Machine Learning

A. Supervised Learning

A.6. Decision Trees

Lars Schmidt-Thieme, Nicolas Schilling

Information Systems and Machine Learning Lab (ISMLL)
Institute for Computer Science
University of Hildesheim, Germany

Outline

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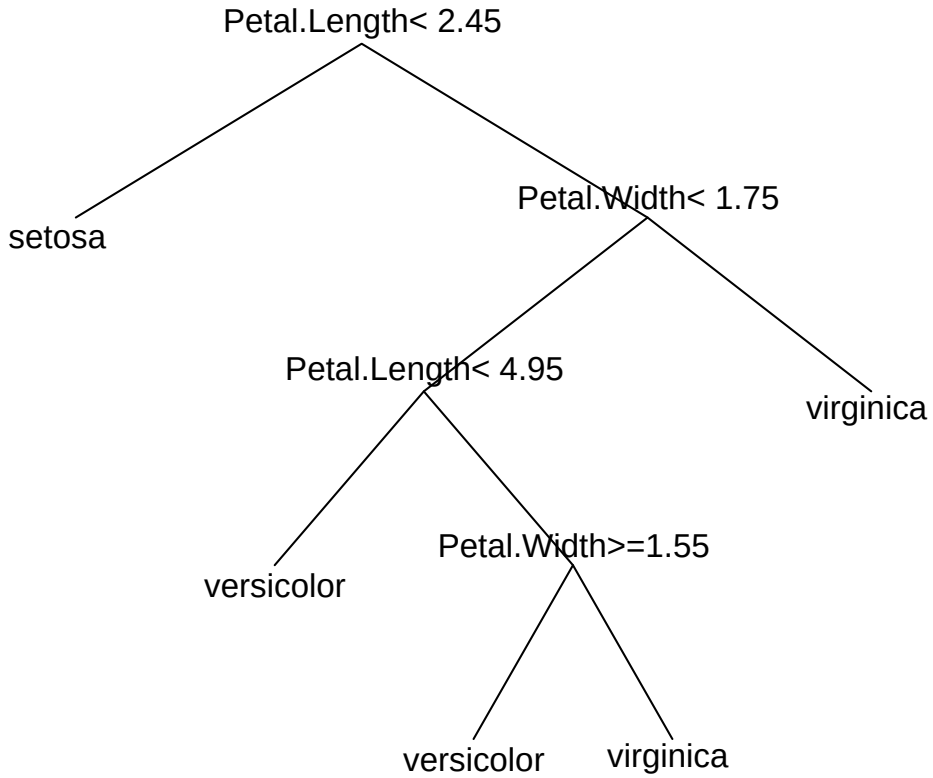
Decision Tree

A **decision 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 **prediction** (class label).

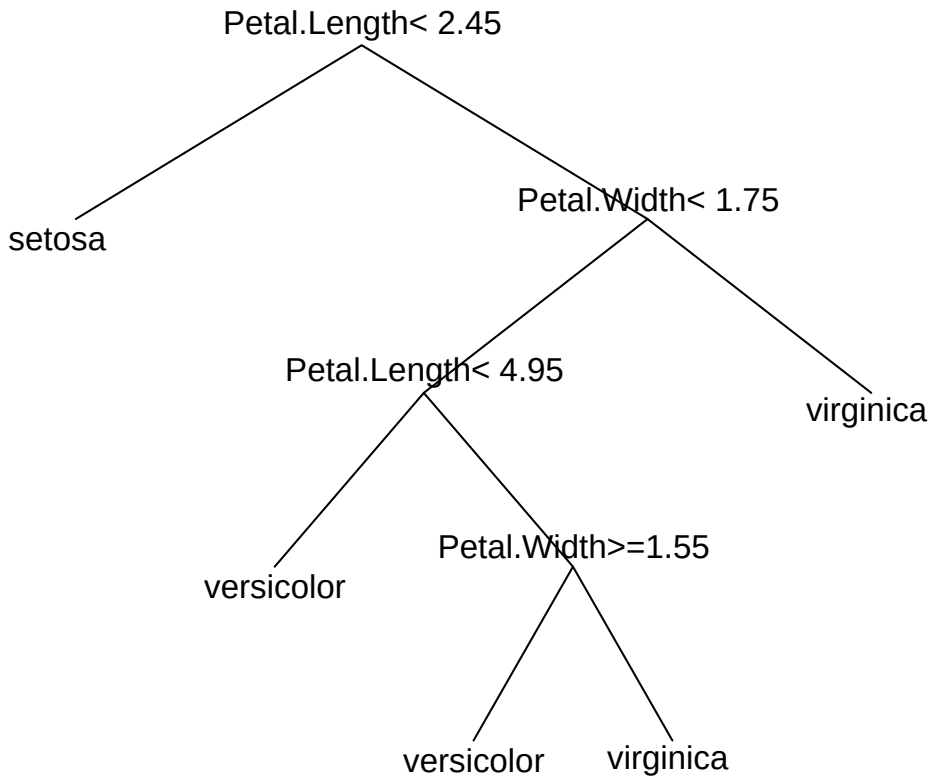


Note: The splitting rule is also called **decision rule**, the prediction the **decision**.

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.

