrightarrow$ has been empirically shown to yield good error rate estimates

Stratified cross-validation – each class should be represented in roughly the same proportion as in the entire data set

$\longrightarrow$ if data sets are small, the risk of purely ramdom split should be avoided

Leave-one-out cross-validation (LOOCV)

Extreme case: $k = n$, where n is the size of the development data set
$\longrightarrow$ leave-one-out method (LOOCV)

Advantages

- using maximum training sets $\rightarrow$ low bias
- no randomness in data splitting

Disadvantages

- training sets are almost identical(!) $\rightarrow$ high variance of the estimate
  – variance is high, because LOOCV averages the outputs of n models that are highly positively correlated with each other
  – high variance is the reason why k-fold CV with moderate k often gives more accurate estimates of the test error than does LOOCV
- may be (typically) too time-consuming
- similar class distribution in training and test data is not guaranteed
  – The extreme case: 50 % class A, 50 % class B. Then the trivial MFC classifier has true error 50 %, BUT the LOOCV error estimate is 100 % (!).

Recommended evaluation procedure

Typically, use k-fold cross-validation for $k = 5$ or $k = 10$ for estimating the performance (accuracy, etc.)

Then compute

- the mean value of performance estimate
- standard deviation
- confidence intervals

Report mean values of performance estimates and their standard deviations, or (better) 95 % confidence intervals around the mean.

A simple sampling method

Motivation: When the total number of examples is very small (≤ 50), even the leave-one-out method becomes unreliable.

- repeat 2-fold cross-validation (e.g. 100 times)
- it has been shown that the average quality of estimation is better than the leave-one-out method

Bootstrapping principle

Bootstrap sampling – generating different training subsets

- New data sets $D_1, \ldots, D_K$ are drawn from an original data set D *with replacement*, each of the same size as the original $|D| = n$.

- Then in the i-th step of the iteration, D_i is used as a training set, while all the other examples $\mathbf{x} \in D \setminus D_i$ form the actual test set.

How many examples will appear in the bootstrap samples?

- The probability that we pick an instance is $1/n$, and the probability that we do not pick an instance is $1 - 1/n$. The probability that we do not pick an instance after n draws is $(1 - 1/n)^n \approx e^{-1} \doteq 0.368$.

- It means that for training the system will not use 36.8 % of the data, and thus the error estimate will be rather pessimistic.

A simple bootstrap heuristic

- Suppose a development data set of n examples
- An optimistic error rate e_ℓ of the model is obtained by building and testing on all available examples
  - Train a model using all n examples

  – Get training error = optimistic estimate e_ℓ.
- A pesimistic error rate e_0 is obtained by making 200 bootstrap samples
  - Randomly select n examples with replacement and train a model
    – on average, it will be 63.2 % of the original set
  - Test the model on the examples not used in the training
    – on average, it will be 36.8 % of the original set
  - Get the test error

  – Get mean test error as an average quality = pesimistic estimate e_0.
- Finally, the error ".632 estimator" is defined as a linear combination

$$e = 0.368 \cdot e_\ell + 0.632 \cdot e_0$$

Notes

The .632 estimator can break down in overfitting situations (when e_ℓ is close to 0).

The error estimation obtained by a hundred 2-fold CV runs may be used instead of e_0.

General principles of hypothesis testing
Example 1 – historical

Lady tasting tea – a famous example introduced by R. Fisher (1935)

The example is based on a real story. Fisher met a lady (Muriel Bristol) who claimed to be able to tell whether the tea or the milk was added first to a cup.

First we need to design an experiment to test her ability.
Then we need to meaningfully evaluate the result of the experiment.

Lady tasting tea – Experiment 1

The Lady is provided with 2 randomly ordered cups of tea – 1 prepared by first adding milk, the other prepared by first adding the tea. She should select the one prepared by first adding milk.

Result: The Lady selected the cup prepared by first adding milk.

What can we conclude from this experiment?

