Machine Learning: Symbolische Ansätze

- Introduction
  - Decision Trees
  - TDIDT: Top-Down Induction of Decision Trees
- ID3
  - Attribute selection
  - Entropy, Information, Information Gain
  - Gain Ratio
- C4.5
  - Numeric Values
  - Missing Values
  - Pruning
- Regression and Model Trees

Acknowledgements:
Many slides based on Frank & Witten, a few on Kan, Steinbach & Kumar

Decision Trees

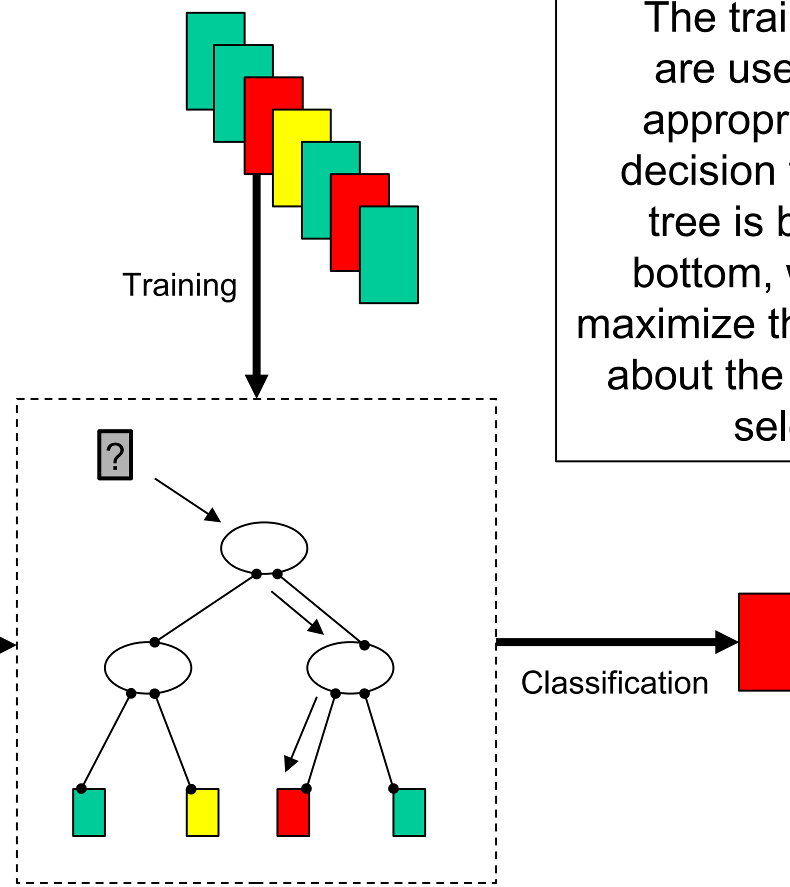
- a decision tree consists of
  - **Nodes:**
    - test for the value of a certain attribute
  - **Edges:**
    - correspond to the outcome of a test
    - connect to the next node or leaf
  - **Leaves:**
    - terminal nodes that predict the outcome

to classifiy an example:

1. start at the root
2. perform the test
3. follow the edge corresponding to outcome
4. goto 2. unless leaf
5. predict that outcome associated with the leaf

Decision Tree Learning

In ***Decision Tree Learning***, a new example is classified by submitting it to a series of tests that determine the class label of the example.These tests are organized in a hierarchical structure called a *decision tree*.



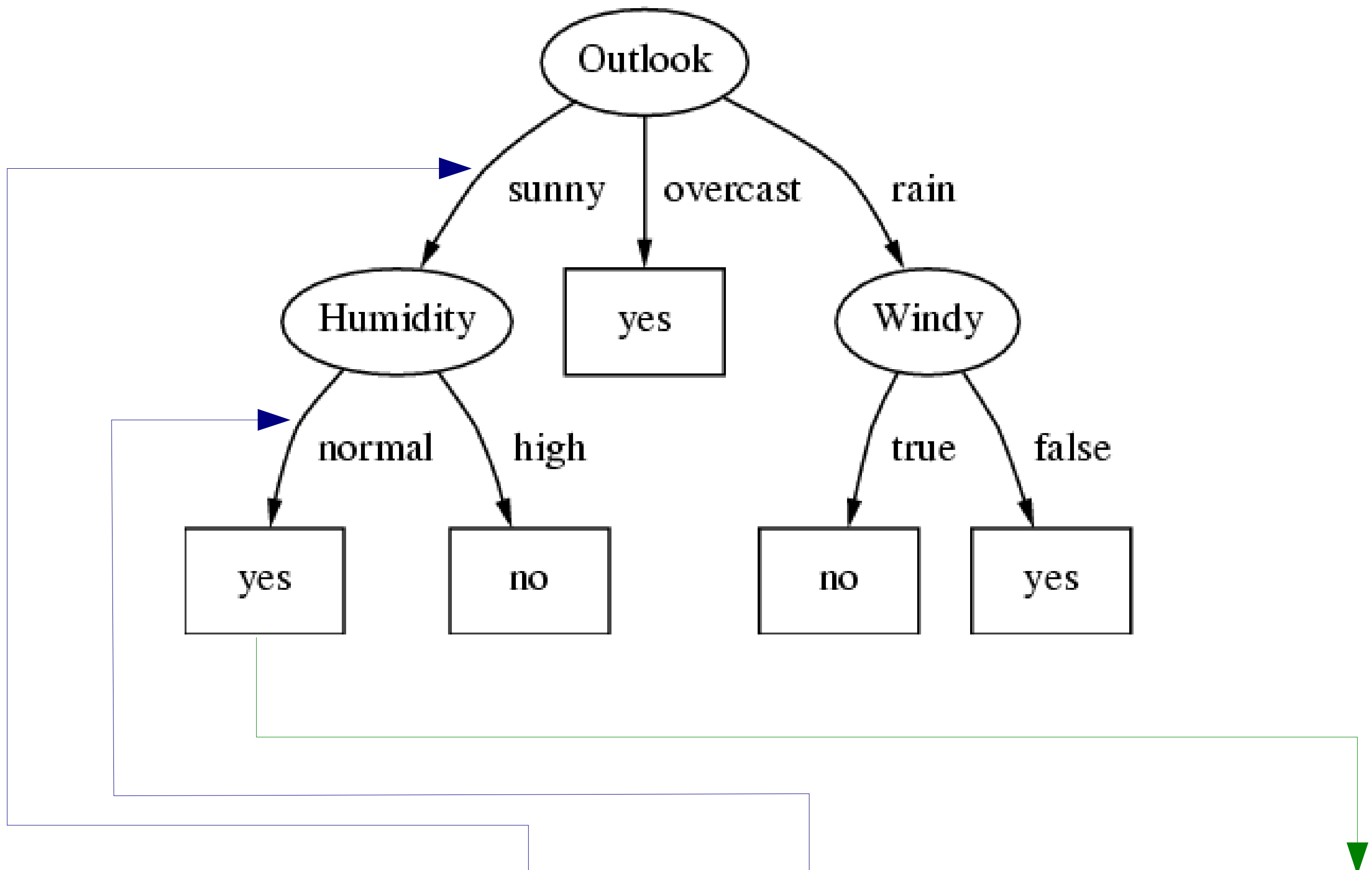
The training examples are used for choosing appropriate tests in the decision tree. Typically, a tree is built from top to bottom, where tests that maximize the information gain about the classification are selected first.

A Sample Task

Day	Temperature	Outlook	Humidity	Windy	Play Golf?
07-05	hot	sunny	high	false	no
07-06	hot	sunny	high	true	no
07-07	hot	overcast	high	false	yes
07-09	cool	rain	normal	false	yes
07-10	cool	overcast	normal	true	yes
07-12	mild	sunny	high	false	no
07-14	cool	sunny	normal	false	yes
07-15	mild	rain	normal	false	yes
07-20	mild	sunny	normal	true	yes
07-21	mild	overcast	high	true	yes
07-22	hot	overcast	normal	false	yes
07-23	mild	rain	high	true	no
07-26	cool	rain	normal	true	no
07-30	mild	rain	high	false	yes

today	cool	sunny	normal	false	?
tomorrow	mild	sunny	normal	false	?

Decision Tree Learning



tomorrow	mild	sunny	normal	false	?

Divide-And-Conquer Algorithms

- Family of decision tree learning algorithms
  - TDIDT: Top-Down Induction of Decision Trees
- Learn trees in a Top-Down fashion:
  - divide the problem in subproblems
  - solve each problem

Basic Divide-And-Conquer Algorithm:

1. select a test for root node
   Create branch for each possible outcome of the test
2. split instances into subsets
   One for each branch extending from the node
3. repeat recursively for each branch, using only instances that reach the branch
4. stop recursion for a branch if all its instances have the same class