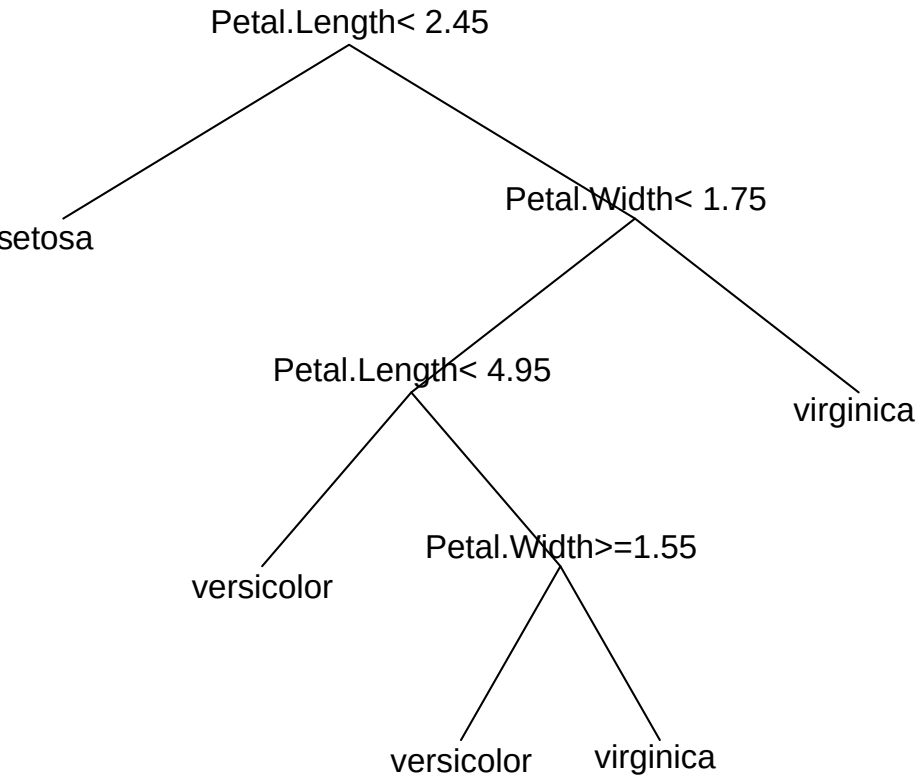


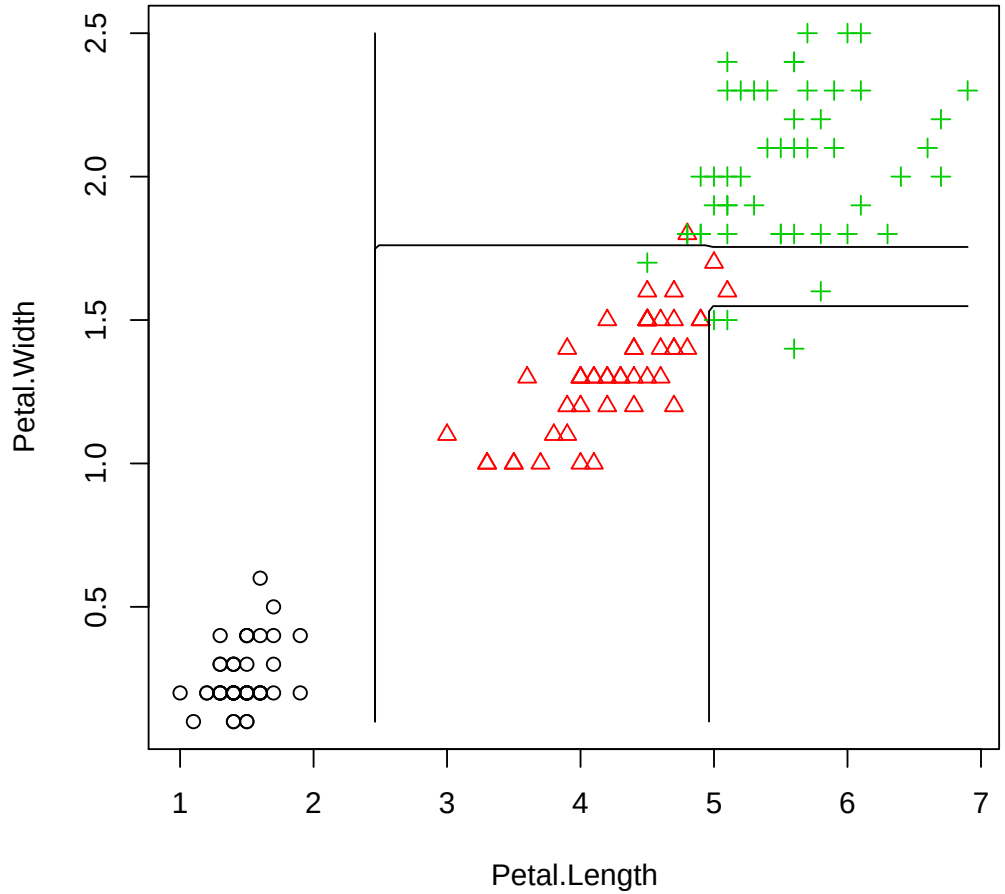
Example:

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

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

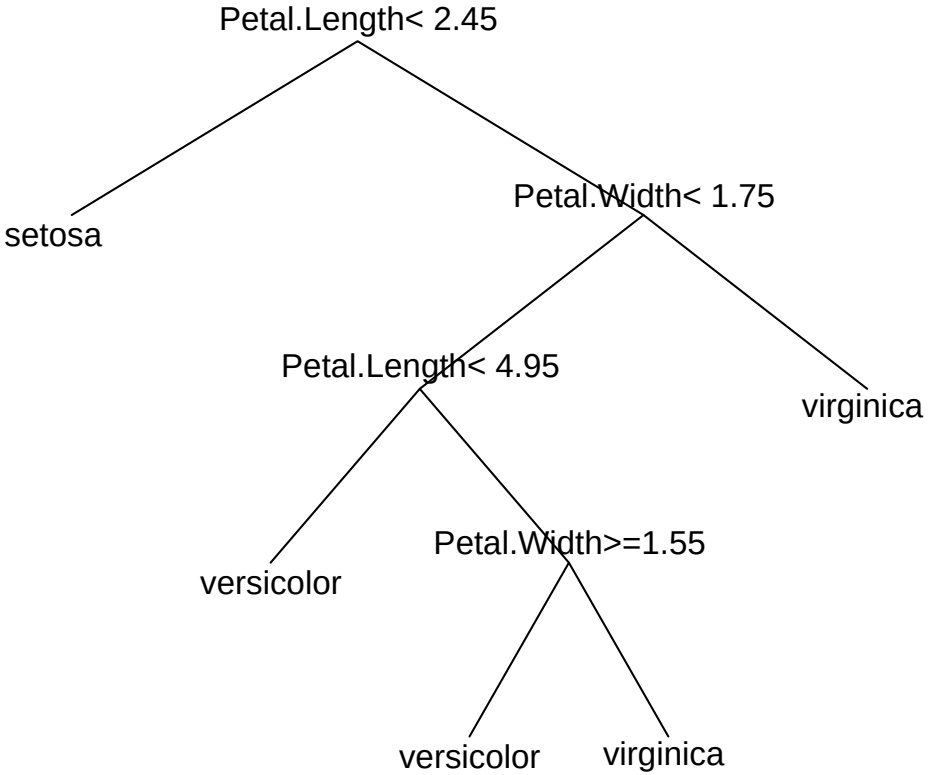
1. at each **inner node** has a **splitting rule** that assigns instances uniquely to child nodes of the actual node, and
2. at each **leaf node** has a **target value**.

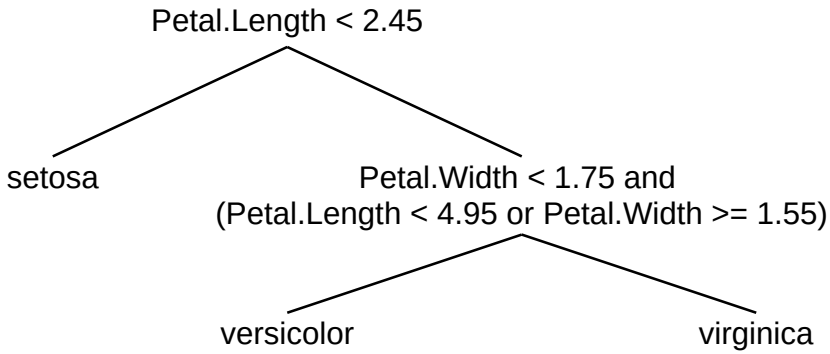
A **probability tree** is a tree that

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**.

Outline

An alternative Decision Tree?





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**.

Example:
"Petal.Width $<$ 1.75" is univariate,
"Petal.Width $<$ 1.75 and Petal.Length $<$ 4.95" is bivariate.

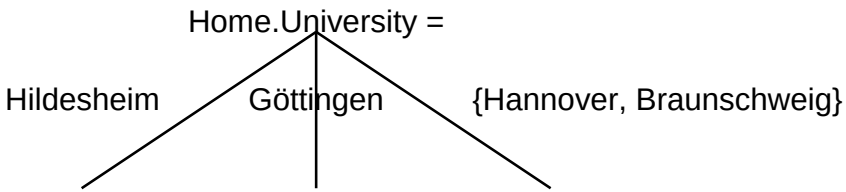
Multivariate splits that are mere conjunctions of univariate splits better would be represented in the tree structure.

But there are also multivariate splits than cannot be represented by a conjunction of univariate splits, e.g.,
"Petal.Width / Petal.Length $<$ 1"

Types of Splits: *n*-ary

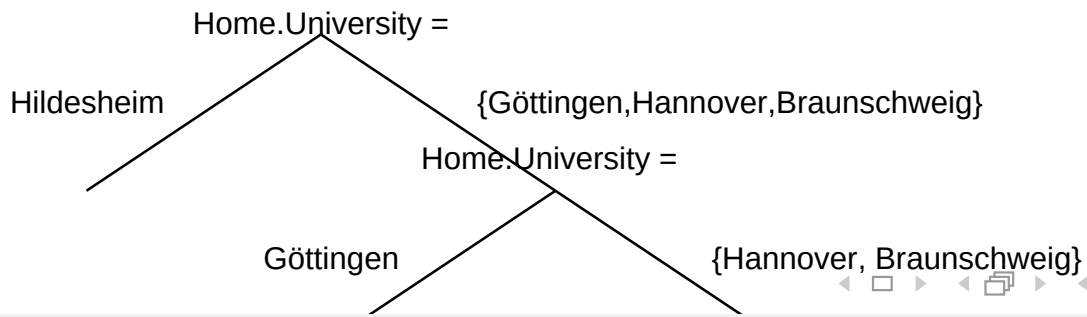
A split is called ***n*-ary** if it has n children.
(**Binary** is used for 2-ary, **ternary** for 3-ary.)