Lady tasting tea – Experiment 2

We repeat the Experiment 1 four times.

The Lady is provided with 4 pairs of 2 randomly ordered cups of tea – in each pair one cup is prepared by first adding milk, the other prepared by first adding the tea. From each pair she should select the one prepared by first adding milk.

Result: The Lady selected the 4 cups prepared by first adding milk.

What can we conclude from this experiment?

Obviously, the Experiment 2 is more convincing than the Experiment 1.

Lady tasting tea – Experiment 3 (Fisher's)

In fact, Fisher proposed to give her eight cups, four of each variety, in random order.

The Lady is provided with 8 randomly ordered cups of tea – 4 prepared by first adding milk, 4 prepared by first adding the tea. She should select the 4 cups prepared by first adding milk.

Result: The Lady selected the 4 cups prepared by first adding milk.

What can we conclude from this experiment?

Both Experiment 2 and Experiment 3 indicate that the results are probably not random. Which one is more convincing?

Fisher's experiment – random selection

Compute the probability of getting the observed result **if** the selection is random?

```
# the eight cups -- four T and four F
> cups = c(T,T,T,T,F,F,F,F)

# one million random experiments
> N = 10^6; s = numeric(N)
> for(i in 1:N) s[i] = sum(sample(cups, 4, rep=F))
> table(s)
s
     0      1      2      3      4
 14433 228323 514215 228763  14266

# the probability of getting 4 T at random is
> mean(s == 4)
[1] 0.014266
```

Or, since the statistic has hypergeometric distribution, you can simply do

```
> dhyper(4,4,4,4)
[1] 0.01428571
```

Lady tasting tea – interpretation and analysis of the experiments

How to interpret the three experiments in the framework of "statistical hypothesis testing" originally coined by R. Fisher?

- The **null hypothesis** H_0 is that the Lady has no such ability to recognize cups prepared by first adding milk.
  – null hypothesis means that she (hypothetically) does random selection
- The **test statistic** is a simple count of the number of successes in selecting the correct cups.
- The probability of getting the observed result (= the statistic value) at random is
  - 50 % in the Experiment 1
  - 6.25 % in the Experiment 2
  - 1.43 % in the Experiment 3

Rejecting the null hypothesis based on p-value

Assuming that the null hypothesis is true, the probability of getting the observed result in Experiment 3 is only 1.43 %, which *could be considered as* a good reason to **reject the null hypothesis**.

P-value
In statistical tests, p-value is the probability of obtaining a test statistic result at least as extreme as the one that was actually observed, assuming that the null hypothesis is true.

The null hypothesis is rejected if the p-value is small enough

So, we need to set a threshold for the p-value.

Test significance level α and confidence level $1 - \alpha$

Could we make wrong decision when rejecting the null hypothesis?

- Yes, in the example above there is 1.43 % chance of getting the result even if the Lady selected randomly!
- Such an error is called error of the first kind or "Type I Error".

The null hypothesis should be only rejected when an error is very unlikely

- Therefore we choose a **significance level** α as a threshold for p-value
  - α is the test's probability of incorrectly rejecting the null hypothesis
- Then the null hypothesis will be only rejected when p-value $< \alpha$
- Usually, $\alpha = 5\,\%$ or $1\,\%$ or $0.5\,\%$ or something like that
- The corresponding value $1 - \alpha$ is called **confidence level**
  - which is the probability of not doing the error of the first kind

Remember: The significance level α is a property of the test itself, while p-value is derived from the observed data!