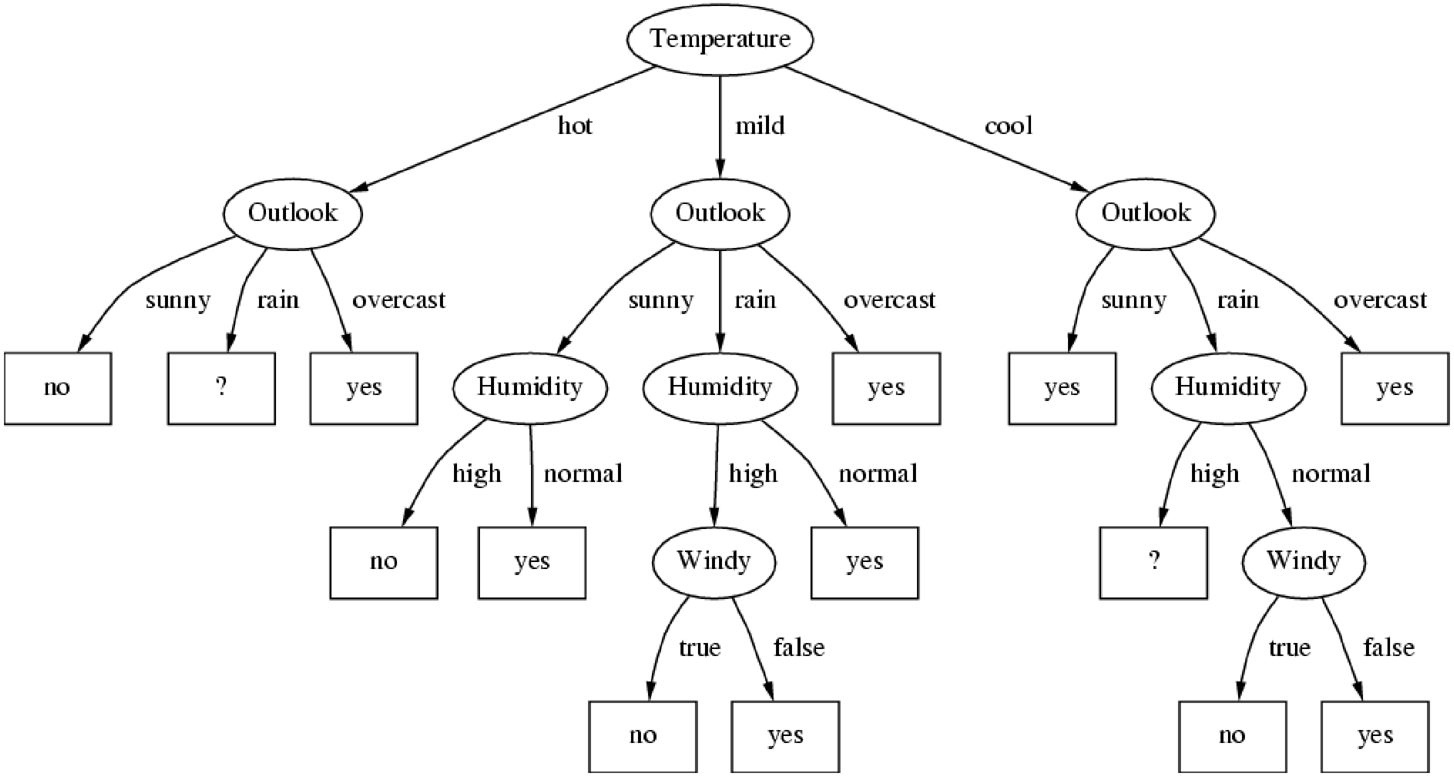
ID3 Algorithm

Function ID3

- **Input:** Example set S
- **Output:** Decision Tree DT

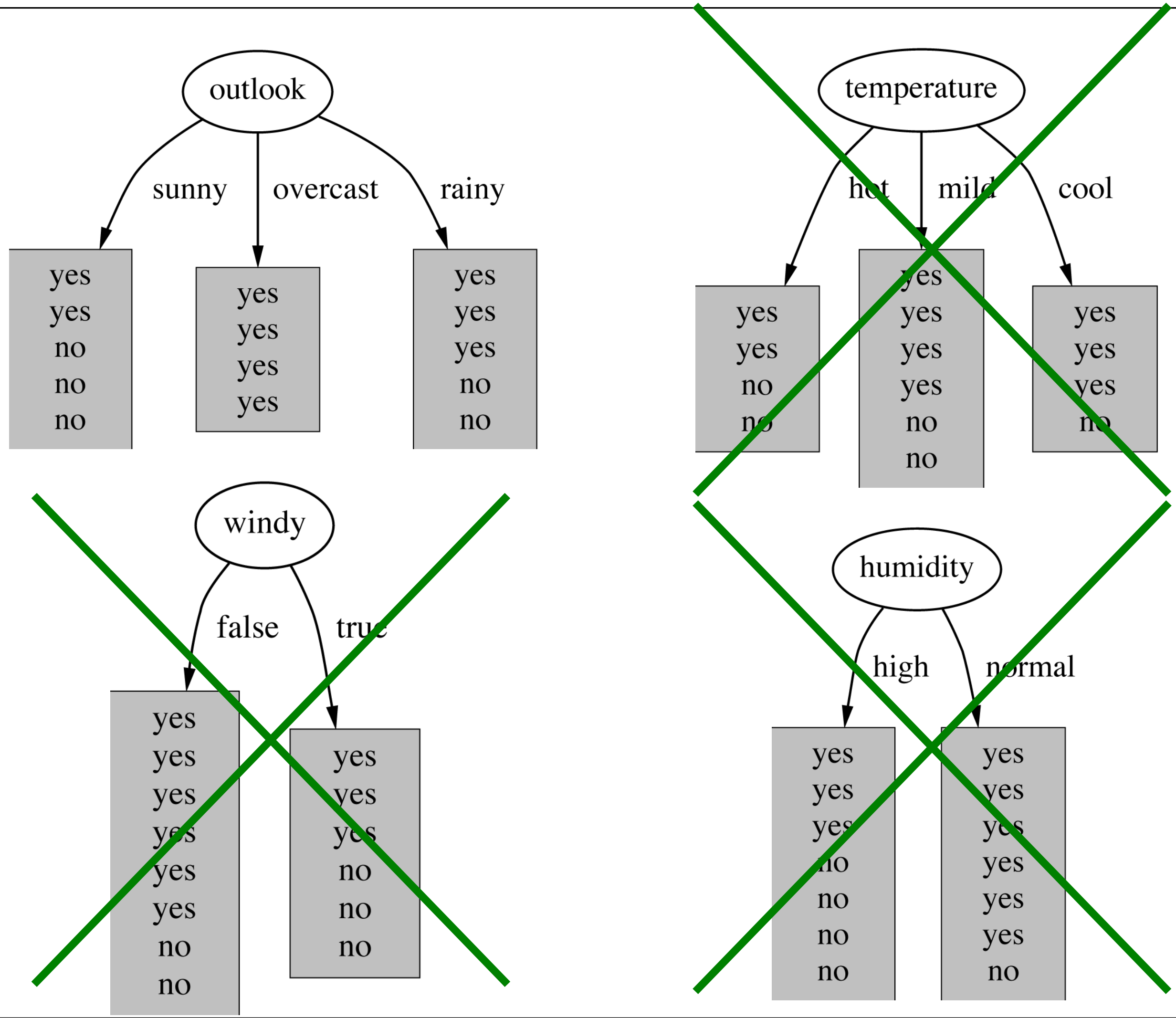
- If all examples in S belong to the same class c
  - return a new leaf and label it with c
- Else
  i. Select an attribute A according to some heuristic function
  ii. Generate a new node DT with A as test
  iii. For each Value v_i of A
    (a) Let S_i = all examples in S with $A = v_i$
    (b) Use ID3 to construct a decision tree DT_i for example set S_i
    (c) Generate an edge that connects DT and DT_i

A Different Decision Tree



- also explains all of the training data
- will it generalize well to new data?

Which attribute to select as the root?



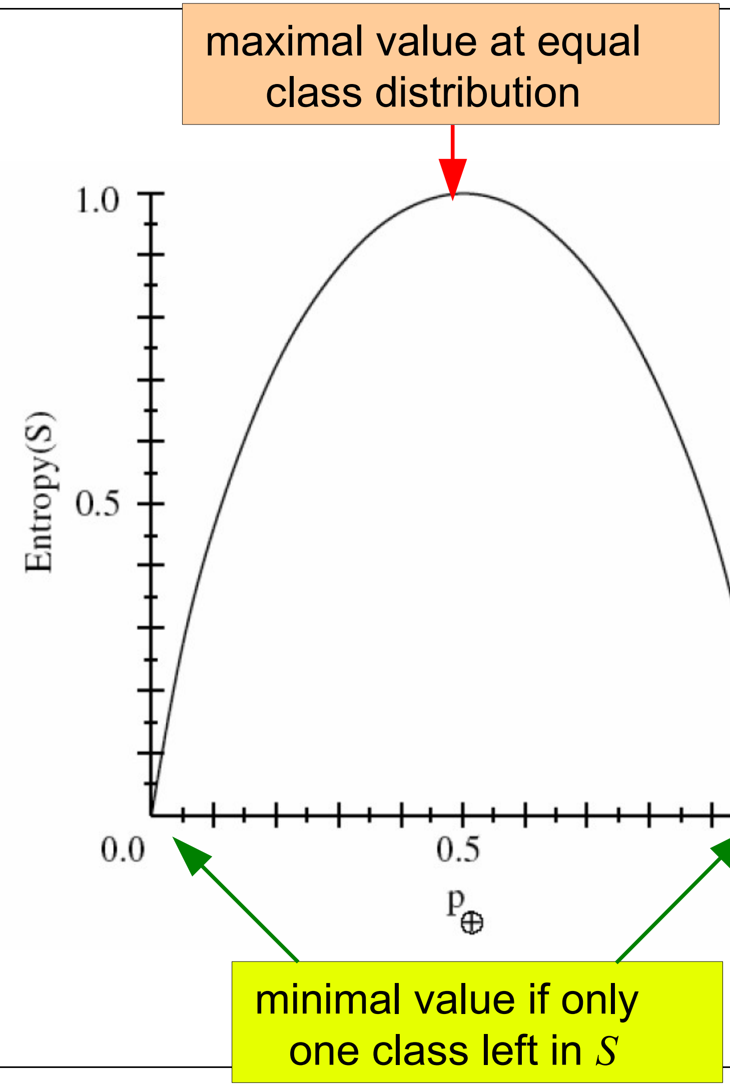
What is a good Attribute?

- We want to grow a simple tree
  → a good heuristic prefers attributes that split the data so that each successor node is as *pure* as posssible
  - i.e., the distribution of examples in each node is so that it mostly contains examples of a single class
- In other words:
  - We want a measure that prefers attributes that have a high degree of „order“:
    - Maximum order: All examples are of the same class
    - Minimum order: All classes are equally likely

  → Entropy is a measure for (un-)orderedness
  - Another interpretation:
    - Entropy is the amount of information that is contained in the node
    - all examples of the same class → no information

Entropy (for two classes)

- S is a set of examples
- $p_\oplus$ is the proportion of examples in class $\oplus$
- $p_\ominus = 1 - p_\oplus$ is the proportion of examples in class $\ominus$



Entropy:

$$E(S) = -p_\oplus \cdot \log_2 p_\oplus - p_\ominus \cdot \log_2 p_\ominus$$

- Interpretation:
  - amount of unorderedness in the class distribution of S

Example: Attribute Outlook

- Outlook = sunny: 2 examples yes, 3 examples no

$$E(\text{Outlook}=\text{sunny}) = -\frac{2}{5}\log_2\left(\frac{2}{5}\right) - \frac{3}{5}\log_2\left(\frac{3}{5}\right) = 0.971$$

- Outlook = overcast: 4 examples yes, 0 examples no

$$E(\text{Outlook}=\text{overcast}) = -1\cdot\log_2(1) - 0\cdot\log_2(0) = 0$$

Note: this is normally undefined. Here: = 0

- Outlook = rainy : 3 examples yes, 2 examples no

$$E(\text{Outlook}=\text{rainy}) = -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$$

Entropy (for more classes)

Entropy can be easily generalized for $n > 2$ classes

- p_i is the proportion of examples in S that belong to the i-th class

$$E(S) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 \ldots - p_n \log_2 p_n = -\sum_{i=1}^{n} p_i \log_2 p_i$$

- Calculation can be simplified using absolute counts c_i of examples in class i instead of fractions
  - If $p_i = \frac{c_i}{|S|}$:

$$E(S) = -\sum_{i=1}^{n} p_i \log_2 p_i = -\frac{1}{|S|} \cdot \left(\sum_{i=1}^{n} c_i \log_2 c_i - |S| \cdot \log_2 |S| \right)$$

  - Example:

$$E([2,3,4]) = -\tfrac{2}{9} \cdot \log_2\left(\tfrac{2}{9}\right) - \tfrac{3}{9} \cdot \log_2\left(\tfrac{3}{9}\right) - \tfrac{4}{9} \cdot \log_2\left(\tfrac{4}{9}\right)$$
$$= -\tfrac{1}{9}\left(2 \cdot \log_2(2) + 3 \cdot \log_2(3) + 4 \cdot \log_2(4) - 9 \cdot \log_2(9)\right)$$

Average Entropy / Information

- **Problem:**
  - Entropy only computes the quality of a single (sub-)set of examples
    - corresponds to a single value
  - How can we compute the quality of the entire split?
    - corresponds to an entire attribute
- **Solution:**
  - Compute the weighted average over all sets resulting from the split
    - weighted by their size

$$I(S, A) = \sum_i \frac{|S_i|}{|S|} \cdot E(S_i)$$

- **Example:**
  - Average entropy for attribute *Outlook*:

$$I(\text{Outlook}) = \frac{5}{14} \cdot 0.971 + \frac{4}{14} \cdot 0 + \frac{5}{14} \cdot 0.971 = 0.693$$

Information Gain

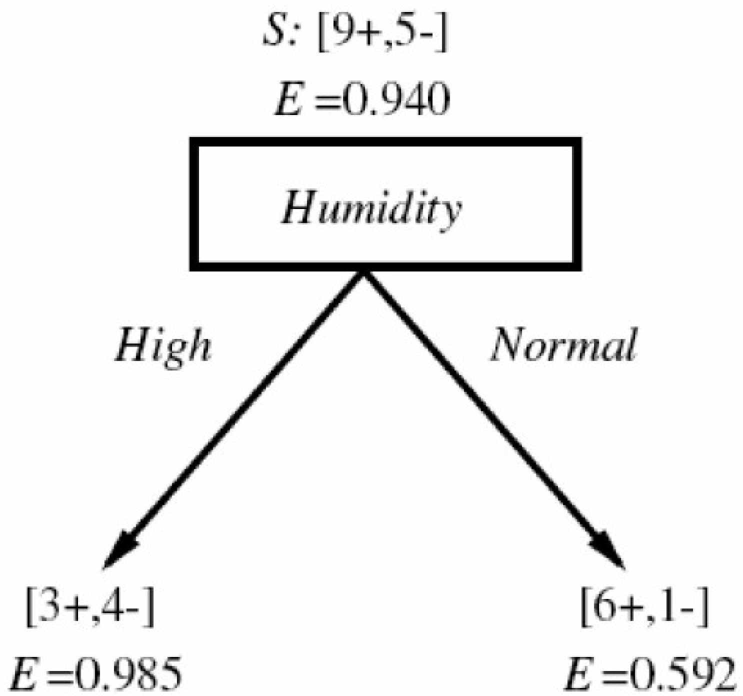
- When an attribute A splits the set S into subsets S_i
  - we compute the average entropy
  - and compare the sum to the entropy of the original set S