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



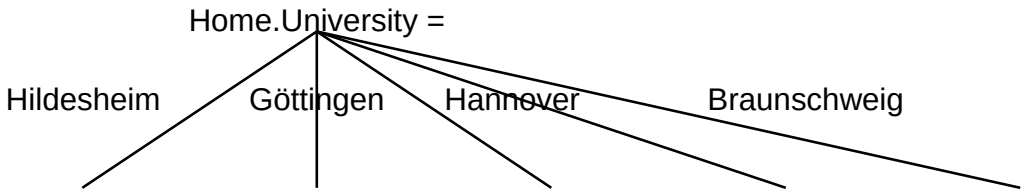
is ternary.

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.

Example:
"Petal.Width $<$ 1.75" is an interval split,
"(i) Petal.Width $<$ 1.45,
(ii) Petal.Width $\geq$ 1.45 and Petal.Width $<$ 1.75,
(iii) Petal.Width $\geq$ 1.75" also is an interval split.

"Petal.Width $<$ 1.75 or Petal.Width $\geq$ 2.4" is not an interval split.

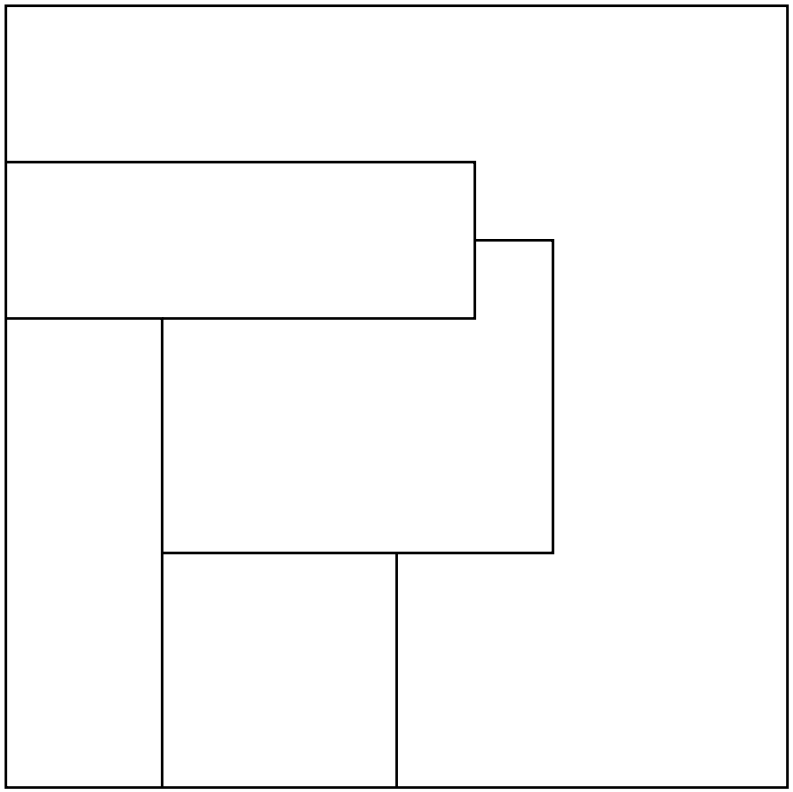
Types of Decision Trees

