

Machine Learning

B. Supervised Learning: Nonlinear Models B.3. Decision Trees

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Syllabus



Fri. 25.10. (1) 0. Introduction

A. Supervised Learning: Linear Models & Fundamentals

- Fri. 1.11. (2) A.1 Linear Regression
- Fri. 8.11. (3) A.2 Linear Classification
- Fri. 15.11. (4) A.3 Regularization
- Fri. 22.11. (5) A.4 High-dimensional Data

B. Supervised Learning: Nonlinear Models

- Fri. 29.11. (6) B.1 Nearest-Neighbor Models
- Fri. 6.12. (7) B.2 Neural Networks
- Fri. 13.12. (8) B.3 Decision Trees
- Fri. 20.12. (9) B.4 Support Vector Machines — Christmas Break —
- Fri. 10.1. (10) B.5 A First Look at Bayesian and Markov Networks

C. Unsupervised Learning

- Fri. 17.1. (11) C.1 Clustering
- Fri. 24.1. (12) C.2 Dimensionality Reduction
- Fri. 31.1. (13) C.3 Frequent Pattern Mining
- Fri. 7.2. (14) Q&A

Outline



- 1. What is a Decision Tree?
- 2. Splits
- 3. Regularization
- 4. Learning Decision Trees
- 5. Split Quality Criteria

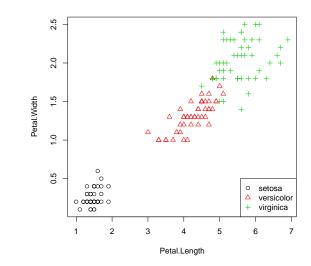
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Decision Tree



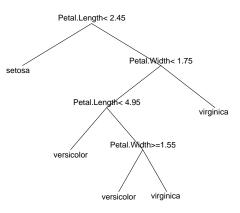


Decision Tree

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A decision tree is a tree that

- at each inner node has a splitting rule that assigns instances uniquely to child nodes of the actual node, and
- 2. at each **leaf node** has a **prediction** (class label).

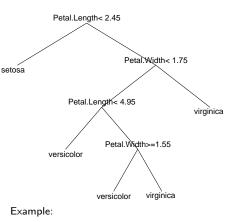


Note: The splitting rule is also called decision rule, the prediction the decision.

Using a Decision Tree

The class of a given case $x \in \mathcal{X}$ is predicted by

- 1. starting at the root node,
- 2. at each interior node
 - evaluate the splitting rule for x and
 - branch to the child node picked by the splitting rule, (default: left = "true", right = "false")
- 3. once a leaf node is reached,
 - predict the class assigned to that node as class of the case x.



x: Petal.Length = 6, Petal.Width = 1.6



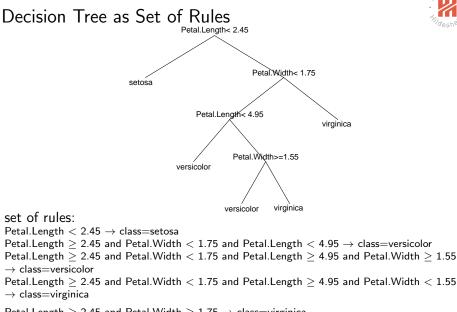
Decision Tree as Set of Rules



Each branch of a decision tree can be formulated as a single conjunctive rule

if condition₁(x) and condition₂(x) and ... and condition_k(x), then y = class label at the leaf of the branch.

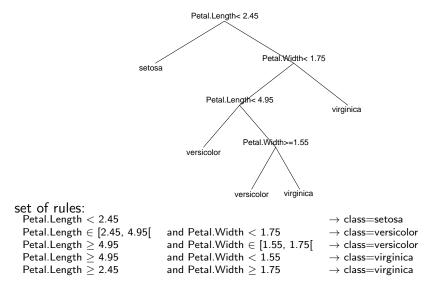
A decision tree is equivalent to a set of such rules, one for each branch.