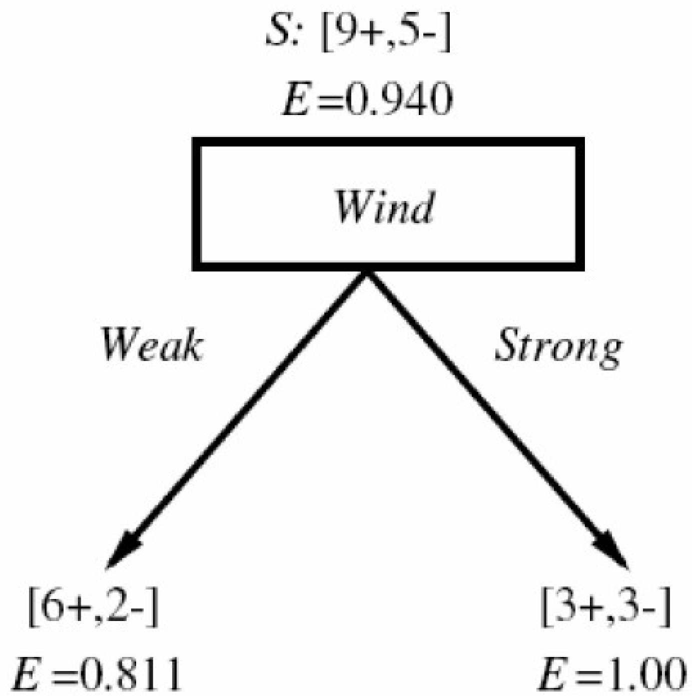
Information Gain for Attribute A

$$Gain(S,A) = E(S) - I(S,A) = E(S) - \sum_i \frac{|S_i|}{|S|} \cdot E(S_i)$$

- The attribute that maximizes the difference is selected
  - i.e., the attribute that reduces the unorderedness most!
- **Note:**
  - maximizing information gain is equivalent to minimizing average entropy, because $E(S)$ is constant for all attributes A

Example





Gain (S, Humidity)

= .940 - (7/14).985 - (7/14).592
= .151

Gain (S, Wind)

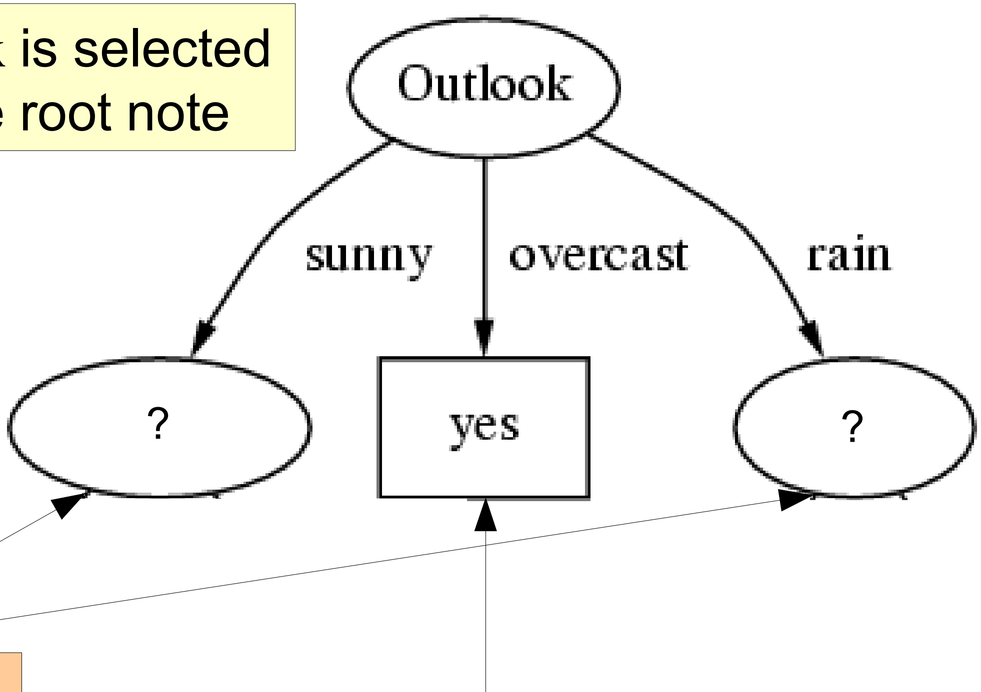
= .940 - (8/14).811 - (6/14)1.0
= .048

$$Gain(S, Outlook) = 0.246$$

$$Gain(S, Temperature) = 0.029$$

Example (Ctd.)

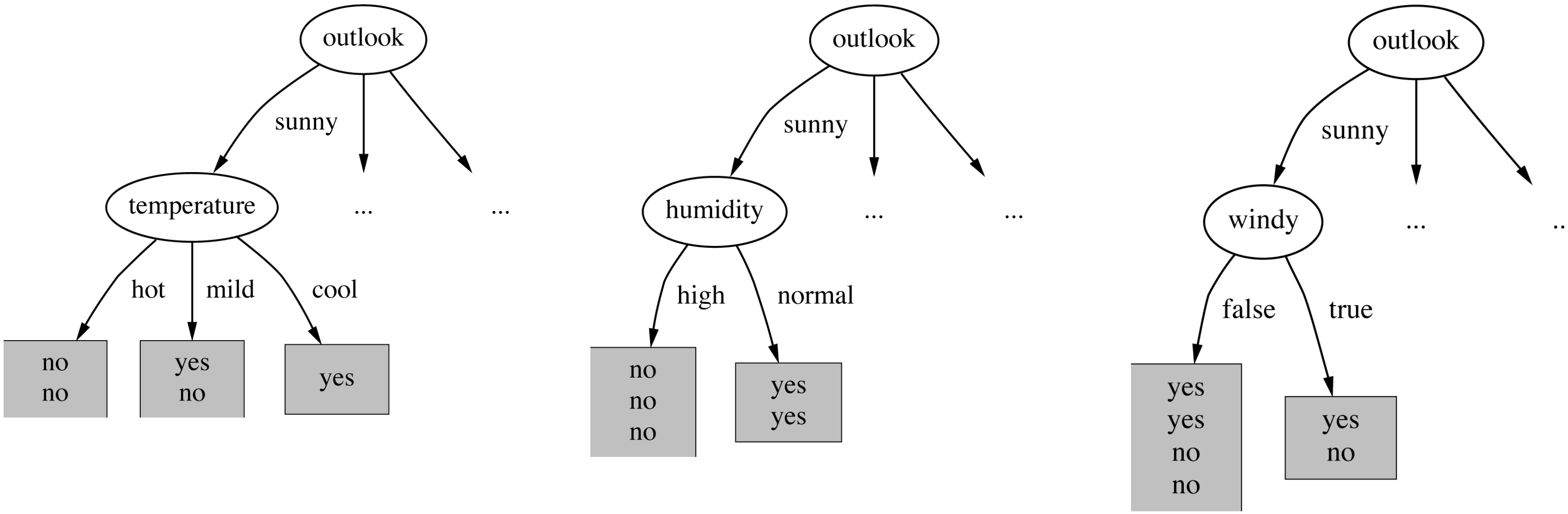
Outlook is selected as the root note



further splitting necessary

Outlook = overcast contains only examples of class **yes**

Example (Ctd.)

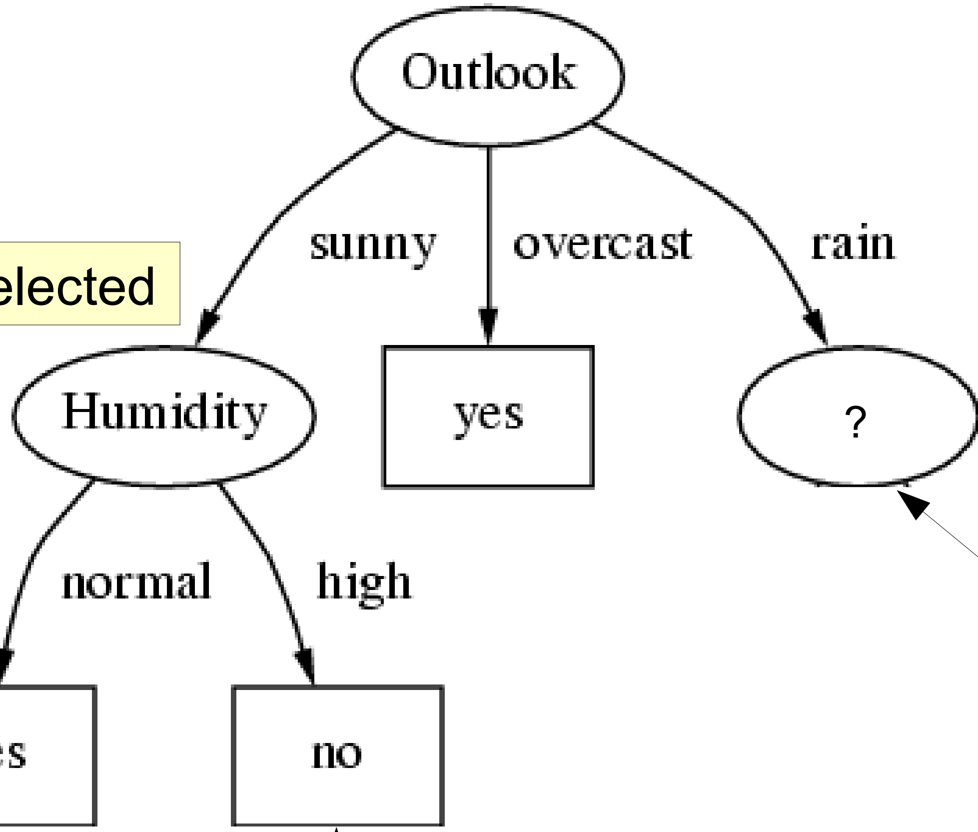


$$\left.\begin{aligned} \text{Gain}(\mathit{Temperature}) &= 0.571 \text{ bits} \\ \text{Gain}(\mathit{Humidity}) &= 0.971 \text{ bits} \\ \text{Gain}(\mathit{Windy}) &= 0.020 \text{ bits} \end{aligned}\right\}$$

Humidity is selected

Example (Ctd.)

