Classification: Decision Trees

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Function Approximation

Problem Setting

- Set of possible instances $\mathcal{X}$
- Set of possible labels $\mathcal{Y}$
- Unknown target function $f : \mathcal{X} \to \mathcal{Y}$
- Set of function hypotheses $H = \{h \mid h : \mathcal{X} \to \mathcal{Y}\}$

Input: Training examples of unknown target function f

$$\{\langle \boldsymbol{x}_i, y_i \rangle\}_{i=1}^{n} = \{\langle \boldsymbol{x}_1, y_1 \rangle, \ldots, \langle \boldsymbol{x}_n, y_n \rangle\}$$

Output: Hypothesis $h \in H$ that best approximates f

Sample Dataset (was Tennis Played?)

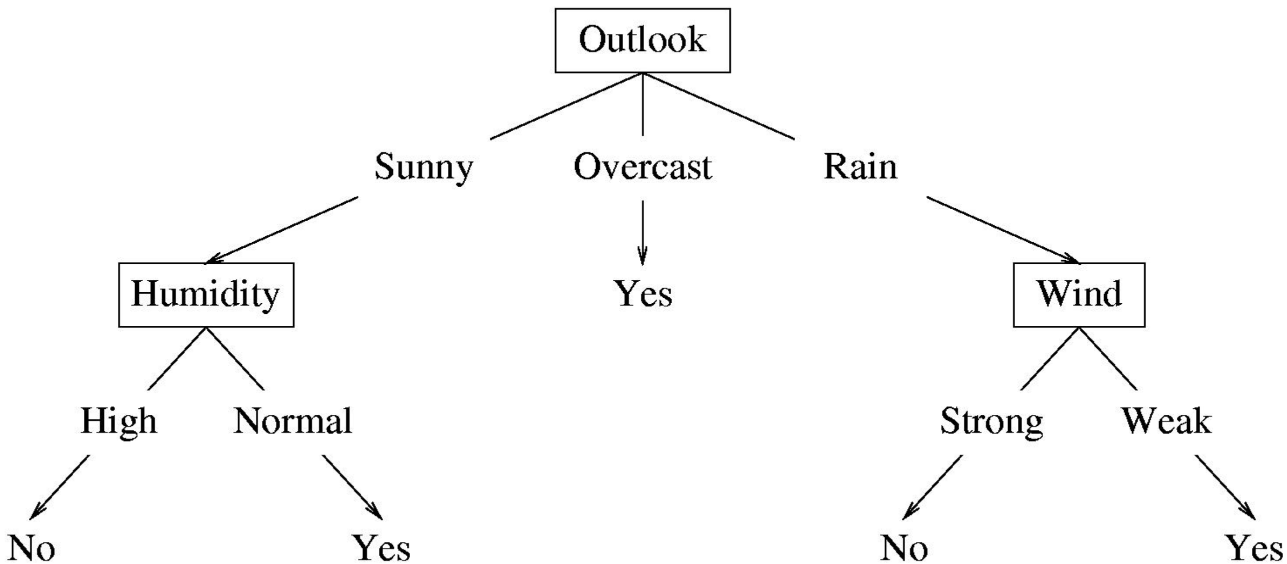
- Columns denote features $\mathrm{X_i}$
- Rows denote labeled instances $\langle \boldsymbol{x}_i, y_i \rangle$
- Class label denotes whether a tennis game was played

$\langle \boldsymbol{x}_i, y_i \rangle$

Predictors				Response
Outlook	**Temperature**	**Humidity**	**Wind**	**Class**
Sunny	Hot	High	Weak	No
Sunny	Hot	High	Strong	No
Overcast	Hot	High	Weak	Yes
Rain	Mild	High	Weak	Yes
Rain	Cool	Normal	Weak	Yes
Rain	Cool	Normal	Strong	No
Overcast	Cool	Normal	Strong	Yes
Sunny	Mild	High	Weak	No
Sunny	Cool	Normal	Weak	Yes
Rain	Mild	Normal	Weak	Yes
Sunny	Mild	Normal	Strong	Yes
Overcast	Mild	High	Strong	Yes
Overcast	Hot	Normal	Weak	Yes
Rain	Mild	High	Strong	No