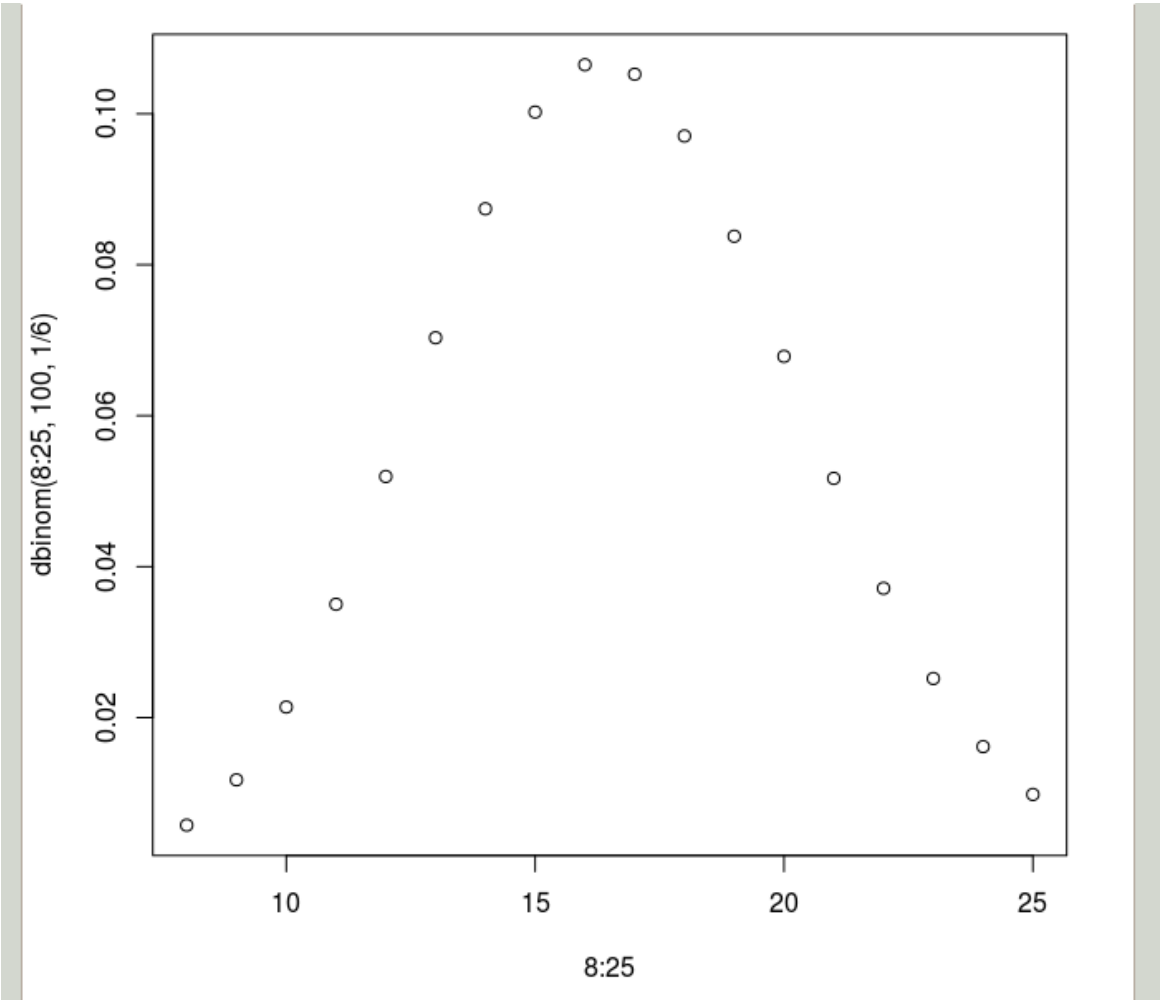
A remark on Czech terms

Česká terminologie

- significance level α = *hladina významnosti testu*
- confidence level $1 - \alpha$ = *hladina spolehlivosti testu*
- interval hodnot statistiky (e.g. t-values), které lze pozorovat s pravděpodobností (pouze) α se nazývá *kritický obor*
  $\longrightarrow$ pokud statistika padne do kritického oboru, zamítáme H_0
- α je míra rizika, že uděláme chybu I. druhu, tj. že chybně zamítneme H_0, ačkoliv ona platí
- p-value = p-hodnota = *dosažená hladina testu*

Example 2 – Is your die fair?