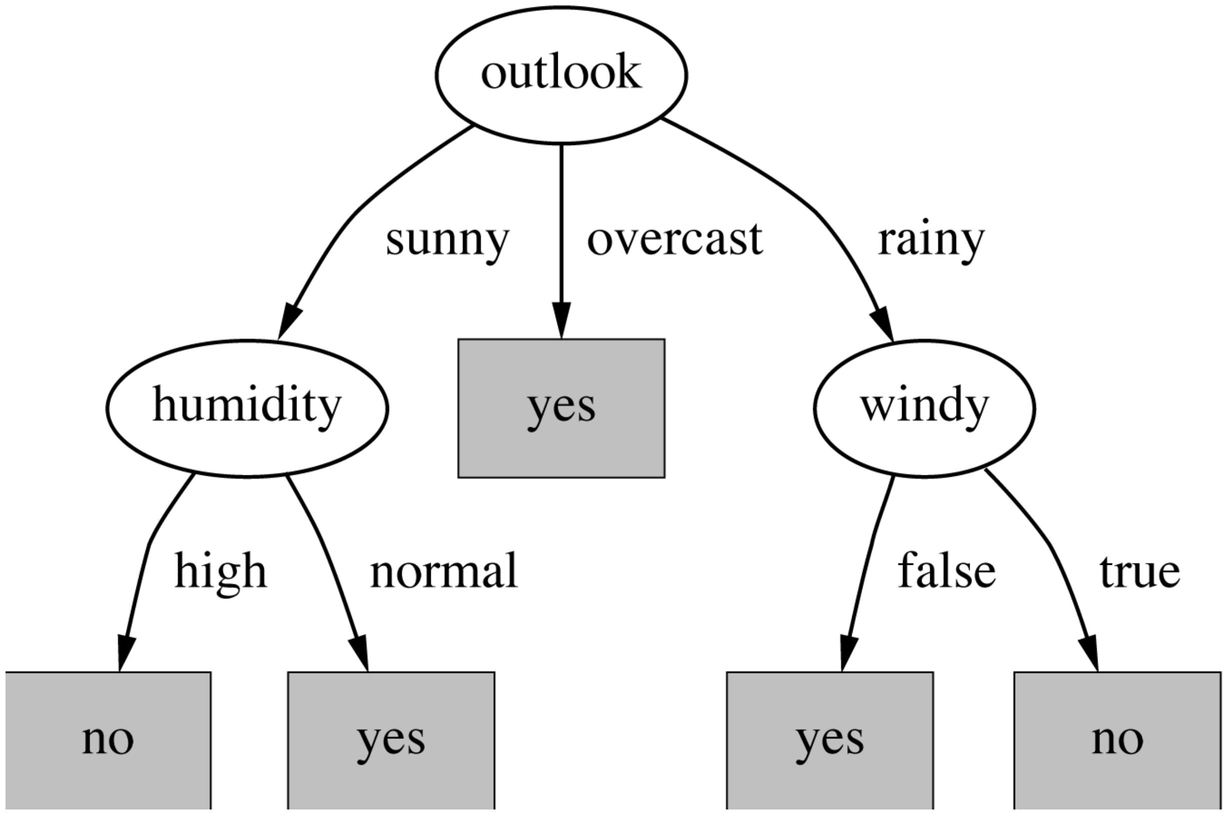
Humidity is selected



further splitting necessary

Pure leaves
→ No further expansion necessary

Final decision tree



Properties of Entropy

Entropy is the only function that satisfies all of the following three properties

1. When node is pure, measure should be zero
2. When impurity is maximal (i.e. all classes equally likely), measure should be maximal
3. Measure should obey multistage property:
   - p, q, r are classes in set S, and T are examples of class $t = q \vee r$

$$E_{p,q,r}(S) = E_{p,t}(S) + \frac{|T|}{|S|} \cdot E_{q,r}(T)$$

   $\rightarrow$ decisions can be made in several stages
   - For example:

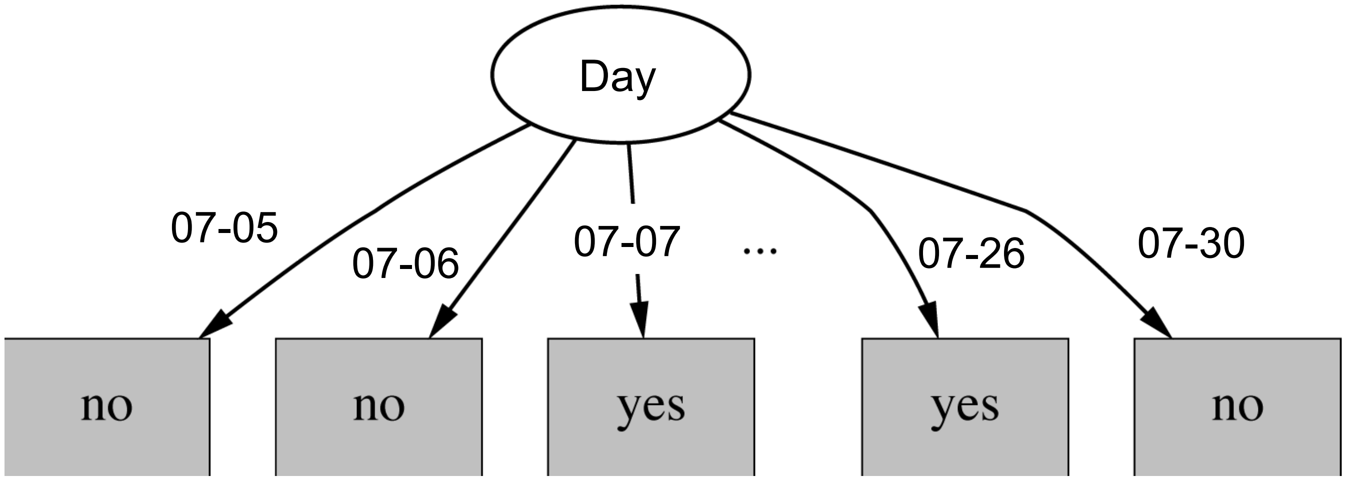
$$E([2,3,4]) = E([2,7]) + \tfrac{7}{9} \cdot E([3,4])$$

Highly-branching attributes

Problematic: attributes with a large number of values

- extreme case: each example has its own value
  - e.g. example ID; Day attribute in weather data
- Subsets are more likely to be pure if there is a large number of different attribute values
  - Information gain is biased towards choosing attributes with a large number of values
- This may cause several problems:
  - Overfitting
    - selection of an attribute that is non-optimal for prediction
  - Fragmentation
    - data are fragmented into (too) many small sets

Decision Tree for Day attribute



- Entropy of split:

$$I(\mathrm{Day}) = \frac{1}{14}\left(E([0,1]) + E([0,1]) + \ldots + E([0,1])\right) = 0$$

  - Information gain is maximal for Day (0.940 bits)

Intrinsic Information of an Attribute

- Intrinsic information of a split
  - entropy of distribution of instances into branches
  - i.e. how much information do we need to tell which branch an instance belongs to

$$IntI(S, A) = -\sum_i \frac{|S_i|}{|S|} \log_2 \left(\frac{|S_i|}{|S|} \right)$$

- Example:
  - Intrinsic information of Day attribute:

$$IntI(\mathrm{Day}) = 14 \times \left(-\tfrac{1}{14} \cdot \log_2 \left(\tfrac{1}{14} \right) \right) = 3.807$$

- Observation:
  - Attributes with higher intrinsic information are less useful

Gain Ratio

- modification of the information gain that reduces its bias towards multi-valued attributes
- takes number and size of branches into account when choosing an attribute
  - corrects the information gain by taking the *intrinsic information* of a split into account
- Definition of Gain Ratio:

$$GR(S,A) = \frac{Gain(S,A)}{IntI(S,A)}$$

- Example:
  - Gain Ratio of Day attribute

$$GR(\mathrm{Day}) = \frac{0.940}{3{,}807} = 0.246$$

Gain ratios for weather data

Outlook		Temperature	
Info:	0.693	Info:	0.911
Gain: 0.940-0.693	0.247	Gain: 0.940-0.911	0.029
Split info: info([5,4,5])	1.577	Split info: info([4,6,4])	1.557
Gain ratio: 0.247/1.577	0.157	Gain ratio: 0.029/1.557	0.019
Humidity		**Windy**	
Info:	0.788	Info:	0.892
Gain: 0.940-0.788	0.152	Gain: 0.940-0.892	0.048
Split info: info([7,7])	1.000	Split info: info([8,6])	0.985
Gain ratio: 0.152/1	0.152	Gain ratio: 0.048/0.985	0.049

- Day attribute would still win...
  - one has to be careful which attributes to add...
- Nevertheless: Gain ratio is more reliable than Information Gain

Gini Index

- Many alternative measures to Information Gain
- Most popular altermative: Gini index
  - used in e.g., in CART (Classification And Regression Trees)
  - impurity measure (instead of entropy)

$$Gini(S) = \sum_i p_i \cdot (1 - p_i) = 1 - \sum_i p_i^2$$

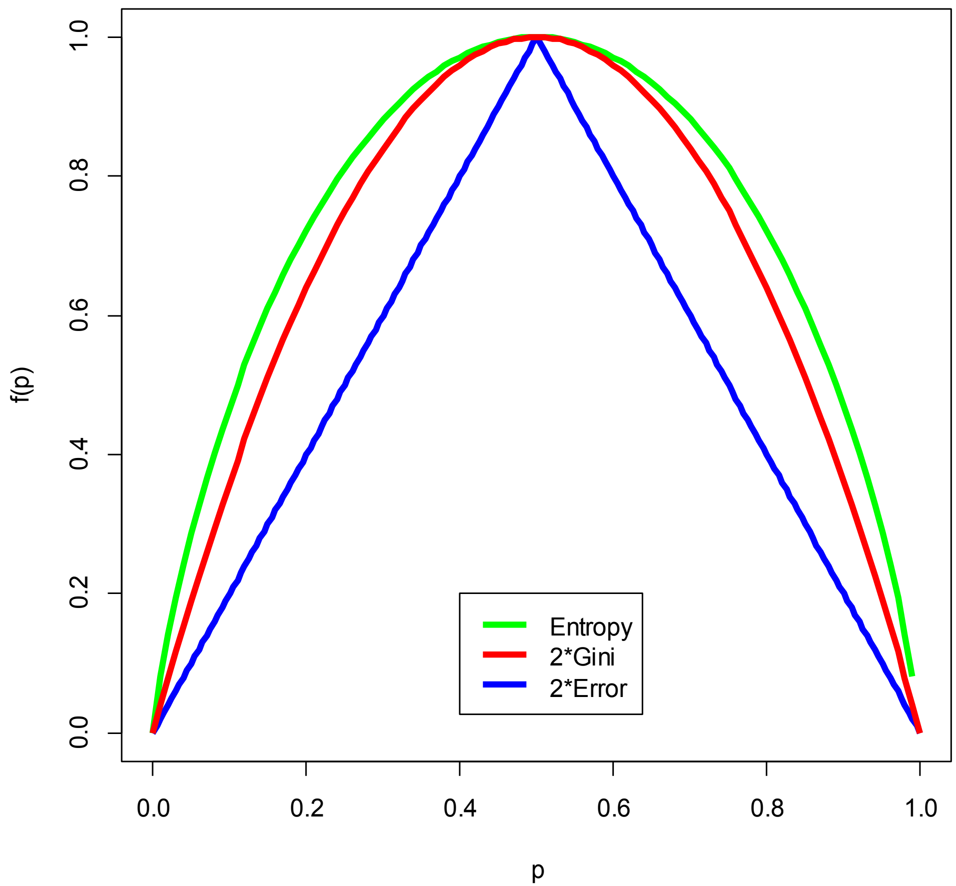
  - average Gini index (instead of average entropy / information)

$$Gini(S, A) = \sum_i \frac{|S_i|}{|S|} \cdot Gini(S_i)$$

- Gini Gain
  - could be defined analogously to information gain
  - but typically averageGini index is minimized instead of maximizing Gini gain

Comparison of Splitting Criteria

For a 2-class problem:



Why not use Error as a Splitting Criterion?

