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

Outline

- **Decision Trees**
  — Key problems of Decision Trees learning
  — Impurity measure
  — Heuristic algorithms for building Decision Trees
  — Evaluation and tuning
  — Weak spots of Decision Trees

- **Ensemble learning and Random Forests**
  — Ensemble classifiers – a motivation exercise
  — Combining classifiers into ensembles – general scheme
  — Generating random samples by bootstrapping
  — Bagging – a simple ensemble classifier
  — Random Forests: Bootstrapping extension of Decision Trees

Learning a decision tree – key problems

Each node of a decision tree is associated with a subset of traning data

Building a decision tree means to make a hierarchical sequence of splits. Each practical algorithm must be able to efficiently decide the following key questions:

(1) **How to choose a suitable splitting condition?**

(2) **When to stop the splitting process?**

Learning a decision tree – key problems

Each node of a decision tree is associated with a subset of traning data

Building a decision tree means to make a hierarchical sequence of splits. Each practical algorithm must be able to efficiently decide the following key questions:

(1) How to choose a suitable splitting condition?

(2) When to stop the splitting process?

A practical answer to problem (1) is to employ entropy or another similar measure. Each node is defined by an associated subset of examples with a specific distribution of target values. After a split, the entropy in child nodes should decrease in comparison with entropy in the parent node.

Learning a decision tree – key problems

Each node of a decision tree is associated with a subset of traning data

Building a decision tree means to make a hierarchical sequence of splits. Each practical algorithm must be able to efficiently decide the following key questions:

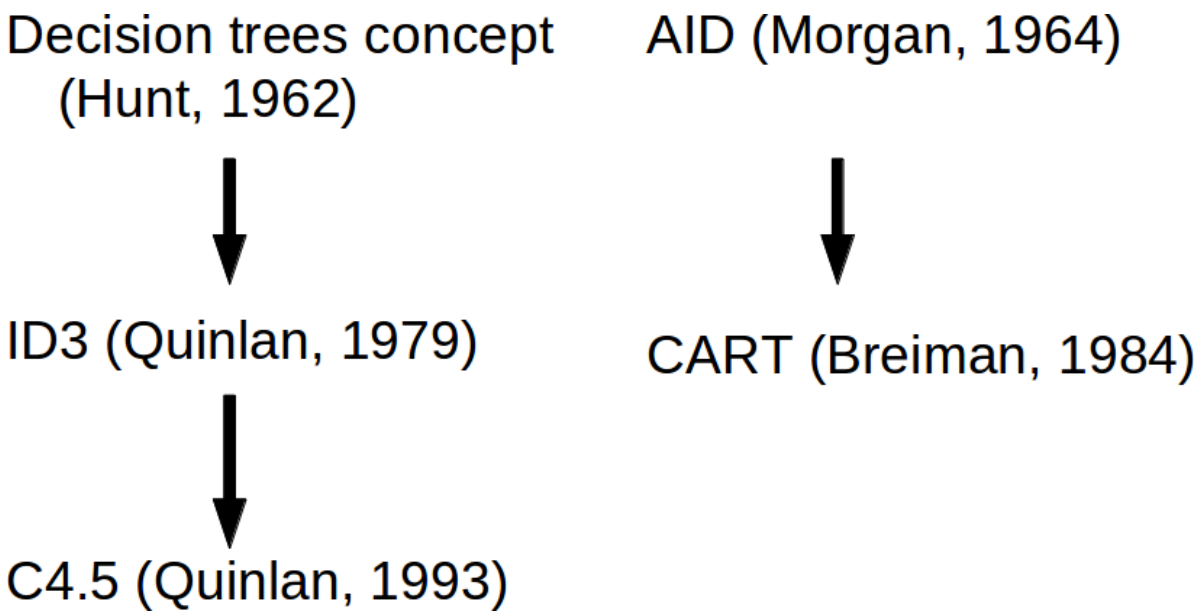
(1) How to choose a suitable splitting condition?

(2) When to stop the splitting process?

A practical answer to problem (1) is to employ entropy or another similar measure. Each node is defined by an associated subset of examples with a specific distribution of target values. After a split, the entropy in child nodes should decrease in comparison with entropy in the parent node.