You have got only 10 sixes when rolling a die 100 times



Example 3 – Classifier accuracy

Example

Test sample size = 100; there are 73 correctly classified instances.
– Is it possible that classifier accuracy is 76 %?

Example 4 – men's height mean

Assume that the population of men's height is normally distributed with the known variance $\sigma^2 = 100$ and an unknown mean μ. In other words, the men's height will be represented by a continuous random variable X so that

$$X \sim \mathrm{N}(\mu = ?,\ \sigma^2 = 100).$$

We have a sample of $n = 10$ men's heights:

```
> observation
 [1] 174.7 178.0 195.9 181.0 181.6 197.5 184.9 167.6 173.4 175.8
```

Are we able to reliably estimate the mean of the population?

The best estimate is given by the **sample mean**:

```
> mean(observation)
 [1] 181.04
```

Why do you believe that this estimate is the best one?
How confident are you about the estimated mean?

Men's height mean – test statistic distribution

The sample average $\bar{x} = \frac{1}{n}\sum x_i$ will be used as a **test statistic**.

- What is the distribution of the average represented by the random variable $\bar{X}$ when we randomly sample the population?

Theorem

If $X_1, \ldots, X_n$ are independent and have the same distribution $\mathrm{N}(\mu, \sigma^2)$, then

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \quad \text{has the distribution} \quad \mathrm{N}\left(\mu, \frac{\sigma^2}{n}\right).$$

When we formulate a hypothesis about the population mean, we will know the hypothetical distribution of the statistic. Hence, we will be able to compute the probability of the observed statistic.

Men's height mean – first example hypothesis

Let us consider the following null hypothesis about the populatin mean
$H_0 : \mu = 190$.

Under that assumption the distribution of the sample average is
$\bar{X} \sim \mathrm{N}(\mu = 190, \sigma^2 = 100/10)$. (orig. σ^2 is divided by the averaged sample size)

Then, what is the probability that $\bar{X} \leq 181.04$?

The answer is 0.23 %.

```
> pnorm(181.04, 190, sqrt(10))
[1] 0.00230278
>
```

Similarly, the probability that $\bar{X} \geq 198.96$ is also 0.23 %.

Conclusion
Assuming that the null hypothesis is true, the probability of obtaining the test statistic $\bar{x}$ as extreme or more extreme as the one that was actually observed is only 0.46 % (= the p-value). Hence, with the significance level $\alpha = 5\,\%$ we will reject the hypothesis.

Men's height mean – second example hypothesis

Let us consider the following null hypothesis about the populatin mean
$H_0 : \mu = 180$.

Under that assumption the distribution of the sample average is
$\bar{X} \sim \mathrm{N}(\mu = 180, \sigma^2 = 100/10)$. (orig. σ^2 is divided by the averaged sample size)

Then, what is the probability that $\bar{X} \geq 181.04$?

The answer is 37.1 %.

```
> 1 - pnorm(181.04, 180, sqrt(10))
[1] 0.3711244
>
```

Similarly, the probability that $\bar{X} \leq 178.96$ is also 37.1 %.

Conclusion
We will not reject the hypothesis. Assuming that the null hypothesis is true, the probability of obtaining the test statistic $\bar{x}$ as extreme or more extreme as the one that was actually observed is 74.2 %. If we rejected the hypothesis, we would take the 74.2 % risk of doing the error of the first kind.

Men's height mean – confidence interval

Obviously, hypothesized values of μ that are relatively close to the observed $\bar{x}$ *would not be rejected*. On the other hand, values that are too far from the observed $\bar{x}$ *would be rejected*.

Question: What is the interval of all possibly hypothesized values of μ that would NOT be rejected?