Decision Tree

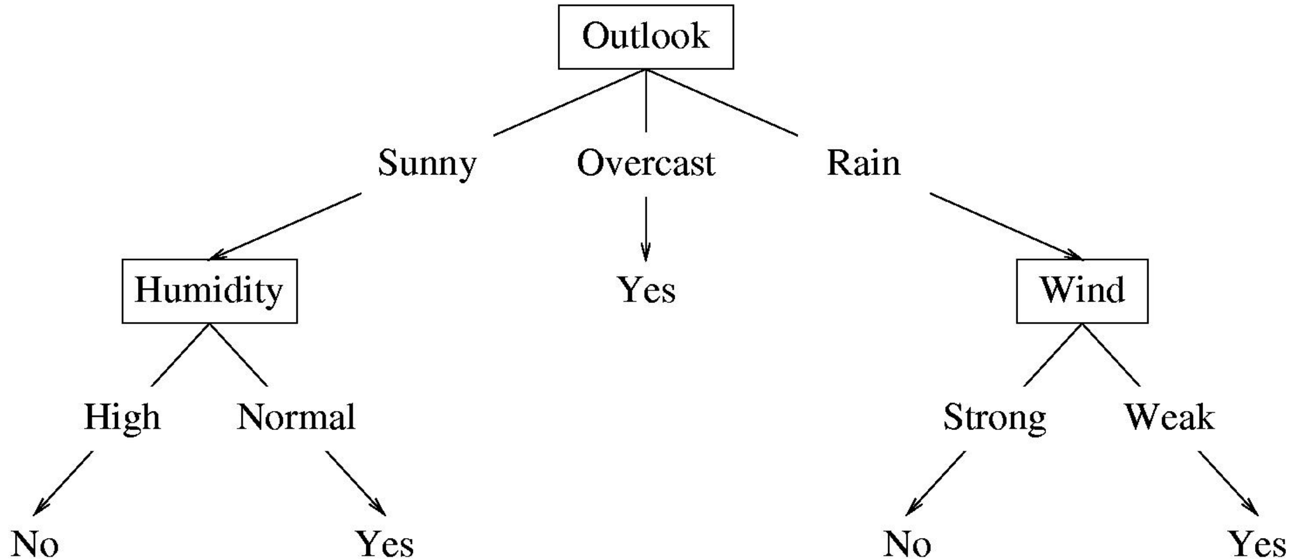
- A possible decision tree for the data:



- Each internal node: test one attribute X_i
- Each branch from a node: selects one value for X_i
- Each leaf node: predict Y

Decision Tree

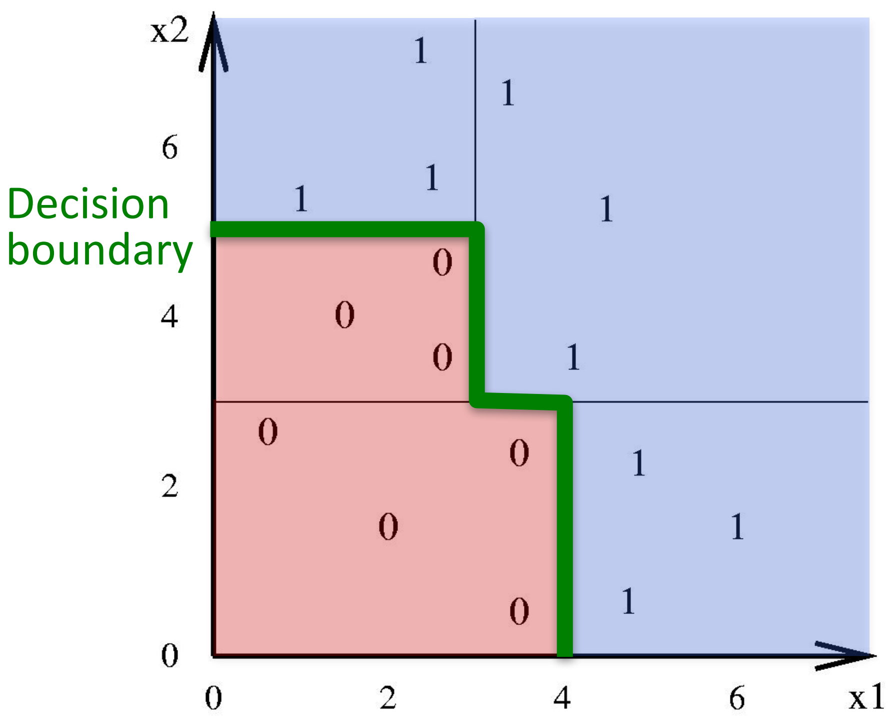
- A possible decision tree for the data:

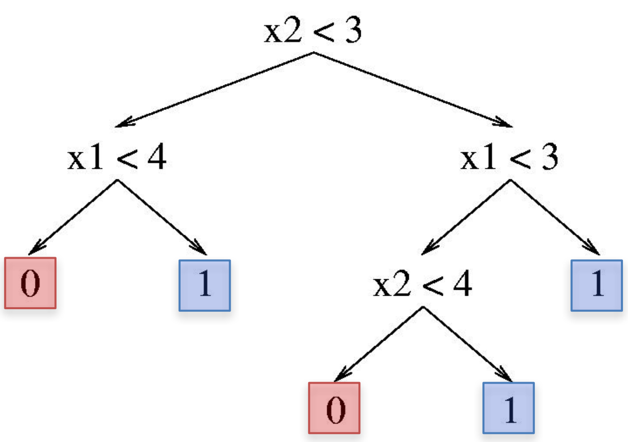


- What prediction would we make for
  <outlook=sunny, temperature=hot, humidity=high, wind=weak> ?

Decision Tree – Decision Boundary

- Decision trees divide the feature space into axis-parallel (hyper-)rectangles
- Each rectangular region is labeled with one label
  - or a probability distribution over labels

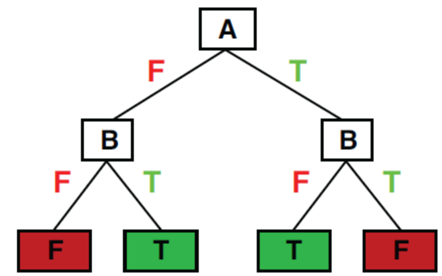




Expressiveness

- Given a particular space of functions, you may not be able to represent everything
- What **functions** can decision trees represent?
- Decision trees can represent any function of the input attributes!
  - Boolean operations (and, or, xor, etc.)?
  - **Yes!**
  - All boolean functions?
  - **Yes!**

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F

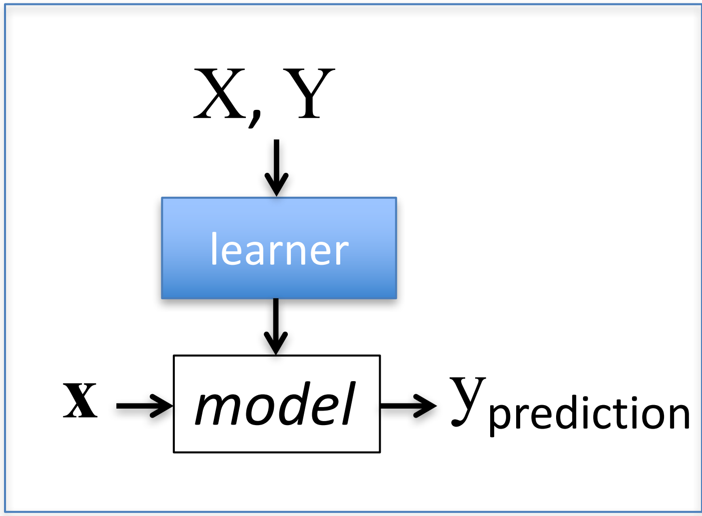


(Figure from Stuart Russell)

Stages of (Batch) Machine Learning

Given: labeled training data $X, Y = \{\langle \boldsymbol{x}_i, y_i \rangle\}_{i=1}^{n}$

- Assumes each $\boldsymbol{x}_i \sim \mathcal{D}(\mathcal{X})$ with $y_i = f_{target}(\boldsymbol{x}_i)$



Train the model:

model ← *classifier*.train(X, Y)

Apply the model to new data:

- Given: new unlabeled instance $\boldsymbol{x} \sim \mathcal{D}(\mathcal{X})$

$y_{\text{prediction}}$ ← *model*.predict(**x**)

Basic Algorithm for Top-Down Learning of Decision Trees

[ID3, C4.5 by Quinlan]

node = root of decision tree

Main loop:

1. *A* ← the "best" decision attribute for the next node.
2. Assign *A* as decision attribute for *node*.
3. For each value of *A*, create a new descendant of *node*.
4. Sort training examples to leaf nodes.
5. If training examples are perfectly classified, stop. Else, recurse over new leaf nodes.