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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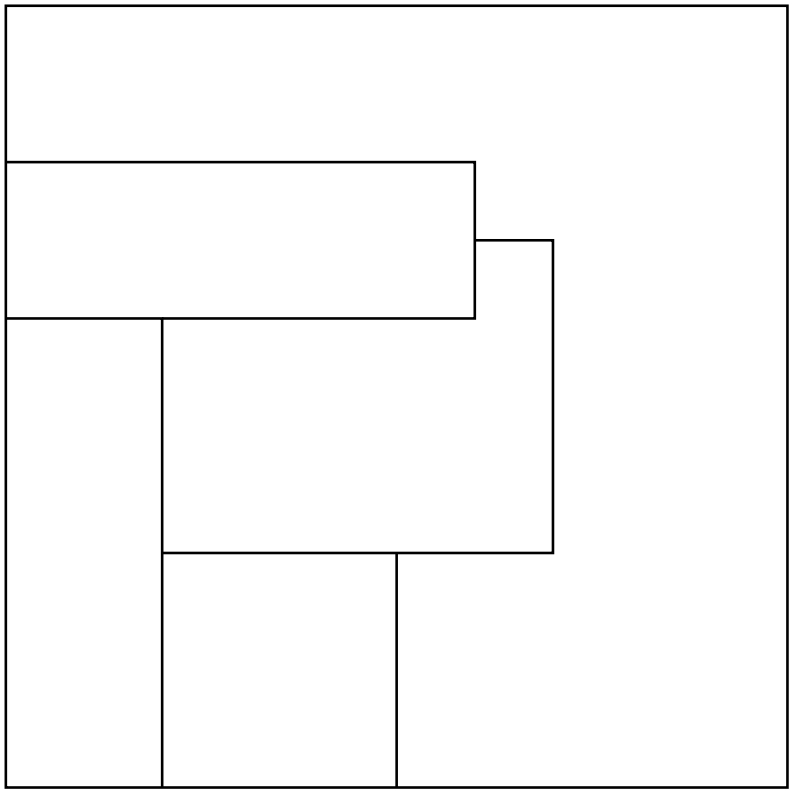
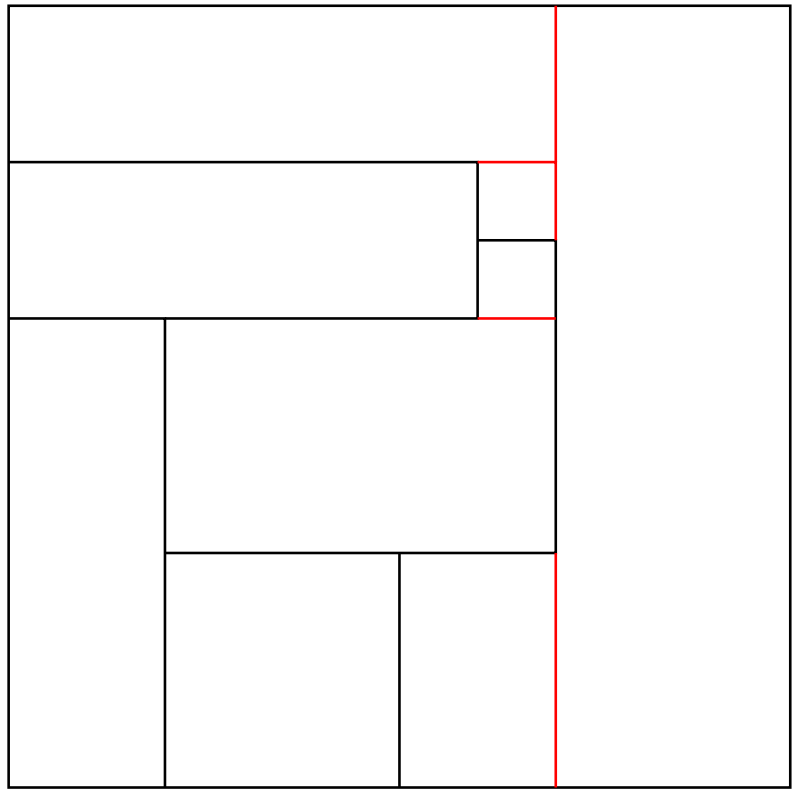




But all partitions can be refined
s.t. they can be created by binary univariate splits.

Outline

Learning Trees (1/2)

For Learning of Decision, Regression or Probability Trees we basically have to do three things:

- Learn the structure of the tree, i.e. all splits
- Assign labels for leaf nodes
- Think of ways how to regularize trees

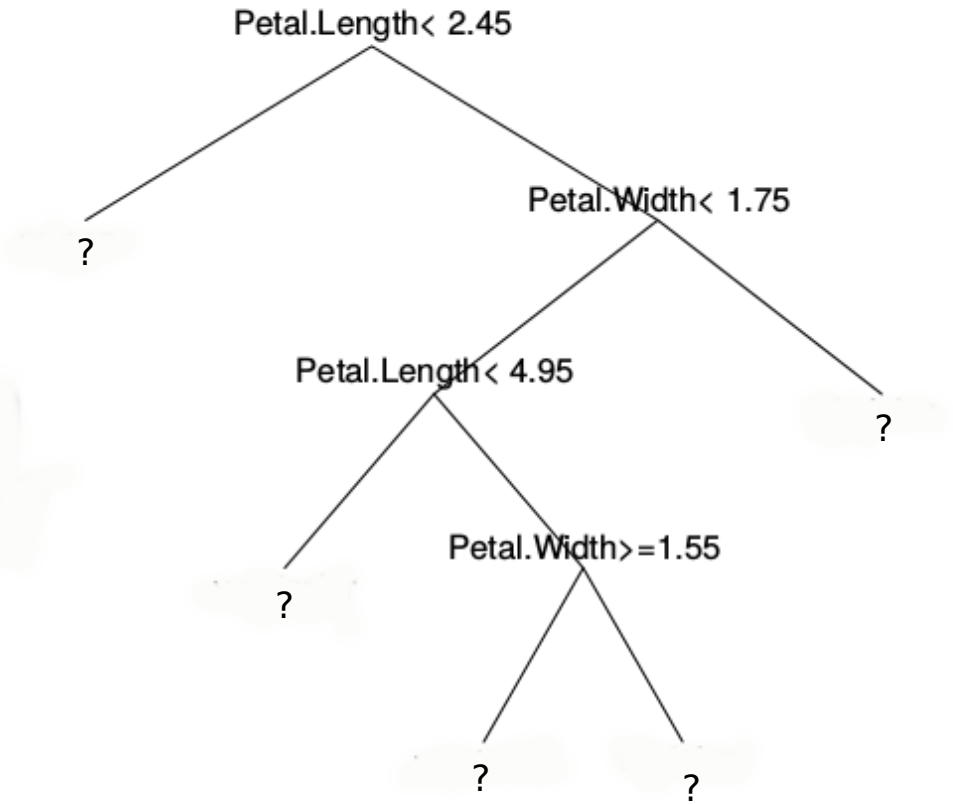
Learning Trees (2/2)