The splitting process should be duly stopped just to not produce model that overfits the training data. To avoid overfitting, practical implementations usually use pruning after building a relatively deep tree.

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**).

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 $p(y_1|t), p(y_2|t), \ldots, p(y_k|t)$,

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

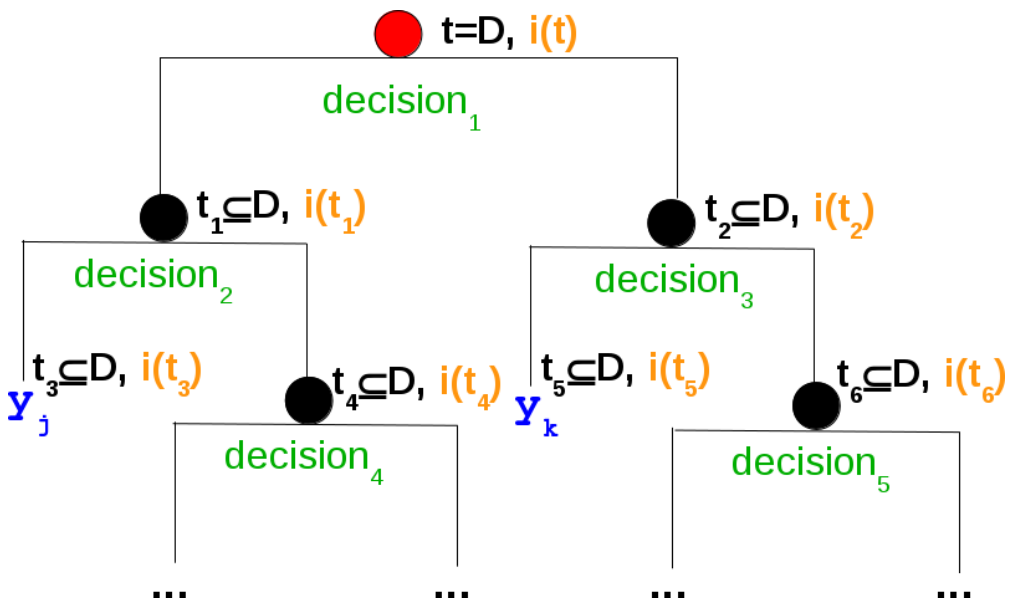
such that

- $\Phi(\frac{1}{k}, \frac{1}{k}, ..., \frac{1}{k}) = max$, 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 $i(t)_{ME}$