<code>Petal.Length \geq 2.45 and <code>Petal.Width \geq 1.75 \rightarrow class=virginica</code></code>

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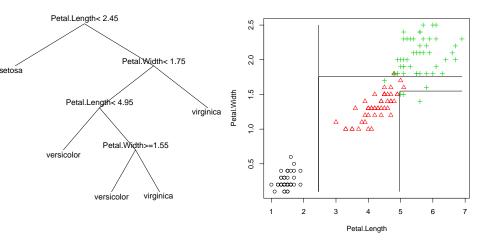
Decision Tree as Set of Rules



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Decision Boundaries

Decision boundaries are rectangular.



Regression Tree

A regression tree is a tree that

- 1. at each **inner node** has a **splitting rule** that assigns instances uniquely to child nodes of the actual node, and
- 2. at each leaf node has a target value.

Regression Tree & Probability Trees

A regression tree is a tree that

- 1. at each **inner node** has a **splitting rule** that assigns instances uniquely to child nodes of the actual node, and
- 2. at each leaf node has a target value.

A probability tree is a tree that

- 1. at each **inner node** has a **splitting rule** that assigns instances uniquely to child nodes of the actual node, and
- 2. at each leaf node has a class probability distribution.



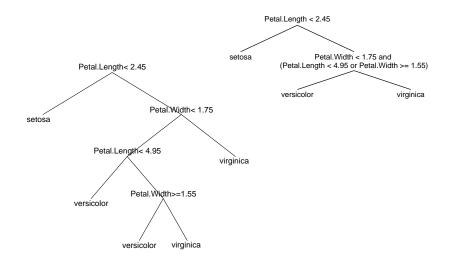
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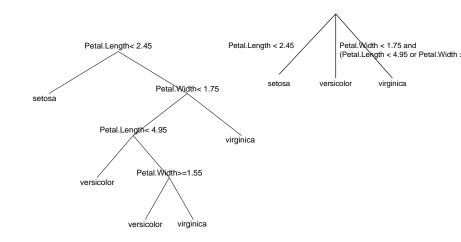
Which Decision Tree is Better?





Which Decision Tree is Better?





Simple Splits



To allow all kinds of splitting rules at the interior nodes (also called **splits**) does not make much sense. The very idea of decision trees is that

- the splits at each node are rather simple and
- more complex structures are captured by chaining several simple decisions in a tree structure.

Therefore, the set of possible splits is kept small by opposing several types of restrictions on possible splits:

- by restricting the number of variables used per split (univariate vs. multivariate decision tree),
- by restricting the number of children per node (binary vs. n-ary decision tree),
- by allowing only some special types of splits (e.g., complete splits, interval splits, etc.).



Types of Splits: Univarite vs. Multivariate

A split is called **univariate** if it uses only a single variable, otherwise **multivariate**.

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Example:

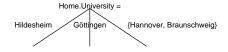
"Petal.Width < 1.75" is univariate,

"Petal.Width < 1.75 and Petal.Length < 4.95" is bivariate.
```

- Multivariate splits that are mere conjunctions of univariate splits better would be represented in the tree structure.
- But there are also multivariate splits than cannot be represented by a conjunction of univariate splits, e.g., "Petal.Width / Petal.Length < 1"
 - can be represented by a univariate split on an additional predictor "Petal.Width / Petal.Length"

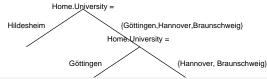
```
Types of Splits: n-ary
A split is called n-ary if it has n children.
(Binary is used for 2-ary, ternary for 3-ary.)
```

Example: "Petal.Length < 1.75" is binary,



is ternary.

► All *n*-ary splits can be also represented as a tree of binary splits, e.g.,



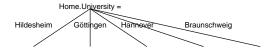


Types of Splits: Complete Splits



A univariate split on a nominal variable is called **complete** if each value is mapped to a child of its own,

i.e., the mapping between values and children is bijective.



 A complete split is *n*-ary (where *n* is the number of different values for the nominal variable).

Types of Splits: Interval Splits



A univariate split on an at least ordinal variable is called **interval split** if for each child all the values assigned to that child are an interval.

Examples: "Petal.Width < 1.75" is an interval split.

 $\label{eq:constraint} \begin{array}{l} \mbox{``(i) Petal.Width < 1.45,} \\ \mbox{(ii) Petal.Width } \geq 1.45 \mbox{ and Petal.Width < 1.75,} \\ \mbox{(iii) Petal.Width } \geq 1.75 \mbox{'' also is an interval split.} \end{array}$

"Petal.Width < 1.75 or Petal.Width ≥ 2.4 " is not an interval split.

Types of Decision Trees



A decision tree is called univariate, n-ary,

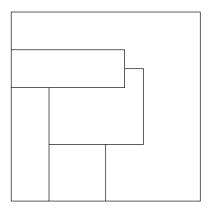
with complete splits or with interval splits,

if **all** its splits have the corresponding property.

Binary Univariate Interval Splits

There are partitions (sets of rules)

that cannot be created by binary univariate splits.

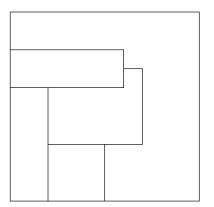


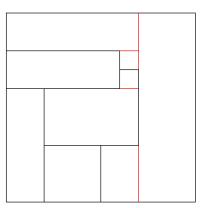


Binary Univariate Interval Splits

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But all partitions can be refined s.t. they can be created by binary univariate splits.



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Learning Regression Trees (1/2)



Imagine, the **tree structure is already given**, thus the partition

$$R_k, \quad k=1,\ldots,K$$

of the predictor space is already given.

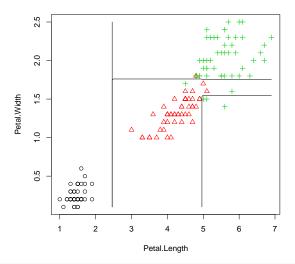
Then the remaining problem is to assign a predicted value

$$\hat{y}_k, \quad k=1,\ldots K$$

to each cell.



Learning Regression Trees (1/2) / Example



Learning Regression Trees (2/2)



Fit criteria such as the **smallest residual sum of squares** can be decomposed in partial criteria for cases falling in each cell:

$$\sum_{n=1}^{N} (y_n - \hat{y}(x_n))^2 = \sum_{k=1}^{K} \sum_{n=1, x_n \in R_k}^{N} (y_n - \hat{y}_k)^2$$

and this sum is minimal if the partial sum for each cell is minimal.

This is the same as fitting a constant model to the points in each cell R_k and thus the \hat{y}_k with smallest RSS are just the means:

$$\hat{y}_k := \operatorname{average}\{y_n \mid n = 1, \dots, N; x_n \in R_k\}$$

Learning Decision Trees

The same argument shows that

 for a probability tree with given structure the class probabilities with maximum likelihood are just the relative frequencies of the classes of the points in that region:

$$\hat{p}(Y = y \mid x \in R_k) = \frac{|\{n \mid n = 1, \dots, N; x_n \in R_k, y_n = y\}|}{|\{n \mid n = 1, \dots, N; x_n \in R_k\}|}$$

And for a decision tree with given structure, that the class label with smallest misclassification rate is just the majority class label of the points in that region:

$$\hat{y}(x \in R_k) = \arg \max_{y} |\{n \mid n = 1, ..., N; x_n \in R_k, y_n = y\}|$$



Possible Tree Structures



- Even when possible splits are restricted,
 - e.g., only binary univariate interval splits are allowed,

then tree structures can be built that separate all cases in tiny cells that contain just a single point

(if there are no points with same predictors).

- For such a very fine-grained partition, the fit criteria would be optimal (RSS=0, misclassification rate=0, likelihood maximal).
- ► Thus, decision trees need some sort of regularization to make sense.

Machine Learning 3. Regularization

Regularization Methods



There are several simple regularization methods:

minimum number of points per cell:

require that each cell (i.e., each leaf node) covers a given minimum number of training points.

maximum number of cells:

limit the maximum number of cells of the partition (i.e., leaf nodes).

maximum depth:

limit the maximum depth of the tree.

The number of points per cell, the number of cells, etc. can be seen as a **hyperparameter** of the decision tree learning method.

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Decision Tree Learning Problem

The decision tree learning problem could be described as follows: Given a dataset

$$\mathcal{D}^{train} := \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$$

find a decision tree $\hat{y}: X \to Y$ that

- ▶ is binary, univariate, and with interval splits,
- ► contains at each leaf a given minimum number *m* of examples,
- ▶ and has minimal misclassification rate

$$\operatorname{mr}(\hat{y}; \mathcal{D}^{\operatorname{train}}) := \frac{1}{N} \sum_{n=1}^{N} \mathbb{I}(y_n \neq \hat{y}(x_n))$$

among all those trees.



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among all those trees.

Unfortunately, this problem is **not feasible** as there are **too many tree structures** / partitions to check and no suitable optimization algorithms to sift efficiently through them.



Greedy Search



Therefore, a greedy search is conducted that

- starting from the root
- builds the tree recursively
- ► by selecting the **locally optimal decision** in each step.
 - ► or alternatively, even just **some locally good** decision.



Greedy Search / Possible Splits (1/2) At each node one tries all possible splits.

For an univariate binary tree with interval splits at the actual node let there still be the data

$$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$$

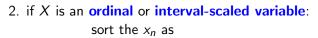
Then check for each predictor variable X with domain \mathcal{X} : 1. if X is a **nominal variable**: (with *m* levels) all $2^{m-1} - 1$ possible splits in two subsets $X_1 \dot{\cup} X_2$.

E.g., for
$$\mathcal{X} = \{Hi, G\ddot{o}, H\}$$
 the splits

$$\begin{cases}
Hi\} & vs. \quad \{G\ddot{o}, H\} \\
Hi, G\ddot{o}\} & vs. \quad \{H\} \\
Hi, H\} & vs. \quad \{G\ddot{o}\}
\end{cases}$$

Machine Learning 4. Learning Decision Trees

Greedy Search / Possible Splits (2/2)



$$x_1' < x_2' < \ldots < x_{n'}', \quad N' \leq N$$

and then test all N' - 1 possible splits at

$$\frac{x'_n + x'_{n+1}}{2}, \quad n = 1, \dots, N' - 1$$

E.g.,

$$(x_1, x_2, \ldots, x_8) = (15, 10, 5, 15, 10, 10, 5, 5), \quad N = 8$$

are sorted as