- to determine this interval you need to know or choose a required significance level α
- this interval is called **confidence interval** for the population mean with the confidence level $1 - \alpha$

Statistical tests – first little summary

Statistical tests are used to test a hypothesis about a population

Always we observe only a sample (often only a small one) of the population.
Then we should make a decision according to this observation.
Having the observed data we compute a test statistic.

The value of the test statistic can be

- in contradiction with the hypothesis
  $\longrightarrow$ then we **reject** the hypothesis

- NOT in contradiction with the hypothesis
  $\longrightarrow$ then we **do not reject** the hypothesis

Example 5 – Confidence interval for the mean of normal population *with known variance* σ^2

Example exercise

Given the confidence level 99 %, find the confidence interval for the men's height population mean based on the given observation. The given assumptions are:

- the men's height population variance $\sigma^2 = 100$
- the observed sample mean $\bar{x} = 181.04$
- the observed sample size $n = 10$

The confidence interval contains all possible values of the population mean that could not be rejected if hypothesized at the given confidence level.

To generally derive how to compute the confidence interval we will use standardized normal distribution and its critical values.

Expected value and variance – basic properties

For any random variables X, Y and any $a, b \in \mathbb{R}$ the following holds true:

- $\mathrm{E}(a + bX) = a + b\,\mathrm{E}X$
- $\mathrm{E}(X + Y) = \mathrm{E}X + \mathrm{E}Y$
- if X and Y are independent, then $\mathrm{E}(XY) = \mathrm{E}X\,\mathrm{E}Y$

Variance of a random variable is defined by

$$\operatorname{var} X = \mathrm{E}(X - \mathrm{E}X)^2.$$

If a random variable X has finite variance, then the following holds true:

- $\operatorname{var} X = \mathrm{E}X^2 - (\mathrm{E}X)^2$
- $\operatorname{var}(a + bX) = b^2 \operatorname{var} X$
- $\sqrt{\operatorname{var}(a + bX)} = |b| \sqrt{\operatorname{var} X}$

Standardized random variable

Definition

If a random variable X has non-zero finite variance, then $Z = \dfrac{X - \mathrm{E}X}{\sqrt{\mathrm{var}\, X}}$ is called *standardized* random variable.

Note: If Z is standardized, then $\mathrm{E}Z = 0$ and $\mathrm{var}\, Z = 1$.

Standardized normal distribution – notation

If $X \sim \mathrm{N}(\mu, \sigma^2)$ then standardized variable $Z = \dfrac{X - \mathrm{E}X}{\sqrt{\mathrm{var}\, X}} = \dfrac{X - \mu}{\sigma}$ has the distribution $\mathrm{N}(0, 1)$. Usual notation for standardized normal distribution is

- φ for the density,
- Φ for the distribution function,
- Φ^{-1} for the quantile function.

Quantiles and critical values

Definition

Quantile function of a random variable X is defined as

$$F_X^{-1}(\alpha) = \inf\{x : F(x) \geq \alpha\},$$

where F_X is the distribution function of X and $\alpha \in (0, 1)$.

Value $F^{-1}(\alpha)$ is called α-*quantile*.

Note: 0.5-quantile $F^{-1}(0.5)$ is called *median*.

Definition

Critical value of the standard normal distribution is defined as $z(\alpha) = \Phi^{-1}(1 - \alpha)$.

Note: If $Z \sim \mathrm{N}(0, 1)$, then

- $\Pr\{Z > z(\alpha)\} = \alpha$
- $\Pr\{|Z| > z(\alpha/2)\} = \alpha$

Computing confidence interval

Example exercise

Given the confidence level 99 %, find the confidence interval for the men's height population mean based on the given observation. The given assumptions are:

- the men's height population variance $\sigma^2 = 100$
- the observed sample mean $\bar{x} = 181.04$
- the observed sample size $n = 10$

The confidence interval contains all possible values of the population mean that could not be rejected if hypothesized at the given confidence level.