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

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 $i(t)_{GI}$

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

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

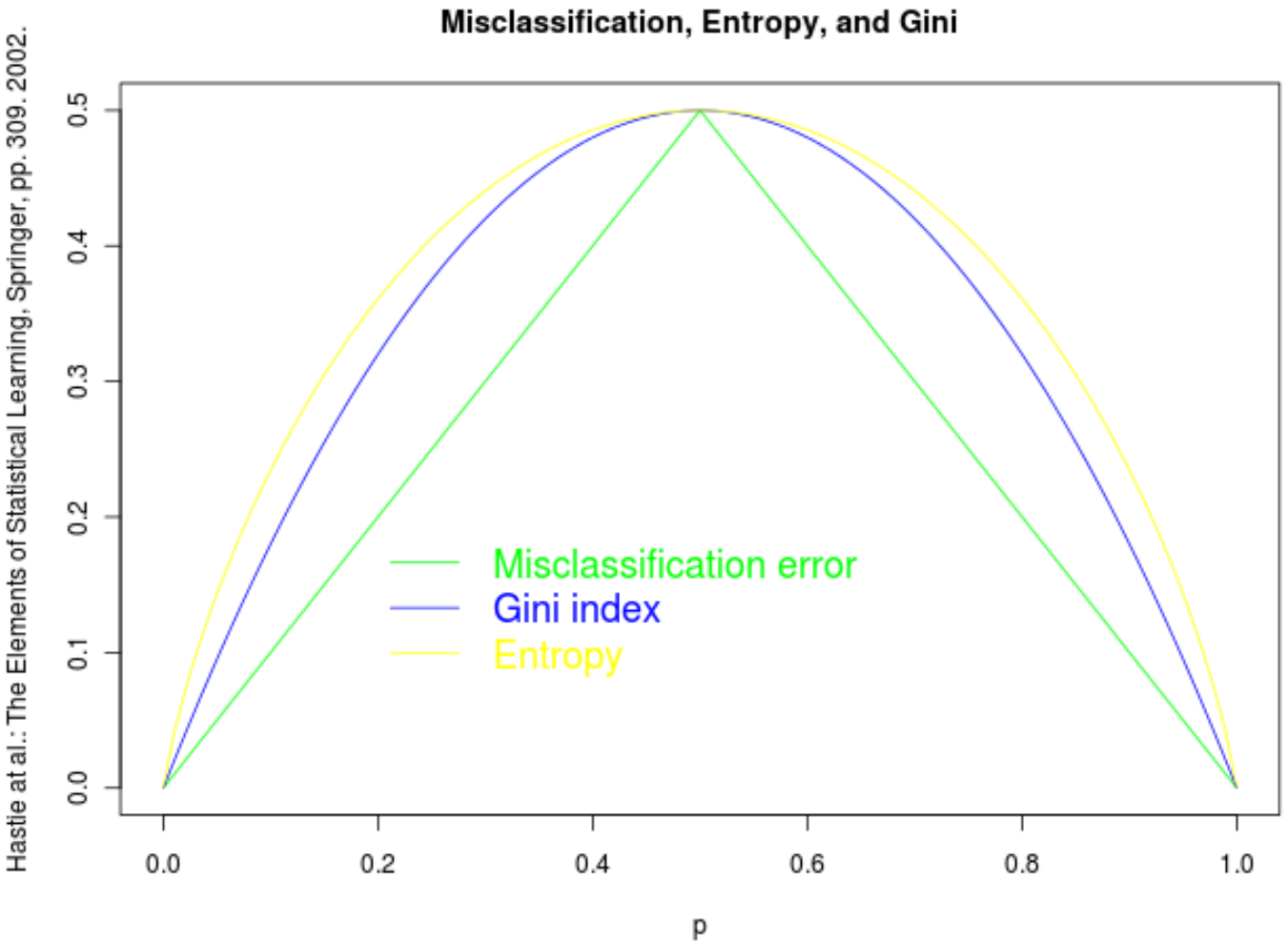
	$\oplus$: 0 $\ominus$: 6	$\oplus$: 1 $\ominus$: 5	$\oplus$: 2 $\oplus$: 4	$\oplus$: 3 $\oplus$: 3
Gini	0	0.278	0.444	0.5
Entropy	0	0.65	0.92	1.0
ME	0	0.17	0.333	0.5

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:

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

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

Decision trees — implementation in R

There are two widely used packages in R

- `rpart`
- `tree`

The algorithms used are very similar.

References

- An Introduction to Recursive Partitioning Using the RPART Routines
  by Terry M. Therneau, Elizabeth J. Atkinson, and Mayo Foundation
  (available online)
- *An Introduction to Statistical Learning with Application in R*
  Chapters 8.1, 8.3.1, and 8.3.2
  by Gareth James, Daniela Witten, Trevor Hastie and Rob Tibshirani
  (available online)
- R packages documentation — `rpart`, `tree`
  (available online)

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

Meaning of the cp parameter

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

⇒ 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?