How do we choose which attribute is best?

Choosing the Best Attribute

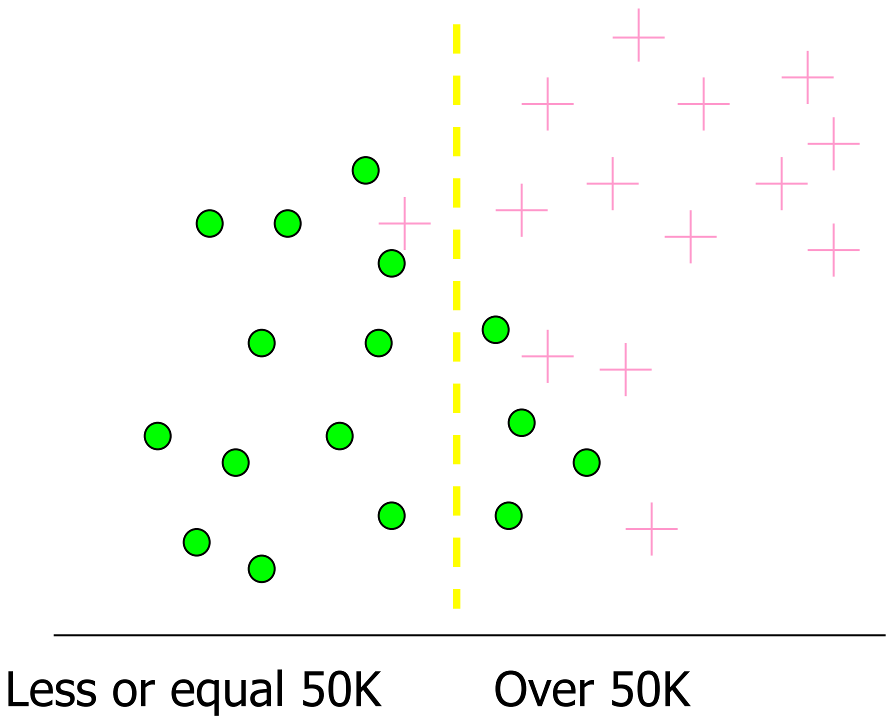
Key problem: choosing which attribute to split a given set of examples

- Some possibilities are:
  - **Random:** Select any attribute at random
  - **Least-Values:** Choose the attribute with the smallest number of possible values
  - **Most-Values:** Choose the attribute with the largest number of possible values
  - **Max-Gain:** Choose the attribute that has the largest expected *information gain*
    - i.e., attribute that results in smallest expected size of subtrees rooted at its children
- The ID3 algorithm uses the Max-Gain method of selecting the best attribute

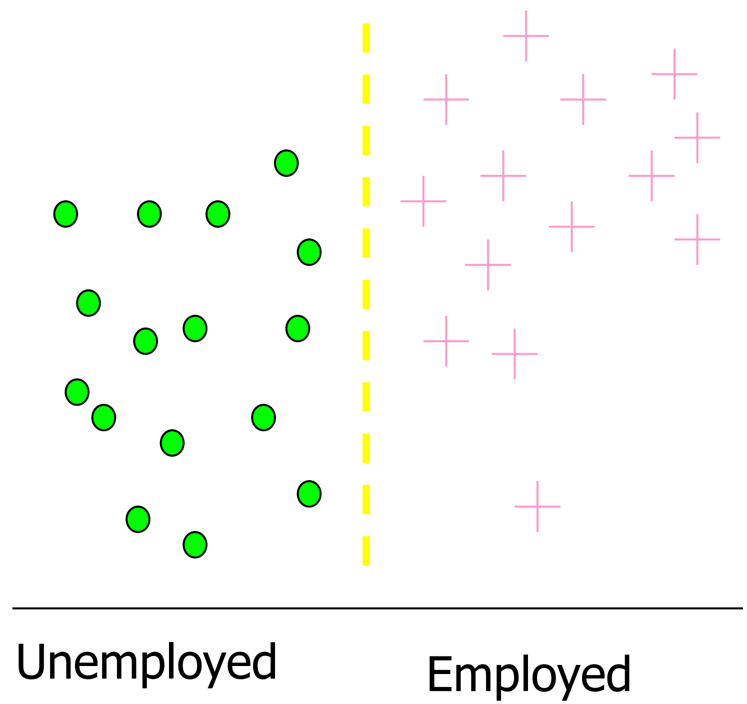
Information Gain

Which test is more informative?