Idea of the solution

The confidence interval is a symmetric interval around the observed sample mean $\bar{x}$. Hence, we are looking for the confidence interval radius r so that the null hypothesis $H_0 : \mu = \mu_0$ is rejected if and only if $|\bar{x} - \mu_0| > r$.

Then the confidence interval will be given by $(\bar{x} - r,\ \bar{x} + r)$.

Assuming that $H_0 : \mu = \mu_0$ is valid, we have $\bar{X} - \mu_0 \sim \mathrm{N}(0, \sigma^2/n)$.

Since the significance level α, which is the probability of incorrectly rejecting the null hypothesis, is given, we should choose the confidence interval radius r so that

$$\Pr\{|\bar{X} - \mu_0| > r\} = \alpha,$$

and after standardization

$$\Pr\left\{\left|\frac{\bar{X} - \mu_0}{\sigma/\sqrt{n}}\right| > \frac{r}{\sigma/\sqrt{n}}\right\} = \alpha,$$

which means that $\dfrac{r}{\sigma/\sqrt{n}} = z(\alpha/2)$, and thus $r = \dfrac{\sigma}{\sqrt{n}}\, z(\alpha/2)$.

Therefore the confidence interval for the population mean μ is

$$\left(\bar{x} - \frac{\sigma}{\sqrt{n}}\, z(\alpha/2),\ \bar{x} + \frac{\sigma}{\sqrt{n}}\, z(\alpha/2)\right),$$

and $\Pr\left\{\bar{X} - \dfrac{\sigma}{\sqrt{n}}\, z(\alpha/2) < \mu < \bar{X} + \dfrac{\sigma}{\sqrt{n}}\, z(\alpha/2)\right\} = 1 - \alpha.$

Example 6 – testing the classifier accuracy mean

You have two models, **A** and **B**, and for each of them 10 results – accuracies obtained from 10-fold cross-validation experiment.

```
> A.acc
 [1] 0.853 0.859 0.863 0.871 0.832 0.848 0.863 0.860 0.850 0.849
> mean(A.acc)
 [1] 0.8548

> B.acc
 [1] 0.851 0.848 0.862 0.871 0.835 0.836 0.860 0.859 0.841 0.843
> mean(B.acc)
 [1] 0.8506
```

The average accuracy of **A** is 85.48 %, while the average accuracy of **B** is only 85.06 %.

Question: Is model A *really* better than model B?

Using t-distribution as the principle of t-test

What if you do NOT know the variance?

When we get k different results from the cross-validation experiment, we can assume that the values are (approximately) normally distributed. Then we use t-test.