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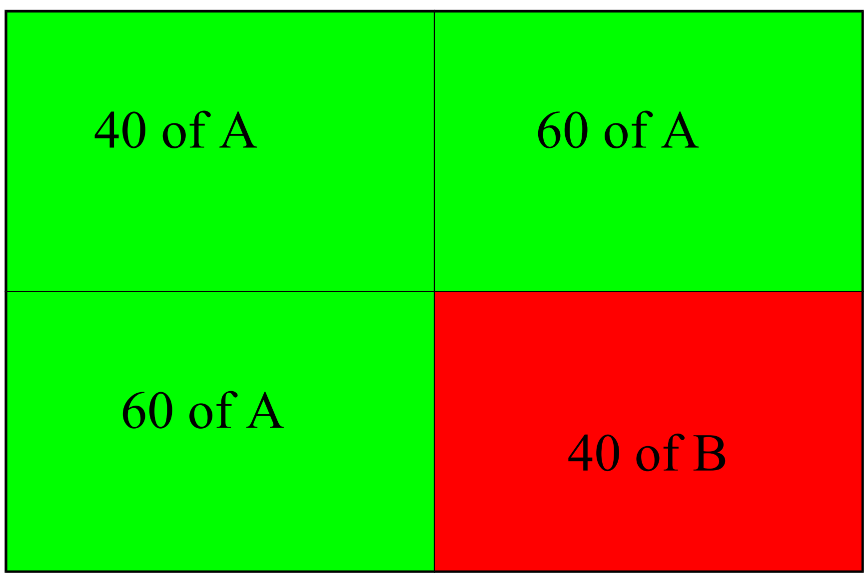
- Reason:
  - The bias towards pure leaves is not strong enough
- Example 1: Data set with 160 Examples A, 40 Examples B
  - → Error rate without splitting is 20%

Split 1



Split 2

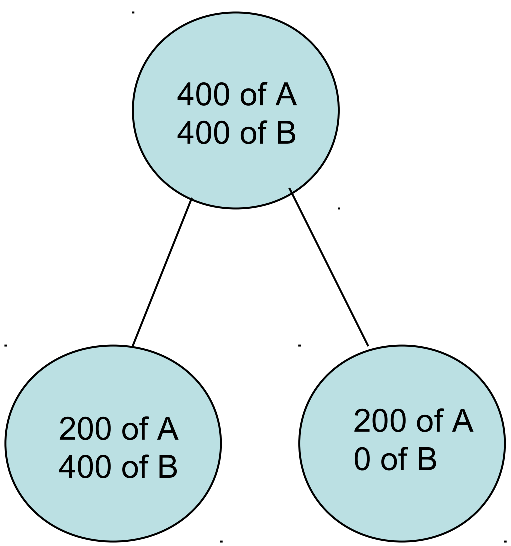
For each of the two splits, the total error after splitting is also (0% + 40%)/2 = 20%
→ no improvement

However, together both splits would give a perfect classfier.

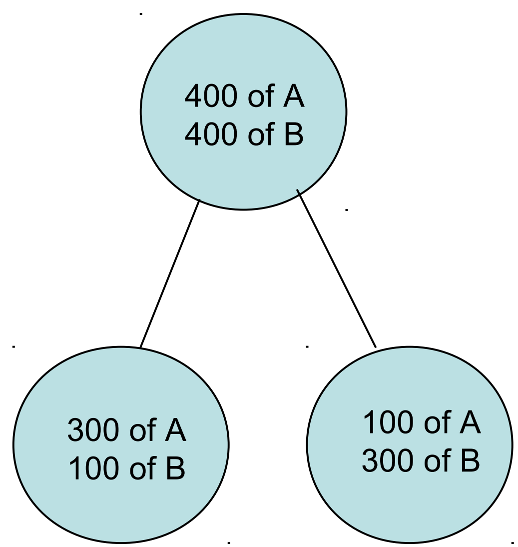
Based on a slide by Richard Lawton

Why not use Error as a Splitting Criterion?

- Reason:
  - The bias towards pure leaves is not strong enough
- Example 2:
  - Dataset with 400 examples of class A and 400 examples of class B



Error rate = 25%



Error rate = 25%

Based on a slide by Richard Lawton

Industrial-strength algorithms

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- For an algorithm to be useful in a wide range of real-world applications it must:
  - Permit numeric attributes
  - Allow missing values
  - Be robust in the presence of noise
  - Be able to approximate arbitrary concept descriptions (at least in principle)

→ ID3 needs to be extended to be able to deal with real-world data

- Result: **C4.5**
  - Best-known and (probably) most widely-used learning algorithm
    - original C-implementation at http://www.rulequest.com/Personal/
  - Re-implementation of C4.5 Release 8 in Weka: J4.8
  - Commercial successor: C5.0

Missing values

- Examples are classified as usual
  - if we are lucky, attributes with missing values are not tested by the tree
- If an attribute with a missing value needs to be tested:
  - split the instance into fractional instances (*pieces*)
  - one piece for each outgoing branch of the node
  - a piece going down a branch receives a weight proportional to the popularity of the branch
  - weights sum to 1
- Info gain or gain ratio work with fractional instances
  - use sums of weights instead of counts
- during classification, split the instance in the same way
  - Merge probability distribution using weights of fractional instances

Numeric attributes

- Standard method: binary splits
  - E.g. temp < 45
- Unlike nominal attributes, every attribute has many possible split points
- Solution is straightforward extension:
  - Evaluate info gain (or other measure) for every possible split point of attribute
  - Choose “best” split point
  - Info gain for best split point is info gain for attribute

→ Computationally more demanding than splits on discrete attributes

Example

- Assume a numerical attribute for Temperature
- First step:
  - Sort all examples according to the value of this attribute
  - Could look like this:

64	65	68	69	70	71	72	72	75	75	80	81	83	85
Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

Temperature < 71.5: yes/4, no/2

Temperature ≥ 71.5: yes/5, no/3

$$I(\text{Temperature} @ 71.5) = \frac{6}{14} \cdot E(\text{Temperature} < 71.5) + \frac{8}{14} E(\text{Temperature} \geq 71.5) = 0.939$$

- Split points can be placed between values or directly at values
- Has to be computed for all pairs of neighboring values

Efficient Computation

- Efficient computation needs only one scan through the values!
  - Linearly scan the sorted values, each time updating the count matrix and computing the evaluation measure
  - Choose the split position that has the best value

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
	Taxable Income									
Sorted Values	60	70	75	85	90	95	100	120	125	220

Split Positions	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
Gini	0.420		0.400		0.375		0.343		0.417		0.400		*0.300*		0.343		0.375		0.400		0.420	

Binary *vs.* Multiway Splits

- Splitting (multi-way) on a nominal attribute exhausts all information in that attribute
  - Nominal attribute is tested (at most) once on any path in the tree
- Not so for binary splits on numeric attributes!
  - Numeric attribute may be tested several times along a path in the tree
- Disadvantage: tree is hard to read
- Remedy:
  - pre-discretize numeric attributes (→ discretization), or
  - use multi-way splits instead of binary ones
    - can, e.g., be computed by building a subtree using a single numerical attribute.
    - subtree can be flattened into a multiway split
    - other methods possible (dynamic programming, greedy...)

Overfitting and Pruning

- The smaller the complexity of a concept, the less danger that it overfits the data
  - A polynomial of degree n can always fit $n+1$ points
- Thus, learning algorithms try to keep the learned concepts simple
  - Note a „perfect“ fit on the training data can always be found for a decision tree! (except when data are contradictory)

Pre-Pruning:

- stop growing a branch when information becomes unreliable

Post-Pruning:

- grow a decision tree that correctly classifies all training data
- simplify it later by replacing some nodes with leafs

- Postpruning preferred in practice—prepruning can “stop early”

Prepruning

- Based on statistical significance test
  - Stop growing the tree when there is no *statistically significant* association between any attribute and the class at a particular node
- Most popular test: *chi-squared test*
- ID3 used chi-squared test in addition to information gain
  - Only statistically significant attributes were allowed to be selected by information gain procedure

- C4.5 uses a simpler strategy
  - but combines it with → post-pruning
  - parameter $-m$: (default value $m=2$)
    each node above a leave must have
    - at least two successors
    - that contain at least m examples

Early Stopping

- Pre-pruning may stop the growth process prematurely: *early stopping*
- Classic example: XOR/Parity-problem
  - No individual attribute exhibits any significant association to the class

	a	b	class
1	0	0	0
2	0	1	1
3	1	0	1
4	1	1	0

→ In a dataset that contains XOR attributes a and b, and several irrelevant (e.g., random) attributes, ID3 can not distinguish between relevant and irrelevant attributes

→ Prepruning won't expand the root node

  - Structure is only visible in fully expanded tree
- But:
  - XOR-type problems rare in practice
  - prepruning is faster than postpruning

Post-Pruning

- basic idea
  - first grow a full tree to capture all possible attribute interactions
  - later remove those that are due to chance

1. learn a complete and consistent decision tree that classifies all examples in the training set correctly
2. as long as the performance increases
   - try simplification operators on the tree
   - evaluate the resulting trees
   - make the replacement that results in the best estimated performance
3. return the resulting decision tree

Postpruning

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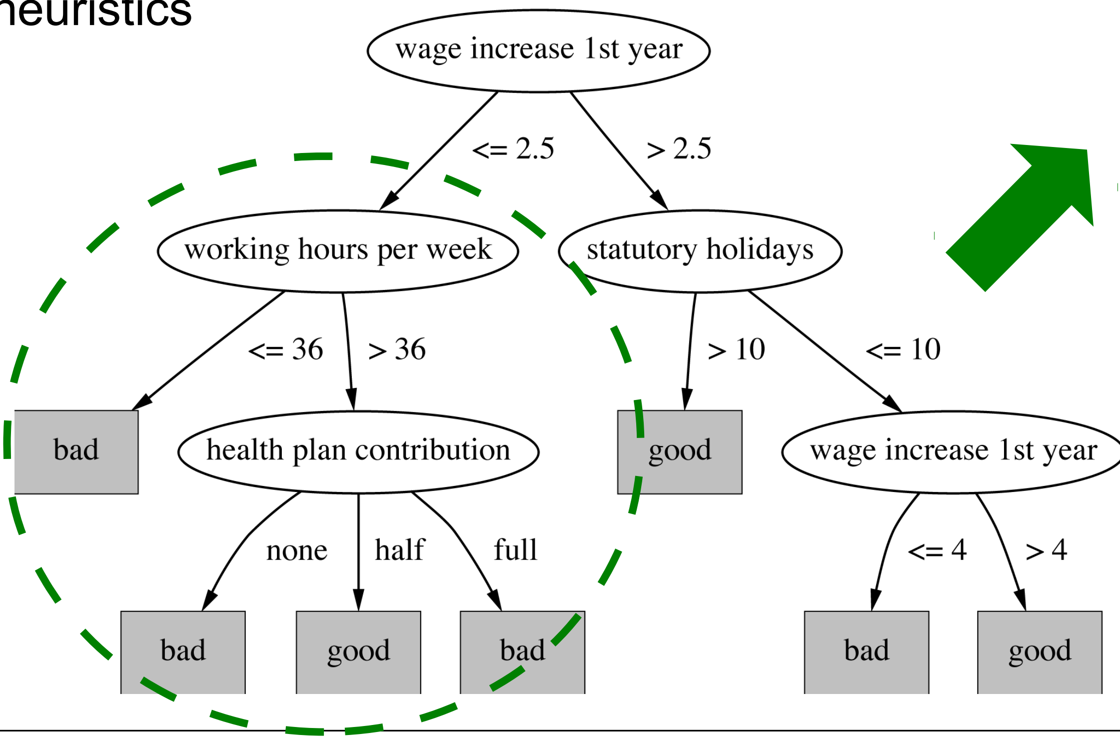
- Two subtree simplification operators
  - Subtree replacement
  - Subtree raising