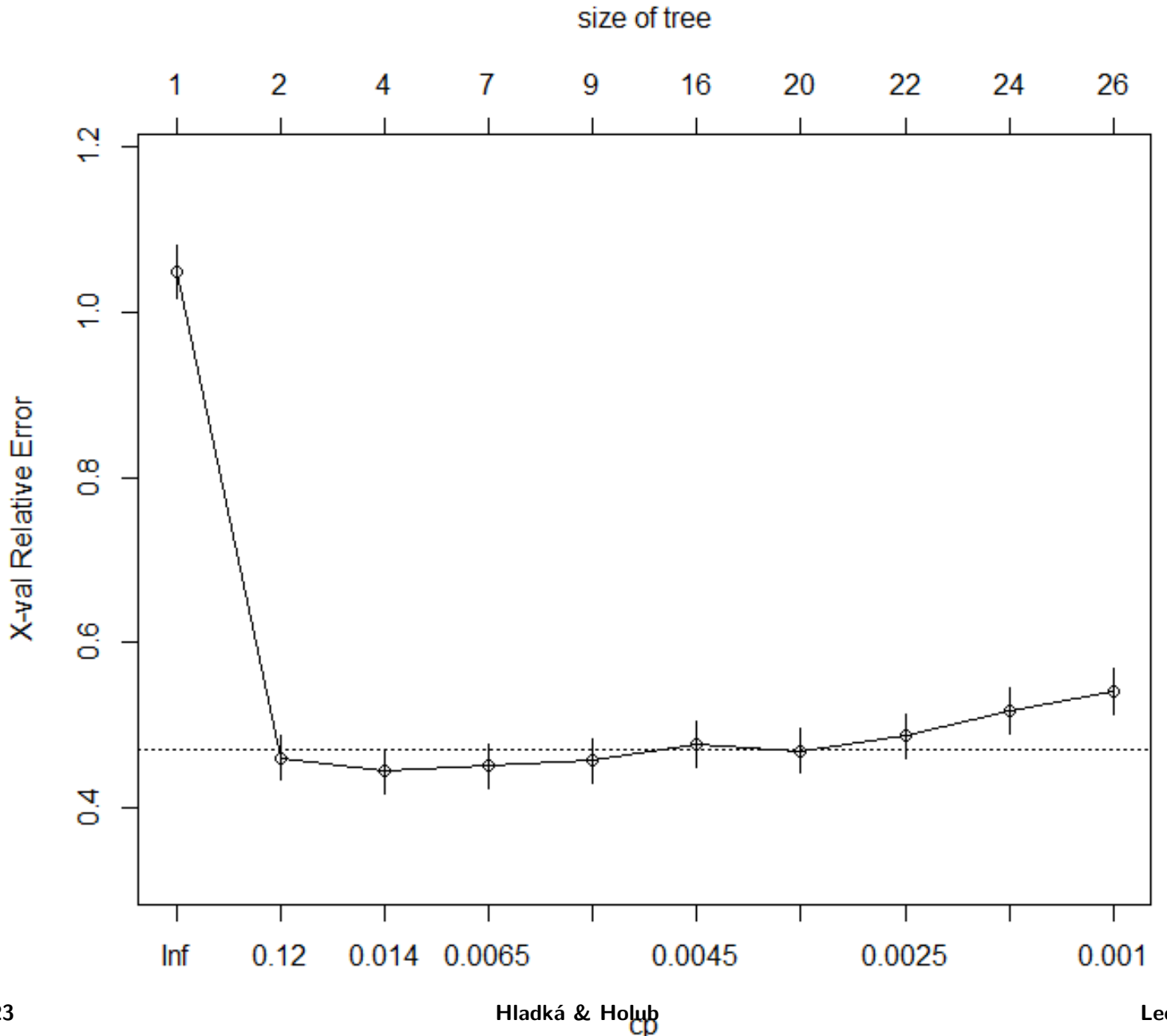
```
> m = rpart(profits ~ category + sales + assets + marketvalue,
            data=F[data.train, 1:8], cp=0.001)
> m$cptable
            CP nsplit rel error    xerror       xstd
1  0.543259557      0 1.0000000 1.0482897 0.03178559
2  0.027162978      1 0.4567404 0.4607646 0.02673551
3  0.007042254      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?



Decision Trees – weak spots

- **data splitting**
  — deeper nodes can learn only from small data portions

- **sensitivity to training data set (unstable algorithm)**
  — learning algorithm is called unstable if small changes in the training set cause large differences in generated models