Split over whether Balance exceeds 50K



Split over whether applicant is employed

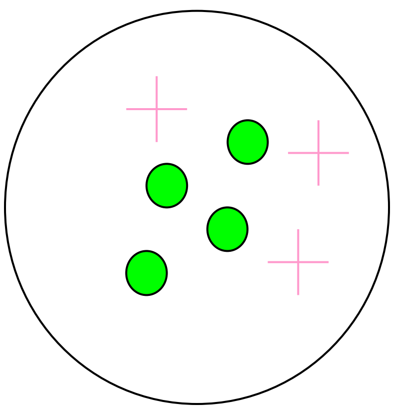


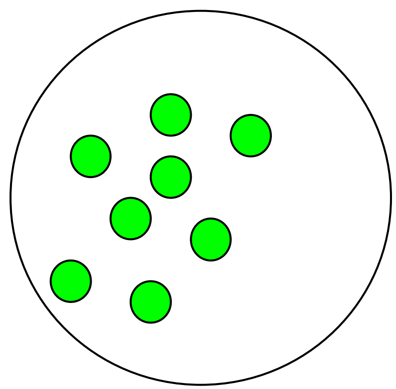
Based on slide by Pedro Domingos

Information Gain

Impurity/Entropy (informal)

– Measures the level of **impurity** in a group of examples





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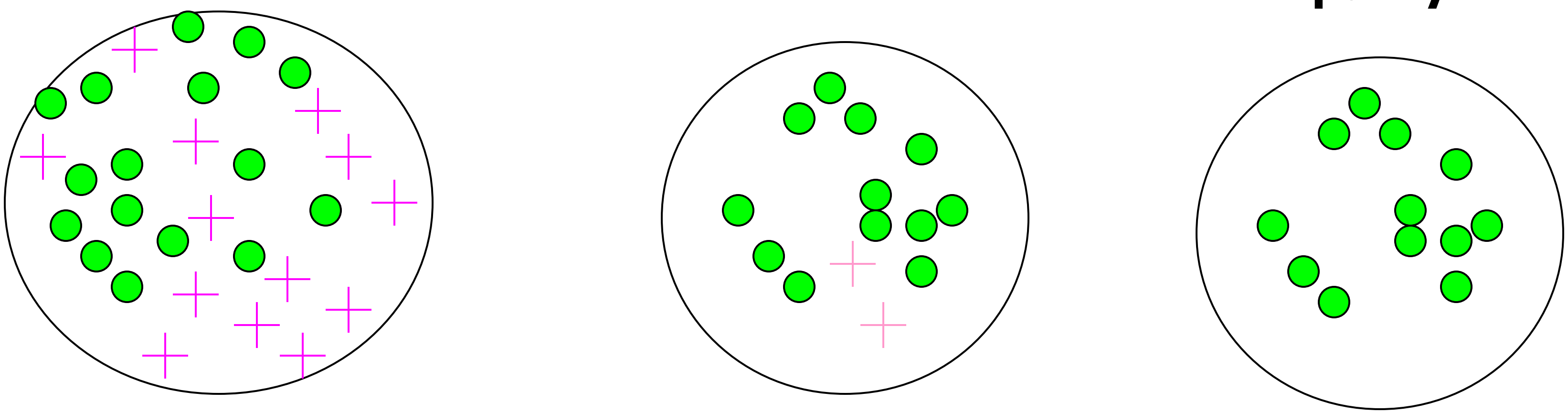
Impurity

Very impure group | **Less impure** | **Minimum impurity**



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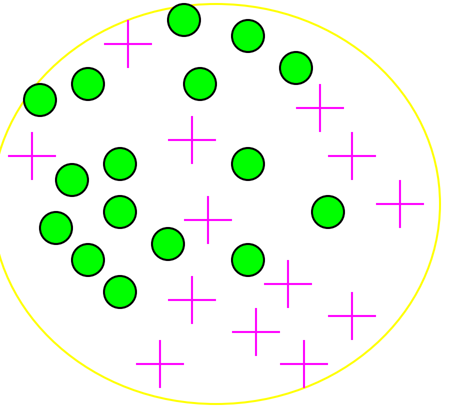
Entropy: a common way to measure impurity

- Entropy = $$\sum_i -p_i \log_2 p_i$$



p_i is the probability of class i

Compute it as the proportion of class i in the set.