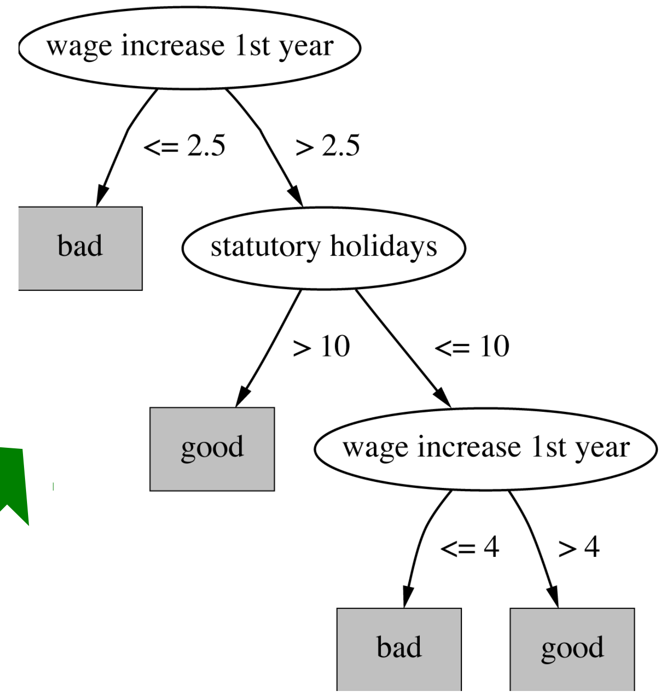
- Possible performance evaluation strategies
  - error estimation
    - on separate pruning set („reduced error pruning“)
    - with confidence intervals (C4.5's method)
  - significance testing
  - MDL principle

Subtree Replacement

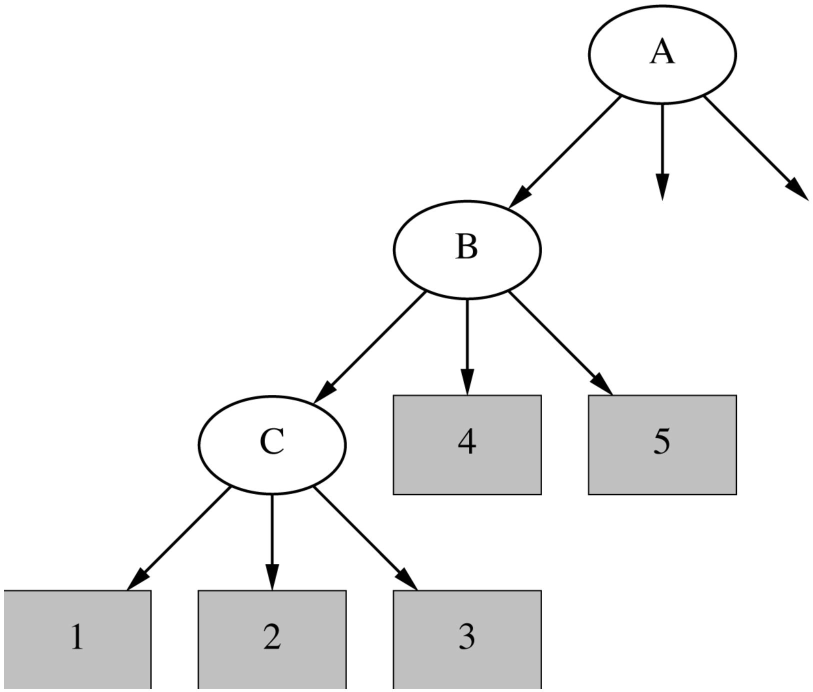
Proceeds Bottom-up:

- consider replacing a tree only after considering all its subtrees
- may make a difference for complexity-based heuristics

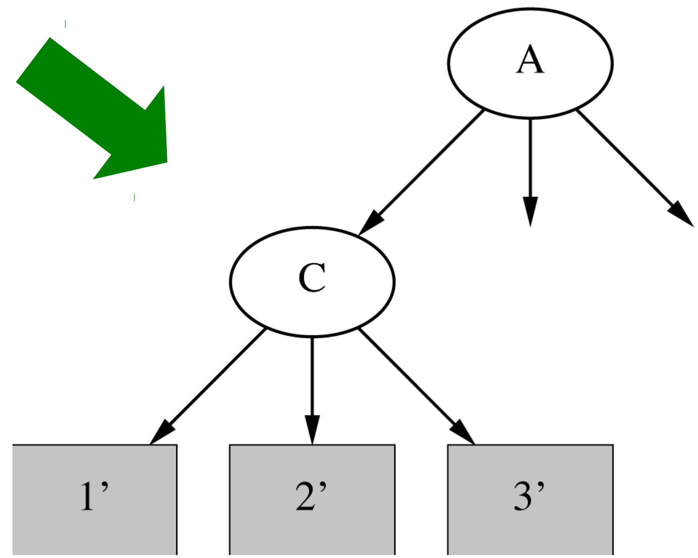




Subtree Raising



- Delete node B
- Redistribute instances of leaves 4 and 5 into C



Estimating Error Rates

- Prune only if it does not increase the estimated error
  - Error on the training data is NOT a useful estimator (would result in almost no pruning)
- Reduced Error Pruning
  - Use hold-out set for pruning
  - Essentially the same as in rule learning
    - only pruning operators differ (subtree replacement)
- C4.5's method
  - Derive confidence interval from training data
    - with a user-provided confidence level
  - Assume that the true error is on the upper bound of this confidence interval (pessimistic error estimate)

Reduced Error Pruning

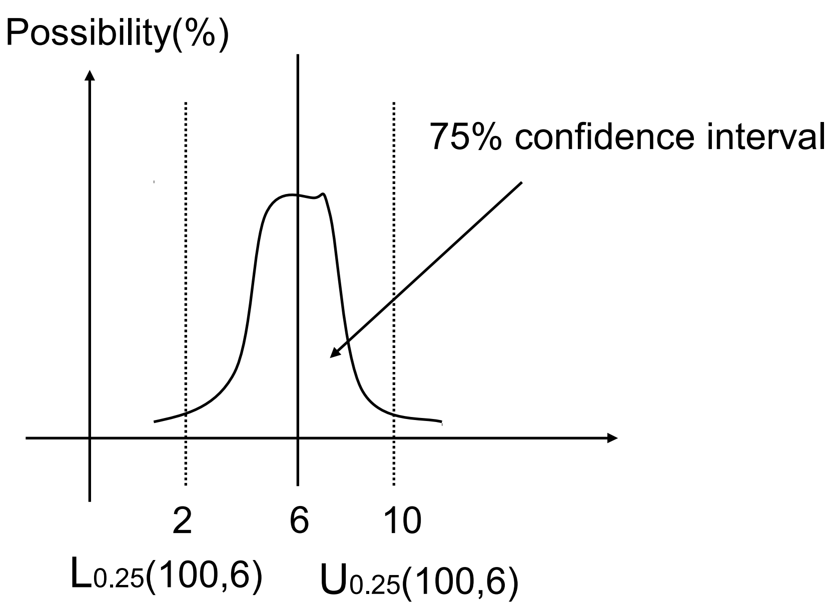
Basic Idea

- optimize the accuracy of a decision tree on a separate pruning set

1. split training data into a growing and a pruning set
2. learn a complete and consistent decision tree that classifies all examples in the growing set correctly
3. as long as the error on the pruning set does not increase
   - try to replace each node by a leaf (predicting the majority class)
   - evaluate the resulting (sub-)tree on the pruning set
   - make the replacement that results in the maximum error reduction
4. return the resulting decision tree

Pessimistic Error Rates

- Consider classifying E examples incorrectly out of N examples as observing E events in N trials in the binomial distribution.
- For a given confidence level CF, the upper limit on the error rate over the whole population is $U_{CF}(E,N)$ with CF% confidence.
- Example:
  - 100 examples in a leaf
  - 6 examples misclassified
  - How large is the true error assuming a pessimistic estimate with a confidence of 25%?
- Note:
  - this is only a heuristic!
  - but one that works well



C4.5's method

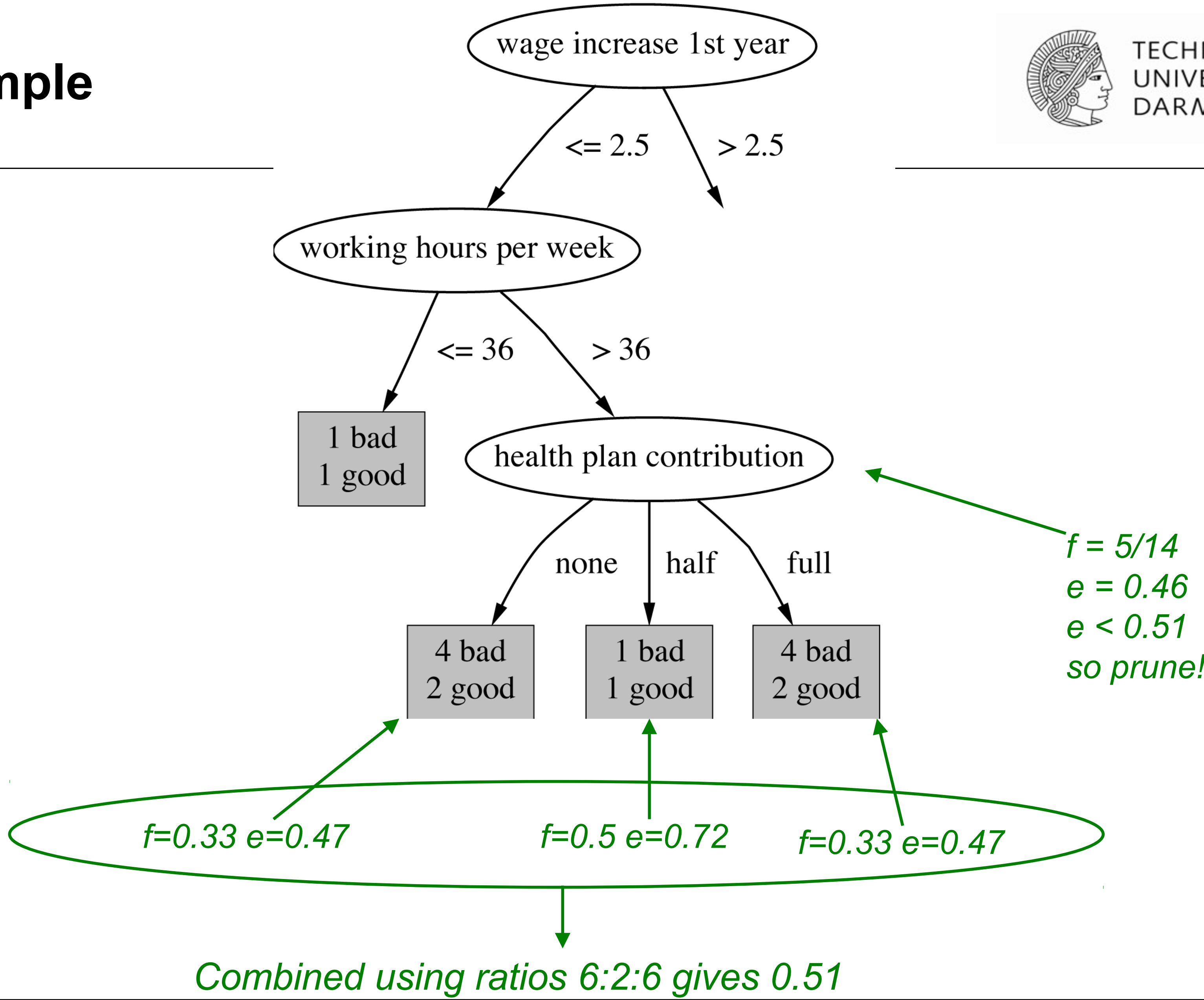
- Pessimistic error estimate for a node

$$e = \frac{f + \frac{z^2}{2N} + z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}}}{1 + \frac{z^2}{N}}$$

  - z is derived from the desired confidence value
    - If $c = 25\%$ then $z = 0.69$ (from normal distribution)
  - f is the error on the training data
  - N is the number of instances covered by the leaf
- Error estimate for subtree is weighted sum of error estimates for all its leaves

→ A node is pruned if error estimate of subtree is lower than error estimate of the node

Example



wage increase 1st year
<= 2.5
> 2.5
working hours per week
<= 36
> 36
1 bad
1 good
health plan contribution
none
half
full
4 bad
2 good
1 bad
1 good
4 bad
2 good
f = 5/14
e = 0.46
e < 0.51
so prune!
f=0.33 e=0.47
f=0.5 e=0.72
f=0.33 e=0.47
Combined using ratios 6:2:6 gives 0.51

C4.5: choices and options

- C4.5 has several parameters
  - `-c` Confidence value (default 25%):
    lower values incur heavier pruning
  - `-m` Minimum number of instances in the two most popular branches (default 2)
  - Others for, e.g., having only two-way splits (also on symbolic attributes), etc.