$$x'_1 := 5 < x'_2 := 10 < x'_3 := 15, \quad N' = 3$$

and then split at 7.5 and 12.5.



Greedy Search / Original Fit Criterion



All possible splits – often called **candidate splits** – are assessed by a **quality criterion**.

For all kinds of trees the original fit criterion can be used, i.e.,

for regression trees:

the residual sum of squares.

for decision trees:

the misclassification rate.

for probability trees:

the likelihood.

The split that gives the best improvement is chosen.

Example



Artificial data about visitors of an online shop:

	<i>x</i> ₁	<i>x</i> ₂	<i>x</i> ₃	у
	referrer	num.visits	duration	buyer
1	search engine	several	15	yes
2	search engine	once	10	yes
3	other	several	5	yes
4	ad	once	15	yes
5	ad	once	10	no
6	other	once	10	no
7	other	once	5	no
8	ad	once	5	no

Learn a decision tree that tries to predict if a visitor will buy.

Example / Root Split Step 1 (root node): The root covers all 8 visitors. There are the following splits:



		buyer		
variable	values	yes	no	errors
referrer	{s}	2	0	2
	{a, o}	2	4	
referrer	{s, a}	3	2	3
	{o}	1	2	
referrer	{s, o}	3	2	3
	$\{a\}$	1	2	
num.visits	once	2	4	2
	several	2	0	
duration	<7.5	1	2	3
	\geq 7.5	3	2	
duration	< 12.5	2	4	2
	≥ 12.5	2	0	

Example / Root Split

The splits

- ▶ referrer = search engine ?
- num.visits = once ?
- duration < 12.5 ?

are locally optimal at the root.

We choose "duration < 12.5":



Note: See backup slides after the end for more examples.



Decision Tree Learning Algorithm

- 1 expand-decision-tree(node T, training data D^{train}) :
- ² if stopping-criterion (\mathcal{D}^{train}):

3
$$T.$$
class := arg max $_{y'} | \{(x, y) \in \mathcal{D}^{train} \mid y = y'\}$

return

4

8

- 5 $s := \operatorname{arg max}_{\operatorname{split} s} \operatorname{quality-criterion}(s)$
- 6 if *s* does not improve:

$$\tau \qquad \mathsf{T.class} = \arg\max_{y'} |\{(x,y) \in \mathcal{D}^{\mathsf{train}} \mid y = y'\}|$$

- return
- 9 *T*.split := *s*
- for $z \in \text{Im}(s)$:
- 11 create new node T'
- 12 T.child[z] := T'
- expand-decision-tree($\mathcal{T}', \{(x, y) \in \mathcal{D}^{\mathsf{train}} \mid s(x) = z\}$)

1 learn-decision-tree(training data \mathcal{D}^{train}) :

- 2 create new node T
- ³ expand-decision-tree(T, D^{train})
- 4 return T



Decision Tree Learning Algorithm / Remarks (1/2)



- ▶ tree nodes *T* with 3 attributes:
 - split and child (inner node)
 - class (leaf node)
- ► stopping-criterion(*X*):

e.g.,

- ▶ all cases in X belong to the same class,
- ► all cases in X have the same predictor values (for all variables),
- ▶ there are less than the minimum number of cases per node to split.
- ► split s:

all possible splits, e.g., all binary univariate interval splits.

quality-criterion(s):

e.g., misclassification rate in X after the split (i.e., if in each child node suggested by the split the majority class is predicted).



Decision Tree Learning Algorithm / Remarks (2/2)

- s does not improve:
 e.g., if the misclassification rate is the same as in the actual node (without the split s).
- Im(s):
 all the possible outcomes of the split,
 e.g., { 0, 1 } for a binary split.
- T.child[z] := T':

keep an array that maps all the possible outcomes of the split to the corresponding child node.

Decision Tree Prediction Algorithm



¹ **predict-decision-tree**(node T, instance $x \in \mathbb{R}^{M}$):

- ² if *T*.split $\neq \emptyset$:
- z := T.split(x)
- 4 T' := T.child[z]
- ⁵ return predict-decision-tree(T', x)
- 6 return T.class

Outline



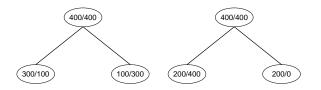