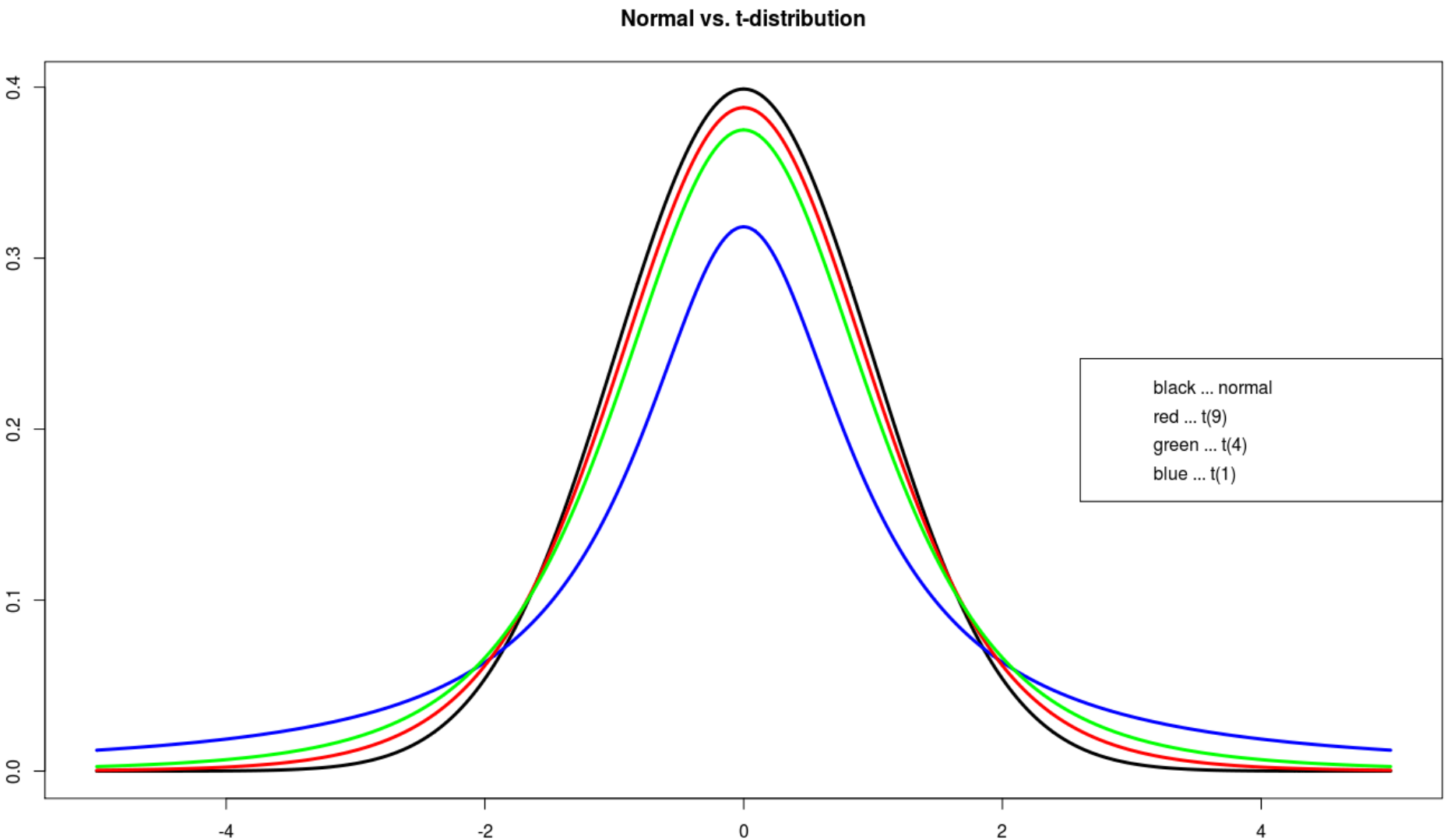
Theorem

If $x_1, \ldots, x_n$ is a random sample of size n selected from a normally distributed population, then

$$T = \frac{\bar{X} - \mu}{S}\sqrt{n} \sim t_{n-1},$$

where n is the sample size, $\bar{X}$ is the sample mean, S is the sample standard deviation, μ is the population mean, T is called t-statistic, and t_{n-1} stands for t-distribution with $n-1$ degrees of freedom.

Normal vs. t-distribution



Using t-test – practical procedure

First, compute **t-value** $T = \frac{\bar{X} - \mu}{S}\sqrt{n}$.
Then compare the t-value with the critical value $t_k(\alpha)$.

Definition

Critical value $t_k(\alpha)$ of the t-distribution t_k is defined by the equation $\Pr\{|T| \geq t_k(\alpha)\} = \alpha$, where α is the test significance level.

Therefore $\Pr\{-t_{n-1}(\alpha) < \frac{\bar{X} - \mu}{S}\sqrt{n} < t_{n-1}(\alpha)\} = 1 - \alpha$

Note: Critical value corresponds to a given significance level and determines the boundary between those samples resulting in a test statistic that leads to rejecting the null hypothesis and those that lead to a decision not to reject the null hypothesis. If the calculated value from the statistical test is greater than the critical value, then the null hypothesis is rejected in favour of the alternative hypothesis, and vice versa.