- Suppose the structure is given in form of regions of the predictor space

$$R_j, \quad j = 1, \ldots, k$$

- Then how do we assign labels?

$$\hat{y}_j, \quad j = 1, \ldots k$$



Learning Regression Trees

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

$$\sum_{n=1}^{N}(y_n - \hat{y}(x_n))^2 = \sum_{j=1}^{k} \sum_{n=1, x_n \in R_j}^{n} (y_n - \hat{y}_j)^2$$

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 and thus the $\hat{y}_j$ with smallest RSS are just the **means**:

$$\hat{y}_j := \text{average}\{y_n \mid n = 1, \ldots, N; x_n \in R_j\}$$

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:

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

- 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:

$$\hat{y}(x \in R_j) = \arg\max_y |\{n \,|\, n = 1, \ldots, N; x_n \in R_j, y_n = y\}|$$

Possible Tree Structures

If we have no duplicate instances, then it is **generally possible to build trees where in each leaf node there is only one instance**:

$$|R_j| = 1 \quad \forall j$$

- we obtain a very fine grained partition
- fit criteria would be optimal for every case
- RSS $= 0$, misclassification rate $= 0$, maximal likelihood

$\Rightarrow$ We need to regularize trees in order for them to make sense

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.

Decision Tree Learning Problem

The decision tree learning problem could be described as follows:

Given a dataset

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

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

$$\frac{1}{N} \sum_{n=1}^{N} I(y_n \neq \hat{y}(x_n))$$

among all those trees.

Decision Tree Learning Problem

Unfortunately, this problem is **not feasible** as

- there are **too many possible tree structures** to check
- and **no suitable optimization algorithms** to search efficiently through them.

As an example, consider a real-valued feature, how many possible interval splits exist?

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 a 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 $\mathcal{X}$:

if X is a **nominal variable**:

all $2^{m-1} - 1$ possible splits in two subsets $X_1 \dot{\cup} X_2$.

E.g., for $\mathcal{X} = \{\text{Hi}, \text{Gö}, \text{H}\}$ the splits

$\{\text{Hi}\}$	vs.	$\{\text{Gö}, \text{H}\}$
$\{\text{Hi}, \text{Gö}\}$	vs.	$\{\text{H}\}$
$\{\text{Hi}, \text{H}\}$	vs.	$\{\text{Gö}\}$

Greedy Search / Possible Splits (2/2)

if X is an **ordinal** or **interval-scaled variable**:

sort the x_n as

$$x'_1 < x'_2 < \ldots < x'_{n'}, \quad N' \leq N$$

and then test all $N' - 1$ possible splits at

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

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:

	x_1	x_2	x_3	y
	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

Build 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
	≥ 7.5	3	2	
duration	< 12.5	2	4	2
	≥ 12.5	2	0	

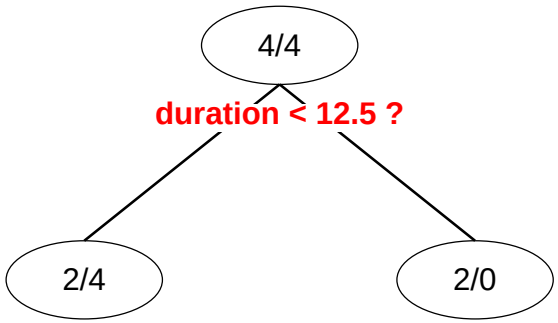
Example / Root Split

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

procedure EXPAND-DECISION-TREE(node T, training data $\mathcal{D}^{\text{train}}$)
  if stopping-criterion($\mathcal{D}^{\text{train}}$) **then**
    T.class $:= \arg\max_{y'} |\{(x, y) \in \mathcal{D}^{\text{train}} \mid y = y'\}|$
    return
  $s := \arg\max_{\text{split } s}$ quality-criterion(s)
  if s does not improve **then**
    T.class $= \arg\max_{y'} |\{(x, y) \in \mathcal{D}^{\text{train}} \mid y = y'\}|$
    return
  T.split $:= s$
  for $z \in \text{Im}(s)$ **do**
    create new node T'
    T.child[z] $:= T'$
    EXPAND-DECISION-TREE($T', \{(x, y) \in \mathcal{D}^{\text{train}} \mid s(x) = z\}$)

procedure LEARN-DECISION-TREE(training data $\mathcal{D}^{\text{train}}$)
  create new node T
  expand-decision-tree($T, \mathcal{D}^{\text{train}}$)
  return T

Decision Tree Learning Algorithm / Remarks (1/2)

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).

$\text{Im}(s)$:

all the possible outcomes of the split,
e.g., $\{ 0, 1 \}$ for a binary split.