Ensemble classifiers – a motivation exercise

Consider the following task – we have a binary classification problem and a number of predictors, each with error less than 0.5. Will the resulting majority voting ensemble have an error lower than the single classifers?

Ensemble classifiers – a motivation exercise

Consider the following task – we have a binary classification problem and a number of predictors, each with error less than 0.5. Will the resulting majority voting ensemble have an error lower than the single classifers?

Depends on the *accuracy* and the *diversity* of the base learners!

Ensemble classifiers – a motivation exercise

Consider the following task – we have a binary classification problem and a number of predictors, each with error less than 0.5. Will the resulting majority voting ensemble have an error lower than the single classifers?

Depends on the *accuracy* and the *diversity* of the base learners!

Illustrative example

Particular settings – assume that you have

- 21 classifiers
- each with error $p = 0.3$
- their outputs are *statistically independent*

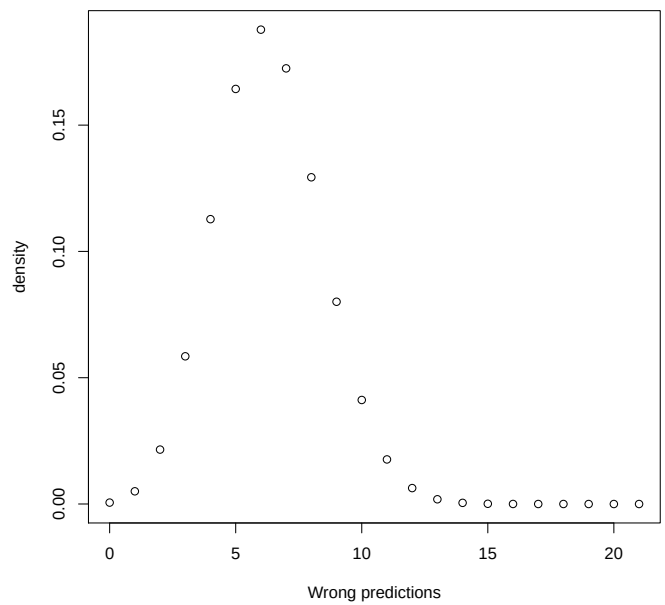
Compute the error of the ensemble under these conditions!

Solution of the exercise

How many classifiers will produce error output?

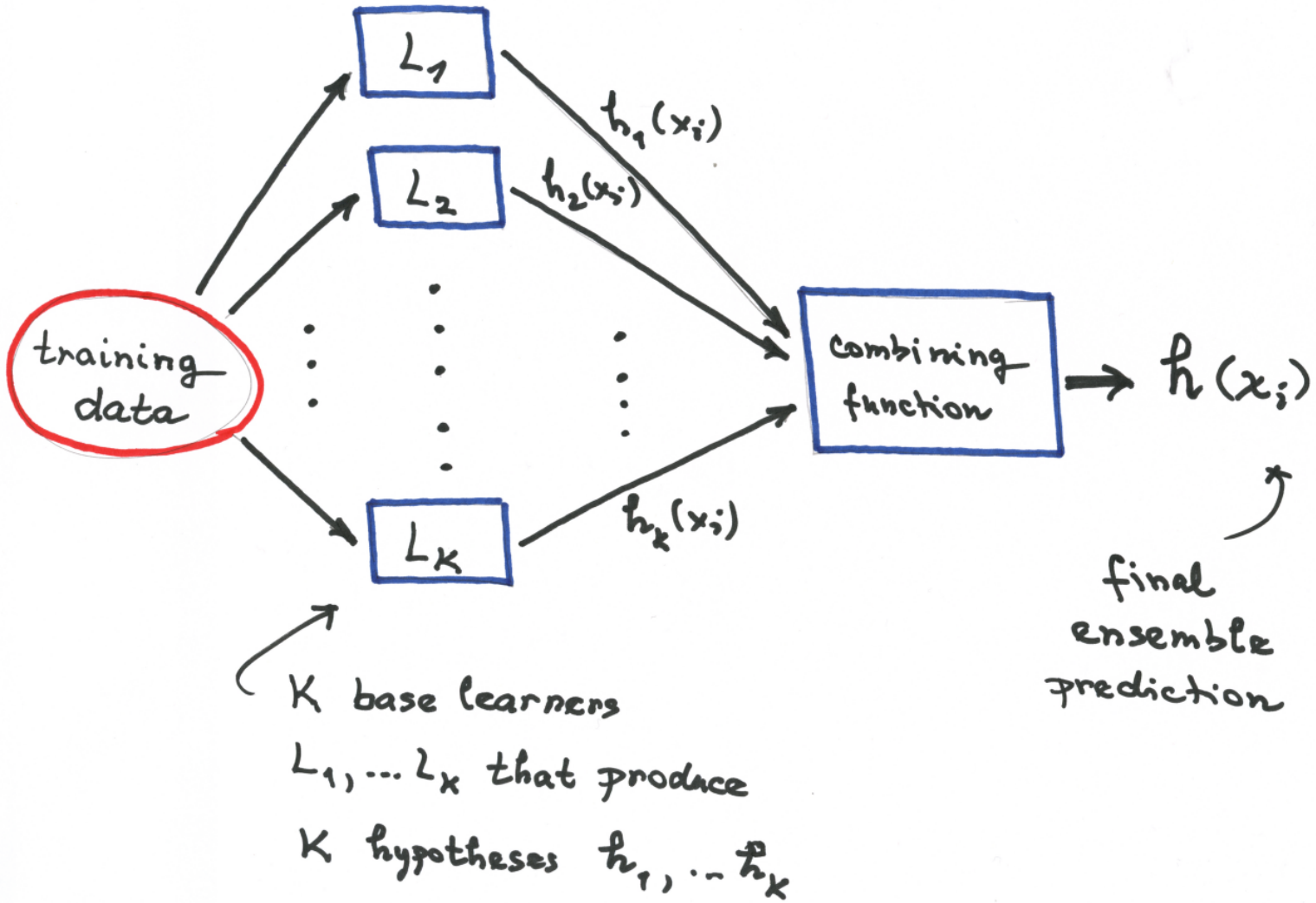
Key idea: The number of them will be binomially distributed! $\sim$ Bi(21, 0.3)