- Entropy comes from information theory. The higher the entropy the more the information content.

What does that mean for learning from examples?

Based on slide by Pedro Domingos

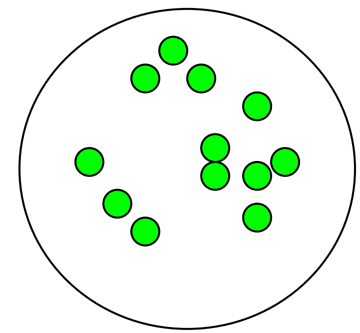
2-Class Cases:

Entropy $$H(x) = -\sum_{i=1}^{n} P(x=i) \log_2 P(x=i)$$

- What is the entropy of a group in which all examples belong to the same class?
  - entropy = - 1 $\log_2 1$ = 0

not a good training set for learning

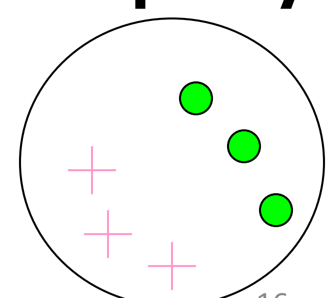
Minimum impurity



- What is the entropy of a group with 50% in either class?
  - entropy = -0.5 $\log_2 0.5$ – 0.5 $\log_2 0.5$ =1

good training set for learning

Maximum impurity



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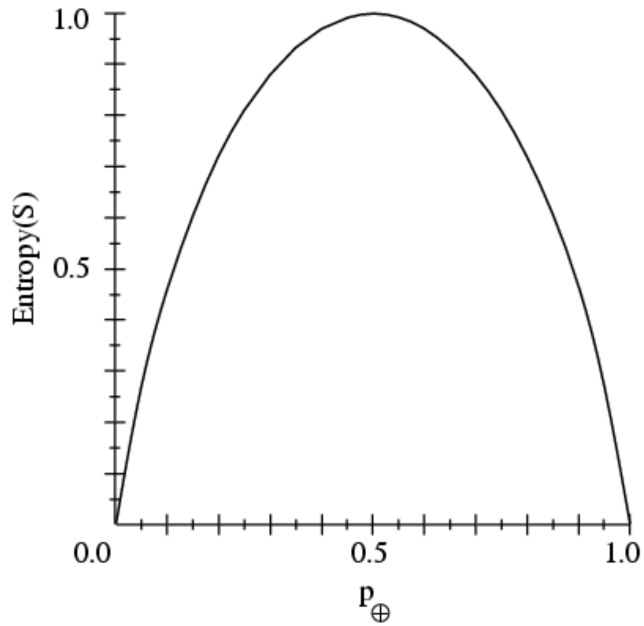
Sample Entropy



- S is a sample of training examples
- $p_\oplus$ is the proportion of positive examples in S
- $p_\ominus$ is the proportion of negative examples in S
- Entropy measures the impurity of S

$$H(S) \equiv -p_\oplus \log_2 p_\oplus - p_\ominus \log_2 p_\ominus$$

Information Gain

- We want to determine which attribute in a given set of training feature vectors is most useful for discriminating between the classes to be learned.
- Information gain tells us how important a given attribute of the feature vectors is.
- We will use it to decide the ordering of attributes in the nodes of a decision tree.

Based on slide by Pedro Domingos

From Entropy to Information Gain

Entropy $H(X)$ of a random variable X

$$\boxed{H(X) = -\sum_{i=1}^{n} P(X=i)\log_2 P(X=i)}$$

Specific conditional entropy $H(X|Y=v)$ of X given $Y=v$:

$$H(X|Y=v) = -\sum_{i=1}^{n} P(X=i|Y=v)\log_2 P(X=i|Y=v)$$

Conditional entropy $H(X|Y)$ of X given Y :

$$H(X|Y) = \sum_{v \in values(Y)} P(Y=v)H(X|Y=v)$$

Mututal information (aka Information Gain) of X and Y :