$T.\text{child}[z] := T'$:

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

Decision Tree Prediction Algorithm

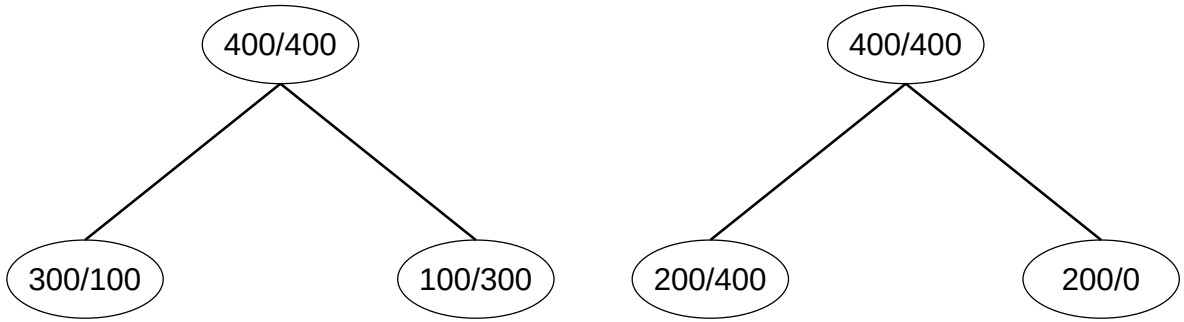
1: **procedure** PREDICT-DECISION-TREE(node T, instance $x \in \mathbb{R}^M$)
2: **if** T.split $\neq \emptyset$ **then**
3: $z := T$.split(x)
4: $T' := T$.child$[z]$
5: **return** PREDICT-DECISION-TREE(T', x)
6: **return** T.class

Outline

Why Misclassification Rate is a Bad Split Quality Criterion

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.

Split Contingency Tables

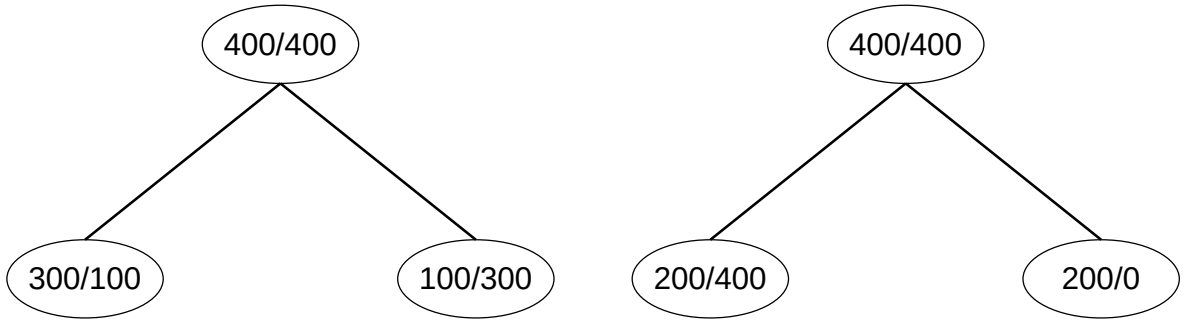
The effects of a split on training data can be described by a **contingency table** $(C_{j,k})_{j \in J, k \in K}$, i.e., a matrix

- 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:

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

Example: Contingency Tables

For both splits:



We would have contingency tables:

$$\begin{pmatrix} 300 & 100 \\ 100 & 300 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 200 & 400 \\ 200 & 0 \end{pmatrix}$$

Entropy

Let

$$P_n := \{(p_1, p_2, \ldots, p_n) \in [0,1]^n \mid \sum_i p_i = 1\}$$

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

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

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

Entropy

Examples:

Cross-Entropy / Deviance:

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

Shannons Entropy:

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

Quadratic Entropy:

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

Entropy for Contingency Tables

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

$$C_{j,.} := \sum_{k \in K} C_{j,k} \qquad \text{sum of row } j$$

$$C_{.,k} := \sum_{j \in J} C_{j,k} \qquad \text{sum of column } k$$

$$C_{.,.} := \sum_{j \in J} \sum_{k \in K} C_{j,k} \qquad \text{sum of matrix}$$

and define the following entropies:

row entropy:

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

column entropy:

$$H_K(C) := H(C_{.,k} \mid k \in K)$$

conditional column entropy:

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

Entropy for Contingency Tables

Suitable split quality criteria are

entropy gain:

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

entropy gain ratio:

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

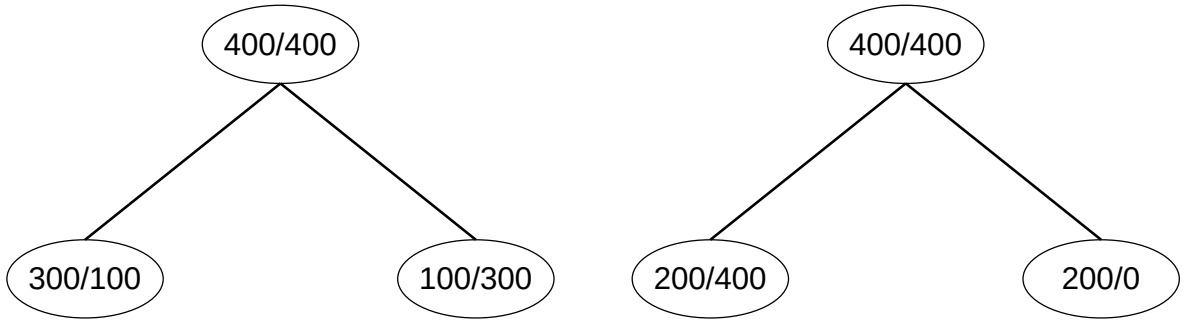
Shannon entropy gain is also called **information gain**:

$$\mathrm{IG}(C) := -\sum_k \frac{C_{.,k}}{C_{.,.}} \log_2 \frac{C_{.,k}}{C_{.,.}} + \sum_j \frac{C_{j,.}}{C_{.,.}} \sum_k \frac{C_{j,k}}{C_{j,.}} \log_2 \frac{C_{j,k}}{C_{j,.}}$$