```
> plot(0:21, dbinom(0:21, 21, 0.3))
> dbinom(11, 21, 0.3)
[1] 0.01764978
> pbinom(10, 21, 0.3)
[1] 0.9736101
```



Conslusion: Accuracy of the ensemble will be more than 97.3 %!

General scheme of combining classifiers



Resampling approach

Resampling can be used as a way to produce diversity among base learners

- Distribute the training data into K portions
- Run the learning process to get K different models
- Collect the output of the K models use a combining function to get a final output value

Bootstrapping principle

- New data sets $Data_1, \ldots, Data_K$ are drawn from $Data$ with replacement, each of the same size as the original $Data$, i.e. n.

- In the i-th step of the iteration, $Data_i$ is used as a training set, while the examples $\{\mathbf{x} \,|\, \mathbf{x} \in Data \wedge \mathbf{x} \notin Data_i\}$ form the test set.

Bootstrapping principle

- New data sets $Data_1, \ldots, Data_K$ are drawn from $Data$ with replacement, each of the same size as the original $Data$, i.e. n.
- In the i-th step of the iteration, $Data_i$ is used as a training set, while the examples $\{\mathbf{x} \,|\, \mathbf{x} \in Data \wedge \mathbf{x} \notin Data_i\}$ form the test set.
- 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 it 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 the error estimate will be pessimistic. So the solution is to repeat the process many times.

Same algorithm, different classifiers

Combining classifiers to improve the performance

Ensemble methods – key ideas

- combining the classification results from different classifiers to produce the final output
- using (un)weighted voting
- different training data – e.g. bootstrapping
- different features
- different values of the relevant paramaters
- performance: complementarity $\longrightarrow$ potential improvement

Two fundamental approaches

- **Bagging** works by taking a bootstrap sample from the training set
- **Boosting** works by changing the weights on the training set

Are ensembles effective?

Combining multiple learners

- the more **complementary** the learners are, the more useful their combining is
- the simpliest way to combine multiple learners is **voting**
- in **weighted voting** the voters (= base-learners) can have different weights

Unstable learning

- learning algorithm is called unstable if small changes in the training set cause large differences in generated models
- typical unstable algorithm is the decision trees learning
- bagging or boosting techniques are a natural remedy for unstable algorithms

Bagging

- Bagging is a voting method that uses slightly different training sets (generated by bootstrap) to make different base-learners.
- Generating complementary base-learners is left to chance and to unstability of the learning method.
- Generally, bagging can be combined with any approach to learning.

Simple bagging algorithm

Bootstrap **AGG**regat**ING**

1. for $i \leftarrow 1$ to K do
2. $Train_i \leftarrow \text{bootstrap}(Data)$
3. $h_i \leftarrow \text{TrainPredictor}(Train_i)$

Combining function

- **Classification:** $h_{final}(\mathbf{x}) = \text{MajorityVote}(\text{h}_1(\mathbf{x}), \text{h}_2(\mathbf{x}), \ldots, \text{h}_\text{K}(\mathbf{x}))$
- **Regression:** $h_{final}(\mathbf{x}) = \text{Mean}(\text{h}_1(\mathbf{x}), \text{h}_2(\mathbf{x}), \ldots, \text{h}_\text{K}(\mathbf{x}))$

Random Forests — an extension of Decision Trees

- Random Forest is another example of bagging
- an ensemble method based on decision trees and bagging
- builds a number of *independent* random decision trees and then uses voting
- introduced by L. Breiman (2001), then developed by L. Breiman and A. Cutler
- very good (state-of-the-art) prediction performance
- a nice page with description
  `www.stat.berkeley.edu/~breiman/RandomForests/cc_home.htm`
- important: Random Forests helps to
  - avoid overfitting (by random sampling the training data set)
  - select important/useful features (by random sampling the feature set)

Building Random Forests

The algorithm for building a tree in the ensemble

1. Having a training set of the size n, sample n cases at random – with replacement, and use the sample to build a decision tree.

2. If there are M input features, choose a less number $m \ll M$. When building the tree, at each node a random sample of m features is selected as split candidates from the full set of M available features. Then the best split on these m features is used to split the node. A fresh sample of m features is taken at each split.
   – m is fixed for the whole procedure

3. Each tree is grown to the largest extent possible. There is no pruning.

The more trees in the ensemble, the better.
There is no risk of overfitting!

R packages for Random Forests

- **randomForest**: Breiman and Cutler's random forests for classification and regression
  – Classification and regression based on a forest of trees using random inputs.

- **RRF**: Regularized Random Forest
  – Feature Selection with Regularized Random Forest. This package is based on the 'randomForest' package by Andy Liaw. The key difference is the RRF function that builds a regularized random forest.
  – `http://cran.r-project.org/web/packages/RRF/index.html`

- **party**: A Laboratory for Recursive Partytioning
  – a computational toolbox for recursive partitioning
  – `cforest()` provides an implementation of Breiman's random forests
  – extensible functionality for visualizing tree-structured regression models is available

Examination requirements

- You should understand the basic ideas of building and using Decision Trees for both classification and regression task.
  - Decision Trees – splitting criteria: typical heuristics
  - Decision Trees – pruning and overfitting: the complexity parameter
  - Decision Trees – practical use of the `rpart()` package
- You should understand Random Forests, which is an important and effective extension of simple Decision Trees.
- You should be able to practically use `rpart()` and `randomForest()` packages in R.
- Also, later we will discuss Random Forests again, in connection with more general ensemble methods.

References – more details on Decision Trees

- Breiman Leo, Friedman Jerome H., Olshen Richard A., Stone Charles J. *Classification and Regression Trees*. Chapman & Hall/CRC, 1984.
- Hunt, E. B. Concept Learning: An Information Processing Problem, Wiley. 1962.
- Morgan, J. N., Sonquist, J. A. Problems in the analysis of survey data, and a proposal. Journal of the American Statistical Association 58, pp. 415–434. 1963.
- Quinlan, J. R. Discovering rules from large collections of examples: A case study, in D. Michie, ed., Expert Systems in the Micro Electronic Age. Edinburgh University Press. 1979.
- Quinlan, J. R. C4.5: Programs for Machine Learning, Morgan Kaufmann, San Mateo, California. 1993.