Confidence interval for the mean μ using t-test

- If $\bar{x}$ is the sample mean of a sample of the size n randomly chosen from a normally distributed population and α is a significance level, then **confidence interval** for the population mean μ is

$$\left(\bar{x} - \frac{S}{\sqrt{n}}\, t_{n-1}(\alpha),\ \bar{x} + \frac{S}{\sqrt{n}}\, t_{n-1}(\alpha)\right)$$

- The probability that the (true) population mean μ lies inside the confidence interval is equal to $1 - \alpha$, which is called **confidence level**.

$$\Pr\left\{\bar{X} - \frac{S}{\sqrt{n}}\, t_{n-1}(\alpha) < \mu < \bar{X} + \frac{S}{\sqrt{n}}\, t_{n-1}(\alpha)\right\} = 1 - \alpha$$

Example 6 – checking the confidence interval

To test if the difference between the models **A** and **B** is **statistically significant** we will check **confidence intervals** for the mean accuracy.

```
### Could the true mean of A accuracy be 0.8506?
> t.test(A.acc, mu=0.8506)
    One Sample t-test

data:  A.acc
t = 1.2195, df = 9, p-value = 0.2537
alternative hypothesis: true mean is not equal to 0.8506
95 percent confidence interval:
 0.8470088 0.8625912
sample estimates:
mean of x
   0.8548
```

We cannot reject the null hypothesis that the mean of A accuracy is equal to 0.8506. The t-test says that the true mean of A accuracy could be between 0.847 and 0.863, which is the confidence interval at the significance level $\alpha = 5\,\%$.

Similarly, you can check the confidence interval for the mean accuracy of classifier B:

```
### Could the true mean of B accuracy be 0.8548?
> t.test(B.acc, mu = 0.8548)

    One Sample t-test

data:  B.acc
t = -1.0974, df = 9, p-value = 0.301
alternative hypothesis: true mean is not equal to 0.8548
95 percent confidence interval:
 0.8419418 0.8592582
sample estimates:
mean of x
   0.8506
```

Using t-tests

When you get k different results from the cross-validation experiment, what can you conclude then?

1. **One Sample t-test**
   – to test if the mean of a (normally distributed) population is equal to a given value

2. **Paired Two-Sample t-test**
   – to test if the difference of the means of two populations is equal to zero (or to another given value)
   – assuming that the given samples contain paired individuals

Example 7 – paired t-test

Using the same input data as in Example 6

```
### Could the true mean of the difference be equal to zero?
> t.test(A.acc, B.acc, paired=T)

        Paired t-test

data:  A.acc and B.acc
t = 2.6296, df = 9, p-value = 0.02738
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 0.0005868378 0.0078131622
sample estimates:
mean of the differences
                 0.0042
```

This test says that we can reject the null hypothesis that the mean of the difference between A accuracy and B accuracy is equal to 0.

Because the paired t-test shows that the true mean of the difference could be between (approximately) 0.00058 and 0.0078, which is the confidence interval at the significance level $\alpha = 5\,\%$.

Homework exercises

Go through all examples in the presentation and make sure that you understand them

Get familiar with the hypergeometric distribution

- Compute analytically and exactly the probability distribution of the test statistic from the Example 1, Experiment 3
- Get familiar with the `dhyper()` function in R

Compute the confidence interval for men's height population mean at confidence levels 90 %, 95 %, and 99 %.

= the exercise from page 49 (Example 4)

Go through the tutorial posted for the lab session and make sure that you are able to successfully do all the exercises!

Summary of evaluation and statistical tests Examination requirements

You should understand and should be able to practically use

- sample error and generalization error
- cross-validation and LOOCV methods
- bootstrap heuristic for true error estimate
- general principles of statistical tests
  - significance and confidence levels, critical values, p-values
- confidence intervals for the mean of normal and t distributions
  - you do not have to know the proofs
- practical use of t-test for population mean, paired t-test