Quadratic entropy gain is also called **Gini index**:

$$\mathrm{Gini}(C) := -\sum_k (\frac{C_{.,k}}{C_{.,.}})^2 + \sum_j \frac{C_{j,.}}{C_{.,.}} \sum_k (\frac{C_{j,k}}{C_{j,.}})^2$$

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

$$= \frac{1}{2}((\frac{3}{4})^2 + (\frac{1}{4})^2) + \frac{1}{2}((\frac{3}{4})^2 + (\frac{1}{4})^2)$$
$$= 0.625$$

Gini-Impurity

$$= \frac{3}{4}((\frac{1}{3})^2 + (\frac{2}{3})^2) + \frac{1}{4}(1^2 + 0^2)$$
$$\approx 0.667$$

Summary

- Decision trees are trees having
  - **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**).

Further Readings

- [HTFF05, chapter 9.2+6+7], [Mur12, chapter 16.1–2], [JWHT13, chapter 8.1+3].

References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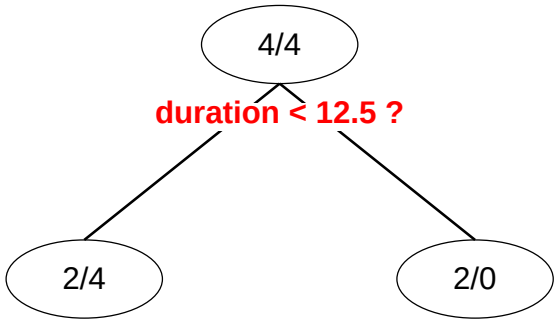
Example / Node 2 Split



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:

		buyer		
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	

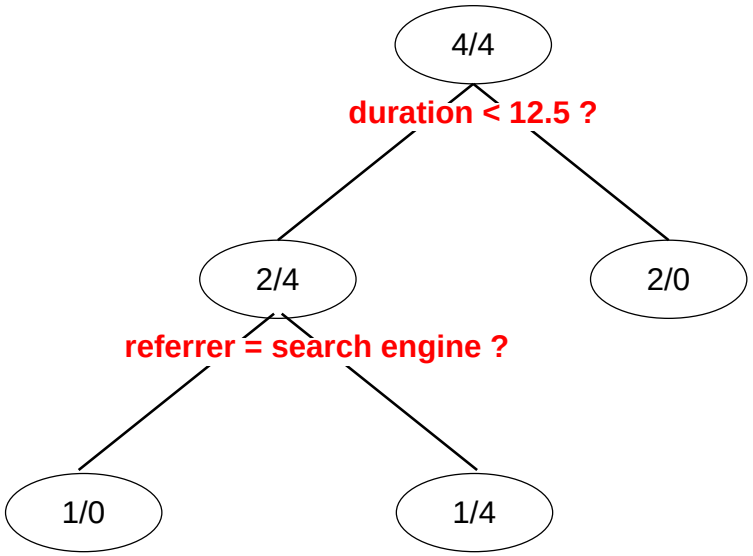
Again, the splits

- 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:

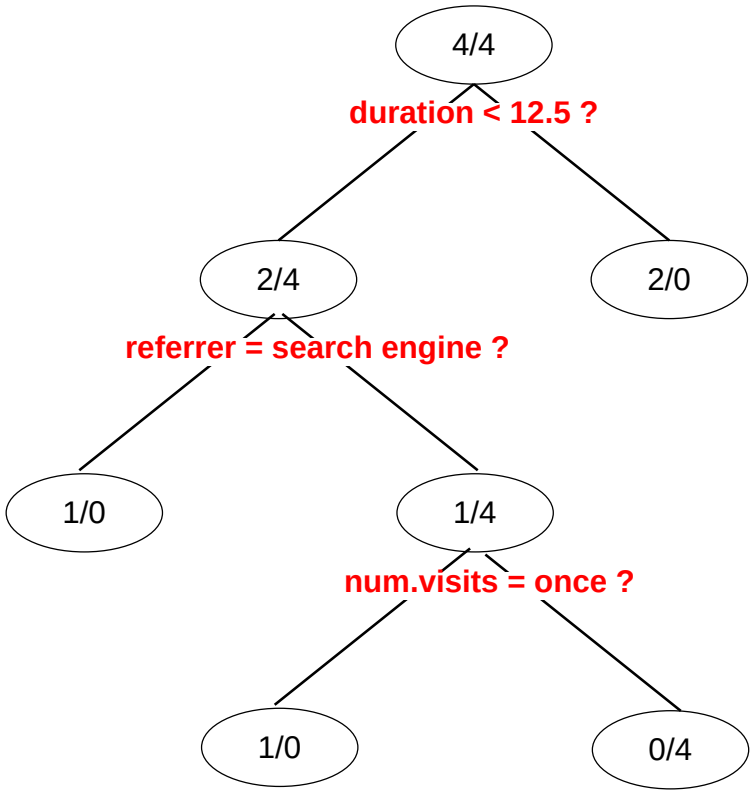
	referrer	num.visits	duration	buyer
3	other	several	5	yes
5	ad	once	10	no
6	other	once	10	no
7	other	once	5	no
8	ad	once	5	no

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.