Sample Experimental Evaluation

Parameters	*Tree Size*	*Purity*	*Predictive Accuracy*
No Pruning (`C4.5 -m1`)	547	99.7%	60.3% (± 4.8)
`C4.5 -m2`	314	91.8%	60.1% (± 3.3)
`C4.5 -m5`	170	82.3%	60.4% (± 5.7)
`C4.5 -m10`	90	76.6%	60.0% (± 5.2)
`C4.5 -m15`	62	74.1%	61.6% (± 4.7)
`C4.5 -m20`	47	71.9%	62.7% (± 2.0)
`C4.5 -m25`	37	71.3%	63.0% (± 2.2)
`C4.5 -m30`	26	70.1%	65.1% (± 2.5)
`C4.5 -m35`	22	69.9%	65.0% (± 4.2)
`C4.5 -m40`	20	69.2%	64.8% (± 2.6)
`C4.5 -m50`	24	69.1%	64.5% (± 3.5)
`C4.5 -c75`	524	99.7%	61.0% (± 4.5)
`C4.5 -c50`	357	95.3%	60.2% (± 3.6)
`C4.5 -c25`	257	91.2%	62.3% (± 4.4)
`C4.5 -c15`	137	81.8%	64.8% (± 4.6)
`C4.5 -c10`	75	76.9%	65.9% (± 4.9)
`C4.5 -c5`	53	74.7%	63.8% (± 6.0)
`C4.5 -c1`	27	70.2%	63.4% (± 5.8)
`C4.5` Default	173	86.2%	62.5% (± 5.2)
`C4.5 -m30 -c10`	20	69.6%	66.7% (± 3.7)
Mode Prediction	1	56.8%	56.8%

Typical behavior with growing m and decreasing c

- tree size and training accuracy (= purity)
  - always decrease
- predictive accuracy
  - first increases (overfitting avoidance)
  - then decreases (over-generalization)
- ideal value *on this data set* near
  - $m = 30$
  - $c = 10$

Complexity of tree induction

- Assume
  - m attributes, n training instances
  - tree depth $O(\log n)$
  - tree has $O(n)$ nodes (≤ one leaf per example)

Costs for

- Building a tree $O(m\, n \log n)$
- Subtree replacement $O(n)$
    - counts of covered instances can be reused from training
- Subtree raising $O(n\, (\log n)^2)$
  - Every instance may have to be redistributed at every node between its leaf and the root
  - Cost for redistribution (on average): $O(\log n)$

→ Total cost: $O(m\, n \log n) + O(n\, (\log n)^2)$

Error-Complexity Measure

- CART uses the following measure

$$R_{\alpha}(T) = f(T) + \alpha \cdot L(T)$$

  - f is the error rate on the training data
  - L is the number leaves in the tree
  - α is a parameter that trades off tree complexity vs. test error

- Different values of α prefer different trees
  - smaller values of α prefer different trees with low training error
  - larger values of α prefer different trees with low training error
  - would nowadays be called a *regularization* parameter

Error-Complexity Pruning
(CART, Breiman et al. 1984)

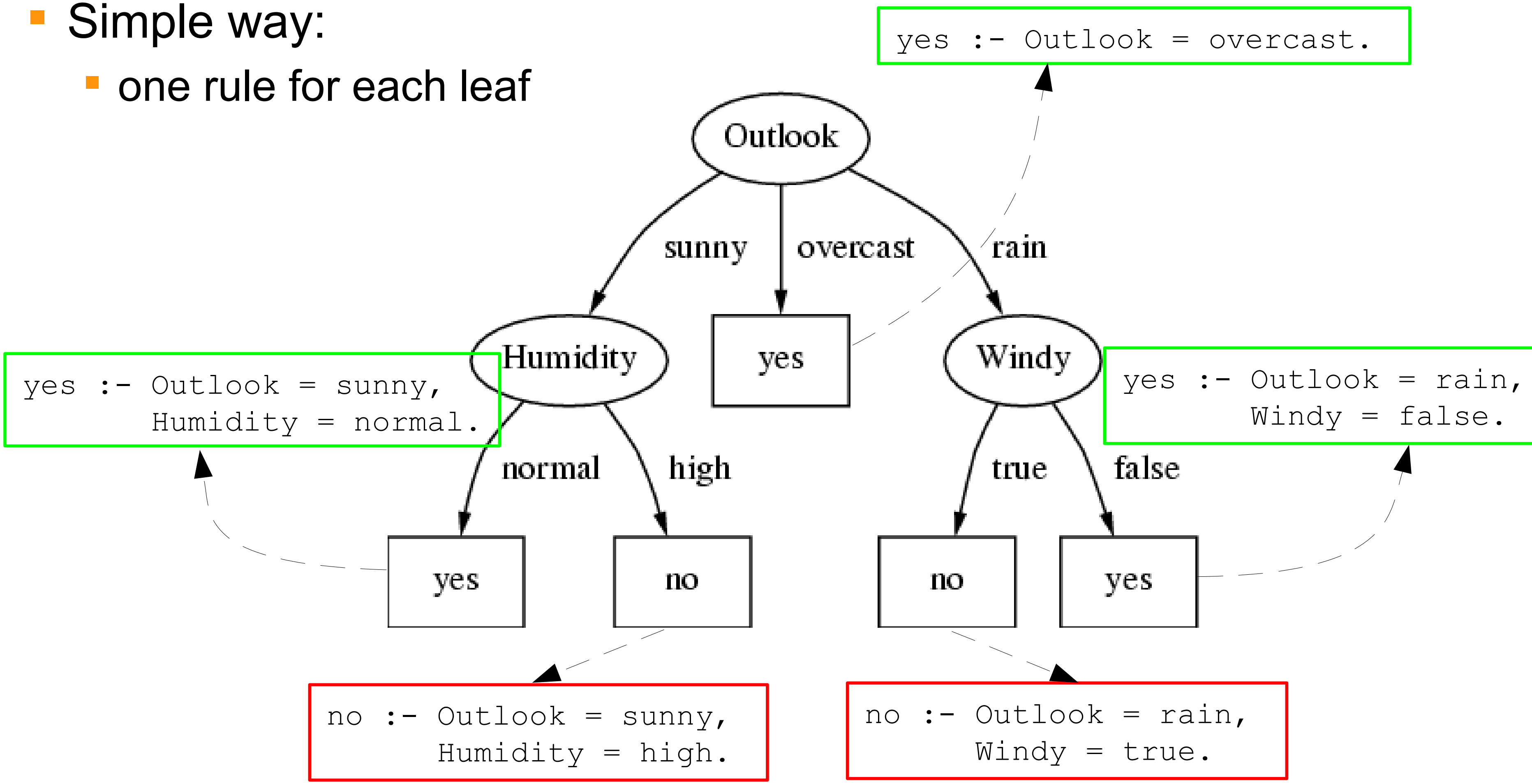
- Generate a sequence of trees with decreasing complexity

$$T_0 \rightarrow T_1 \rightarrow \ldots \rightarrow T_m$$

  - T_0 is the full tree, T_m is the tree that consists only of the root node
  - Each tree is generated from its predecessor by replacing a subtree with a node.
    - It selects the node which results in the smallest increase in the error function, weighted by the number of leaves in the subtree
- this sequence of trees optimizes R_α for successive ranges of α-values
    - T_0 is optimal for the range $[0, \alpha_1]$
    - T_1 is optimal for the range $[\alpha_1, \alpha_2]$
    - ...
- Optimal values for α are then determined with cross-validation on the training data

From Trees To Rules

- Simple way:
  - one rule for each leaf



C4.5rules and successors

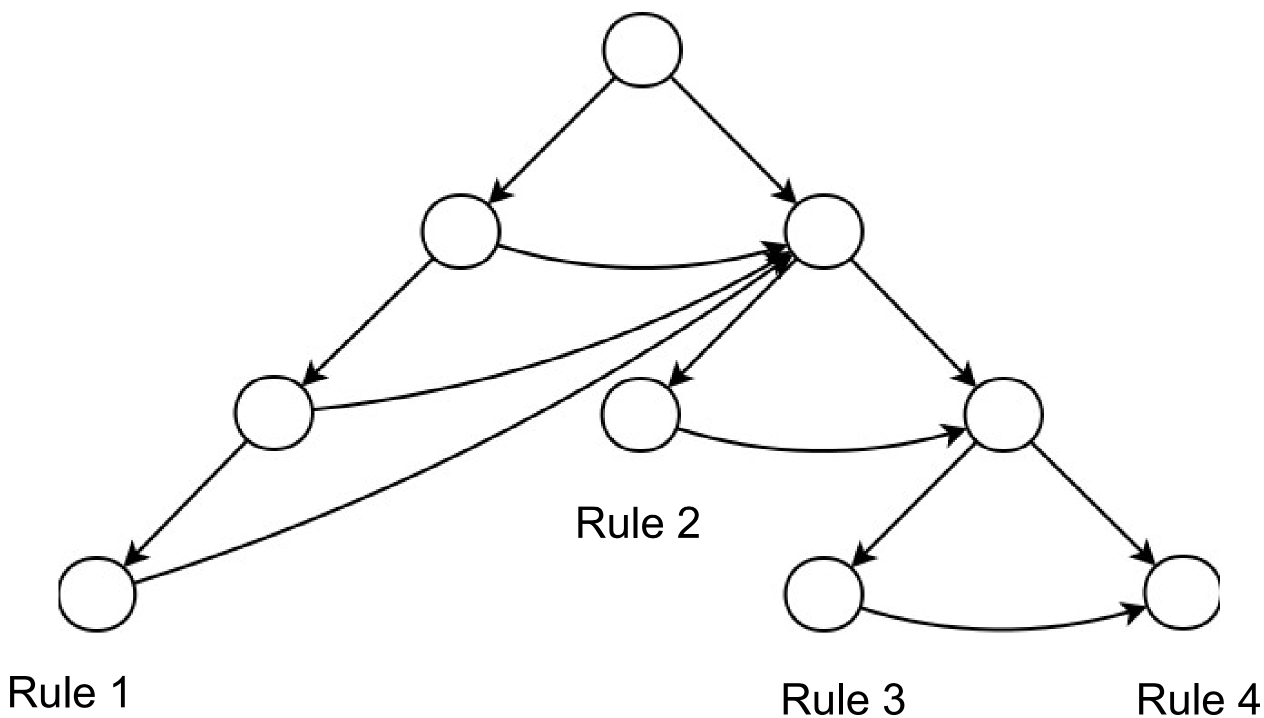
- C4.5rules:
  - greedily prune conditions from each rule if this reduces its estimated error
    - Can produce duplicate rules
    - Check for this at the end
  - Then look at each class in turn
    - consider the rules for that class
    - find a “good” subset (guided by MDL)
    - rank the subsets to avoid conflicts
  - Finally, remove rules (greedily) if this decreases error on the training data
- C4.5rules slow for large and noisy datasets
- Commercial version C5.0rules uses a different technique
  - Much faster and a bit more accurate