$$I(X,Y) = H(X) - H(X|Y) = H(Y) - H(Y|X)$$

Information Gain

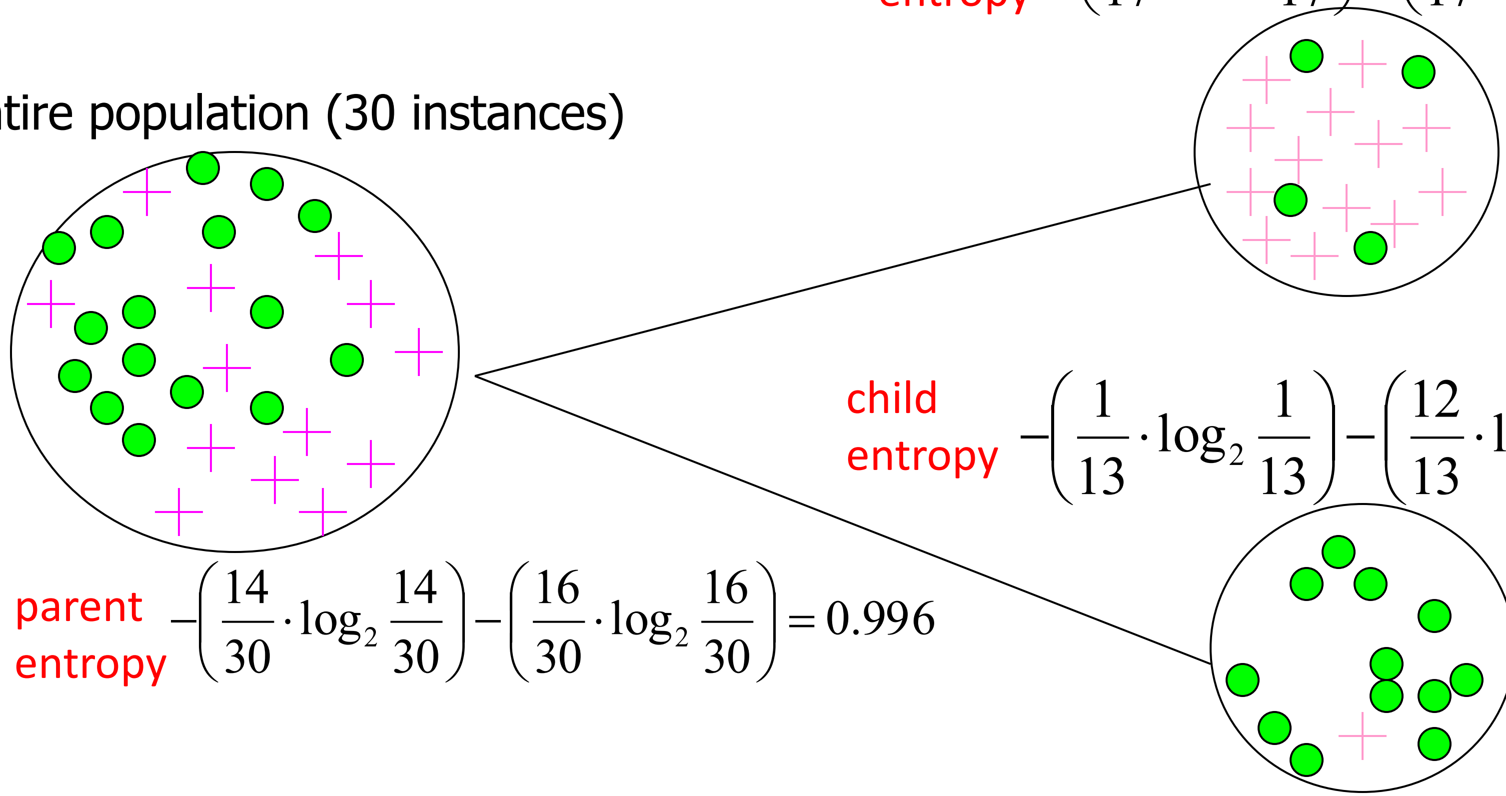
Information Gain is the expected reduction in entropy of target variable Y for data sample S, due to sorting

Calculating Information Gain

Information Gain = entropy(parent) – [average entropy(children)]

child entropy $-\left(\frac{13}{17}\cdot\log_2\frac{13}{17}\right)-\left(\frac{4}{17}\cdot\log_2\frac{4}{17}\right)=0.787$