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Machine Learning 5. Split Quality Criteria

Why Misclassification Rate is a Bad Split Quality Criter Although it is possible to use misclassification rate as quality criterion, it usually is not a good idea.

Imagine a dataset with a binary target variable (zero/one) and 400 cases per class (400/400).

Assume there are two splits:



Both have 200 errors / misclassification rate 0.25.

But the right split may be preferred as it contains a pure node.

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Split Contingency Tables

The effects of a split on training data can be described by a **contingency** table $(C_{j,k})_{j \in J, k \in K}$, i.e., a matrix

- with rows indexed by the different child nodes $j \in J$,
- with columns indexed by the different target classes $k \in K$,
- ► and cells C_{j,k} containing the number of points in class k that the split assigns to child j:

$$C_{j,k} := |\{(x,y) \in \mathcal{D}^{\mathsf{train}} \,|\, s(x) = j \text{ and } y = k\}|$$

Entropy



Let

$$\Delta_N := \{(p_1, p_2, \dots, p_N) \in [0, 1]^N \mid \sum_n p_n = 1\}$$

be the set of multinomial probability distributions on the values $1, \ldots, N$.

An **entropy function** $q: \Delta_N \to \mathbb{R}^+_0$ has the properties

- q is maximal for uniform $p = (\frac{1}{N}, \frac{1}{N}, \dots, \frac{1}{N})$.
- *q* is 0 iff *p* is deterministic
 (one of the *p_n* = 1 and all the others equal 0).

An entropy quantifies the unorder of an distribution.

Entropy / Examples Cross-Entropy / Deviance:

$$H(p_1,\ldots,p_N):=-\sum_{n=1}^N p_n\log(p_n)$$

Shannons Entropy:

$$H(p_1,\ldots,p_N):=-\sum_{i=1}^n p_n \log_2(p_n)$$

Quadratic Entropy:

$$H(p_1,\ldots,p_N) := \sum_{i=1}^n p_n(1-p_n) = 1 - \sum_{n=1}^N p_n^2$$

Entropy measures can be extended to \mathbb{R}^+_0 via

$$q(x_1,\ldots,x_N):=q(\frac{x_1}{\sum_n x_n},\frac{x_2}{\sum_n x_n},\ldots,\frac{x_N}{\sum_n x_n})$$



Entropy for Contingency Tables

For a contingency table $C_{j,k}$ we use the following abbreviations:

$$C_{j,.} := \sum_{k \in K} C_{j,k}$$
$$C_{.,k} := \sum_{j \in J} C_{j,k}$$
$$C_{.,.} := \sum_{j \in J} \sum_{k \in K} C_{j,k}$$

sum of row j

sum of column k

sum of matrix

and define the following entropies:

row entropy:

 $H_J(C) := H(C_{j,.} \mid j \in J)$

column entropy:

 $H_{K}(C) := H(C_{.,k} | k \in K)$ conditional column entropy:

$$H_{K|J}(C) := \sum_{j \in J} \frac{C_{j,.}}{C_{.,.}} H(C_{j,k} \mid k \in K)$$



Machine Learning 5. Split Quality Criteria



Entropy for Contingency Tables Suitable split quality criteria are entropy gain:

$$HG(C) := H_{K}(C) - H_{K|J}(C)$$

entropy gain ratio:

$$HG(C) := \frac{H_{K}(C) - H_{K|J}(C)}{H_{J}(C)}$$

Shannon entropy gain is also called information gain:

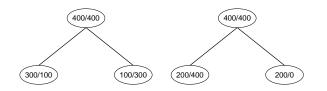
$$\mathsf{IG}(C) := -\sum_{k} \frac{C_{.,k}}{C_{.,.}} \log_2 \frac{C_{.,k}}{C_{.,.}} + \sum_{j} \frac{C_{j,.}}{C_{.,.}} \sum_{k} \frac{C_{j,k}}{C_{j,.}} \log_2 \frac{C_{j,k}}{C_{j,.}}$$

Quadratic entropy gain is also called Gini index:

$$\operatorname{Gini}(C) := -\sum_{k} \left(\frac{C_{.,k}}{C_{.,.}}\right)^{2} + \underbrace{\sum_{j} \frac{C_{j,.}}{C_{.,.}} \sum_{k} \left(\frac{C_{j,k}}{C_{j,.}}\right)^{2}}_{=:\operatorname{gini-impurity}(C)}$$

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Entropy Measures as Split Quality Criterion



Both have 200 errors / misclassification rate 0.25.

But the right split may be preferred as it contains a pure node.

Gini-Impurity