Decision Lists and Decision Graphs

- Decision Lists
  - An ordered list of rules
  - the first rule that fires makes the prediction
  - can be learned with a covering approach
- Decision Graphs
  - Similar to decision trees, but nodes may have multiple predecessors
  - DAGs: Directed, acyclic graphs
  - there are a few algorithms that can learn DAGs
    - learn much smaller structures
    - but in general not very successful
- Special case:
  - a decision list may be viewed as a special case of a DAG

Example

- A decision list for a rule set with rules
  - with 4, 2, 2, 1 conditions, respectively
  - drawn as a decision graph



Rules vs. Trees

- Each decision tree can be converted into a rule set

→ Rule sets are at least as expressive as decision trees

  - a decision tree can be viewed as a set of non-overlapping rules
  - typically learned via *divide-and-conquer* algorithms (recursive partitioning)
- Transformation of rule sets / decision lists into trees is less trivial
  - Many concepts have a shorter description as a rule set
  - low complexity decision lists are more expressive than low complexity decision trees (Rivest, 1987)
  - exceptions: if one or more attributes are relevant for the classification of *all* examples (e.g., parity)
- Learning strategies:
  - Separate-and-Conquer vs. Divide-and-Conquer

Discussion TDIDT

- The most extensively studied method of machine learning used in data mining
- Different criteria for attribute/test selection rarely make a large difference
- Different pruning methods mainly change the size of the resulting pruned tree
- C4.5 builds univariate decision trees
- Some TDIDT systems can build multivariate trees (e.g. CART)
  - multi-variate: a split is not based on a single attribute but on a function defined on multiple attributes

Regression Problems

- Regression Task
  - the target variable $y = f(\mathrm{x})$ is numerical instead of discrete
  - Various error functions, e.g., Mean-squared error:

$$L(f, \hat{f}) = \sum_x (f(x) - \hat{f}(x))^2$$

Two principal approaches

- Discretize the numerical target variable
    - e.g., equal-width intervals, or equal-frequency
  - and use a classification learning algorithm
- Adapt the classification algorithm to regression data
  → Regression Trees and Model Trees

Regression Trees

Differences to Decision Trees (Classification Trees)

- Leaf Nodes:
  - Predict the average value of all instances in this leaf
- Splitting criterion:
  - Minimize the variance of the values in each subset S_i
  - Standard deviation reduction

$$SDR(A,S)=SD(S)-\sum_i \frac{|S_i|}{|S|} SD(S_i)$$

- Termination criteria:
  Very important! (otherwise only single points in each leaf)
  - lower bound on standard deviation in a node
  - lower bound on number of examples in a node
- Pruning criterion:
  - Numeric error measures, e.g. Mean-Squared Error

CART (Breiman et al. 1984)

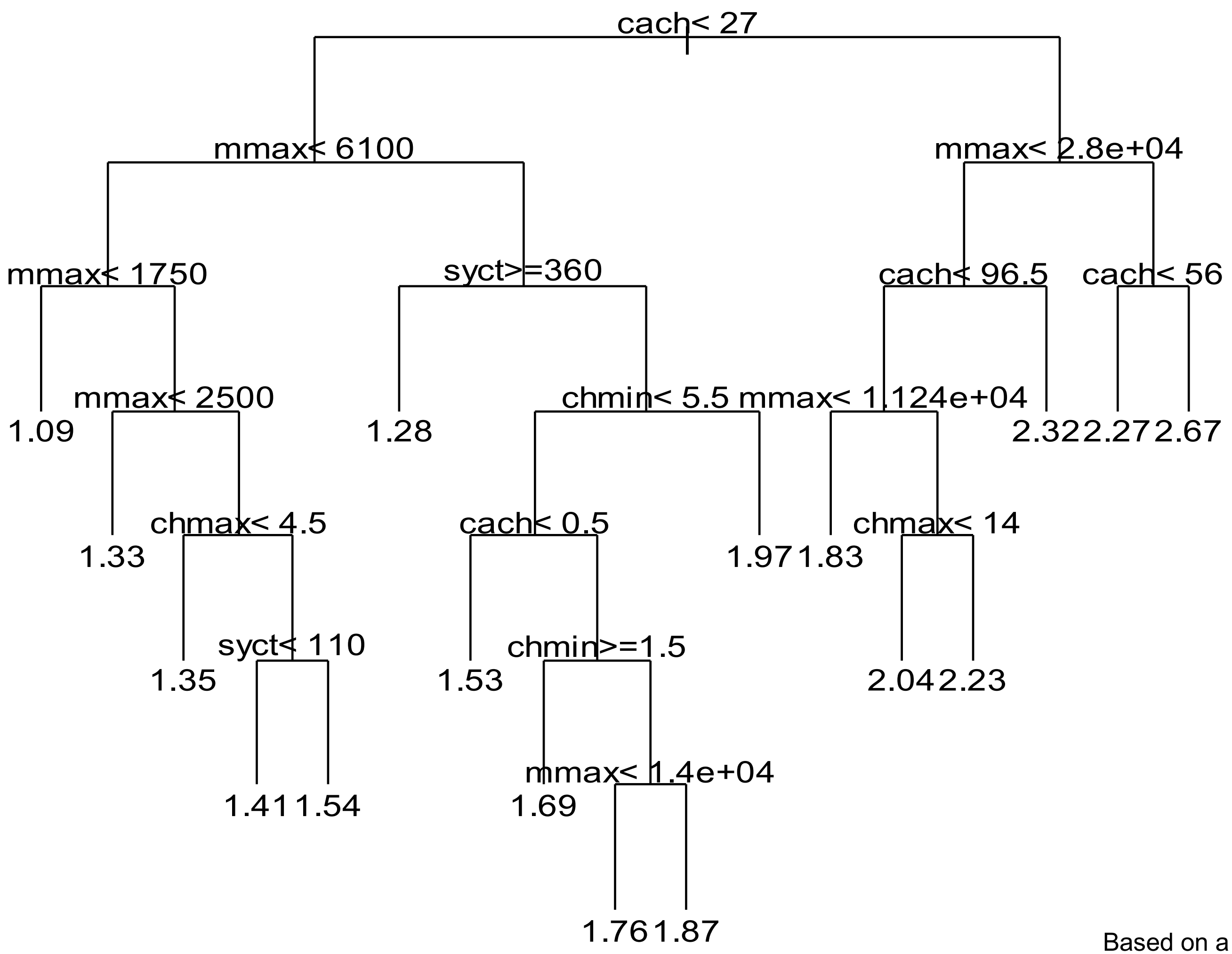
- Algorithm for learning Classification And Regression Trees
  - Quite similar to ID3/C4.5, but developed indepedently in the statistics community
- Splitting criterion:
  - Gini-Index for Classification
  - Sum-of-Squares for Regression
- Pruning:
  - Cost-Complexity Pruning

Regression Tree Example

- Task:
  understand how computer performance is related to a number of variables which describe the features of a PC
- Data:
  - the size of the cache,
  - the cycle time of the computer,
  - the memory size
  - the number of channels (both the last two were not measured but minimum and maximum values obtained).

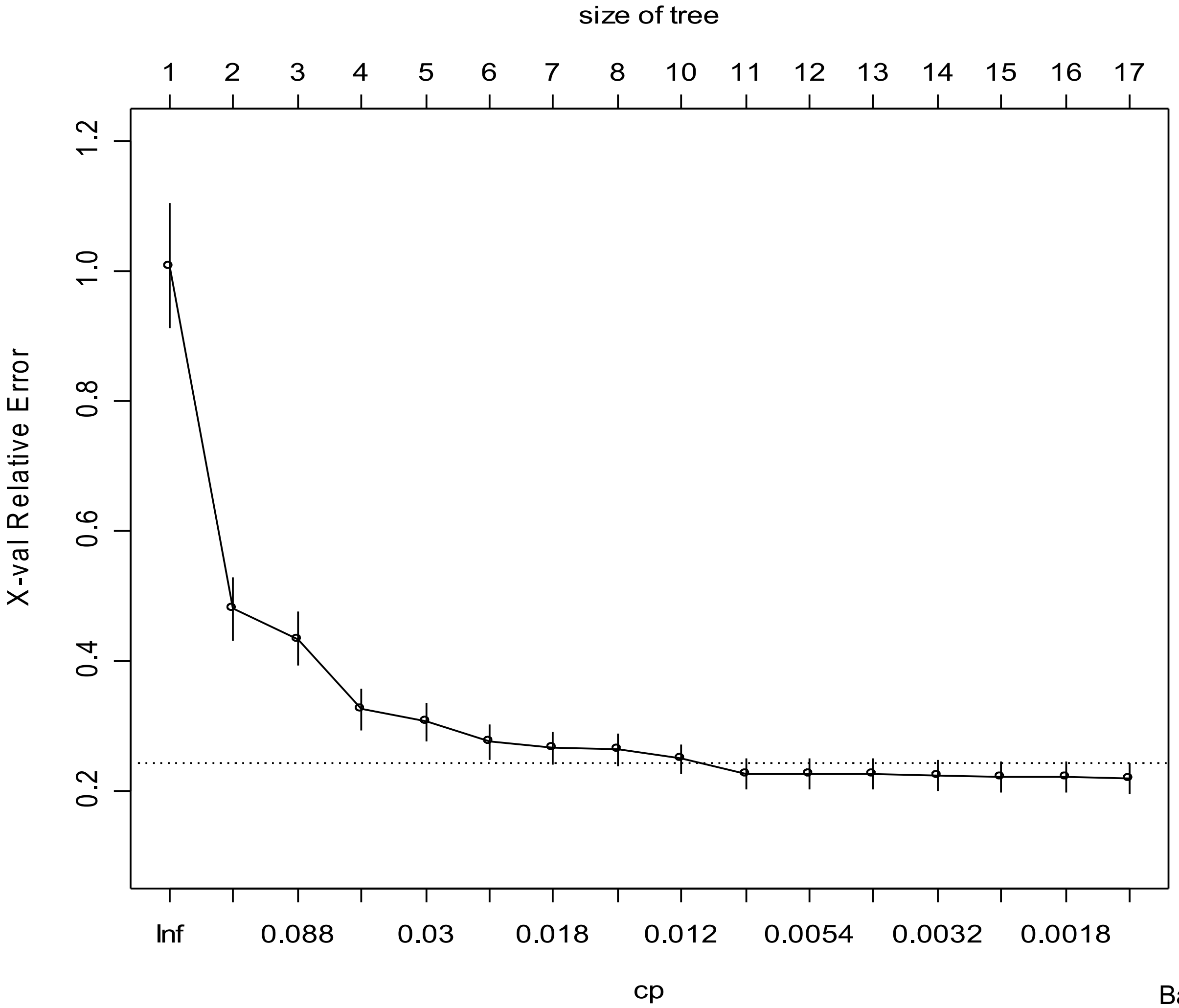
Based on a slide by Richard Lawton

Regression Tree



Based on a slide by Richard Lawton

Estimated Relative Error over Tree Complexity



Based on a slide by Richard Lawton

Model Trees

- In a Leaf node
  - Classification Trees predict a class value
  - Regression Trees predict the average value of all instances in the model
  - Model Trees use a linear model for making the predictions
    - growing of the tree is as with Regression Trees
- Linear Model:
  - $LM(x) = \sum_i w_i v_i(x)$ where $v_i(x)$ is the value of attribute A_i for example x and w_i is a weight
  - The attributes that have been used in the path of the tree can be ignored
- Weights can be fitted with standard math packages
  - Minimize the Mean Squared Error $MSE = \frac{1}{n} \sum_j (y_j - r_j)^2$

Summary

- Classification Problems require the prediction of a discrete target value
  - can be solved using decision tree learning
  - iteratively select the best attribute and split up the values according to this attribute
- Regression Problems require the prediction of a numerical target value
  - can be solved with regression trees and model trees
  - difference is in the models that are used at the leafs
  - are grown like decision trees, but with different splitting criteria
- Overfitting is a serious problem!
  - simpler, seemingly less accurate trees are often preferable
  - evaluation has to be done on separate test sets