$$= \frac{1}{2}((\frac{3}{4})^2 + (\frac{1}{4})^2) + \frac{1}{2}((\frac{3}{4})^2 + (\frac{1}{4})^2) = \frac{3}{4}((\frac{1}{3})^2 + (\frac{2}{3})^2) + \frac{1}{4}(1^2 + 0^2)$$

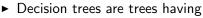
$$= 0.625 \approx 0.667$$

Popular Decision Tree Configurations



name	ChAID	CART	ID3	C4.5
author	Kass 1980	Breiman et al. 1984	Quinlan 1986	Quinlan 1993
selection	χ^2	Gini index,	information gain	information gain
measure		twoing index		ratio
splits	all	binary nominal,	complete	complete,
		binary quantitative,		binary nominal,
		binary bivariate		binary quantitative
		quantitative		
stopping	χ^2 independence	minimum number	χ^2 independence	lower bound on
criterion	test	of cases/node	test	selection measure
pruning	none	error complexity	pessimistic error	pessimistic error
technique		pruning	pruning	pruning, error
				based pruning

Summary



- splitting rules at the inner nodes and
- predictions (decisions) at the leaves.
- Decision trees use only simple splits
 - univariate, binary, interval splits.
- ► Decision trees have to be regularized by constraining their structure
 - ▶ minimum number of examples at inner nodes, maximum depth, etc.
- ► Decision trees are learned by greedy recursive partitioning.
 - As split quality criteria entropy measures are used
 - ► Gini index, information gain ratio, etc.
- Outlook (see lecture Machine Learning 2):
 - ► Sometimes **pruning** is used to make the search less greedy.
 - Decision trees use **surrogate splits** to cope with missing data.
 - Decision trees can be boosted yielding very competitive models (random forests, gradient boosted decision trees).



Further Readings



► [Hastie et al., 2005, chapter 9.2+6+7], [Murphy, 2012, chapter 16.1-2], [James et al., 2013, chapter 8.1+3].

References



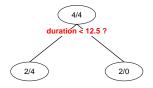
Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin. The Elements of Statistical Learning: Data Mining, Inference and Prediction, volume 27. Springer, 2005.

Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani. An Introduction to Statistical Learning. Springer, 2013.

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Example / Node 2 Split





The right node is pure and thus a leaf.

Step 2 (node 2): The left node (called "node 2") covers the following cases:

	referrer	num.visits	duration	buyer
2	search engine	once	10	yes
3	other	several	5	yes
5	ad	once	10	no
6	other	once	10	no
7	other	once	5	no
8	ad	once	5	no



Example / Node 2 Split

At node 2 are the following splits:

		buy	/er	
variable	values	yes	no	errors
referrer	{s}	1	0	1
	{a, o}	1	4	
referrer	$\{s, a\}$	1	2	2
	{o}	1	2	
referrer	{s, o}	2	2	2
	$\{a\}$	0	2	
num.visits	once	1	4	1
	several	1	0	
duration	<7.5	1	2	2
	≥ 7.5	1	2	

Again, the splits

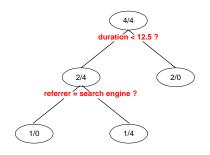
- ▶ referrer = search engine ?
- num.visits = once ?

are locally optimal at node 2.

Example / Node 5 Split

We choose the split "referrer = search engine":





The left node is pure and thus a leaf.

```
The right node (called "node 5") allows further splits.
```



Example / Node 5 Split

Step 3 (node 5): The right node (called "node 5") covers the following cases:

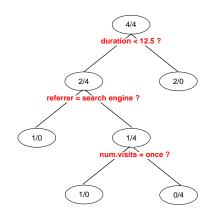
	referrer	num.visits	duration	buyer
3	other	several	5	yes
5	ad	once	10	no
6	other	once	10	no
7	other	once	5	no
8	ad	once	5	no

It allows the following splits:

		buyer		
variable	values	yes	no	errors
referrer	{a}	0	2	1
	{o}	1	2	
num.visits	once	1	0	0
	several	0	4	
duration	<7.5	1	2	1
	≥ 7.5	0	2	



Example / Node 5 Split The split "num.visits = once" is locally optimal.



Both child nodes are pure thus leaf nodes. The algorithm stops.