Entire population (30 instances)



child entropy $-\left(\frac{1}{13}\cdot\log_2\frac{1}{13}\right)-\left(\frac{12}{13}\cdot\log_2\frac{12}{13}\right)=0.391$

parent entropy $-\left(\frac{14}{30}\cdot\log_2\frac{14}{30}\right)-\left(\frac{16}{30}\cdot\log_2\frac{16}{30}\right)=0.996$

(Weighted) Average Entropy of Children = $\left(\frac{17}{30}\cdot 0.787\right)+\left(\frac{13}{30}\cdot 0.391\right)=0.615$

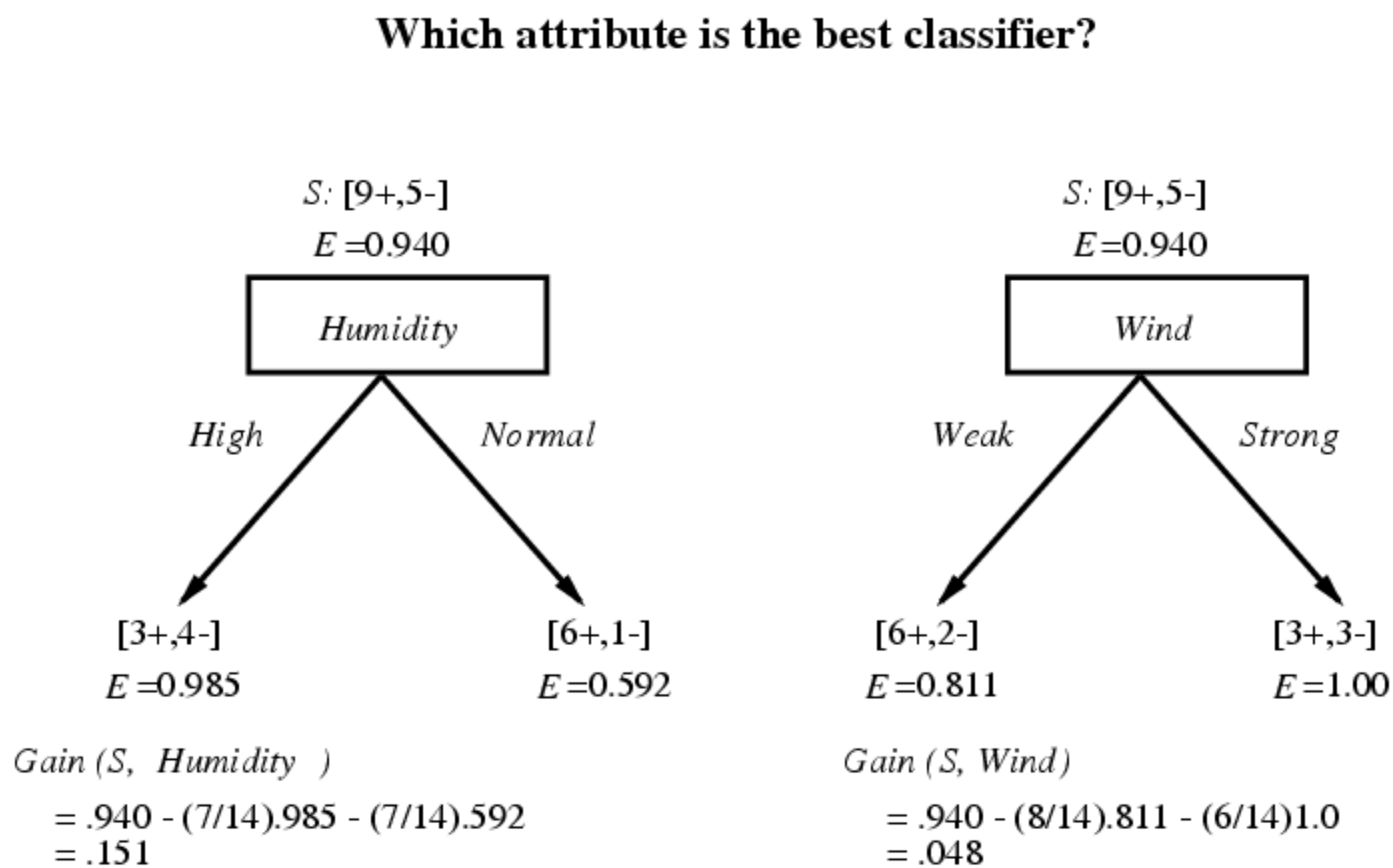
Information Gain= 0.996 - 0.615 = 0.38

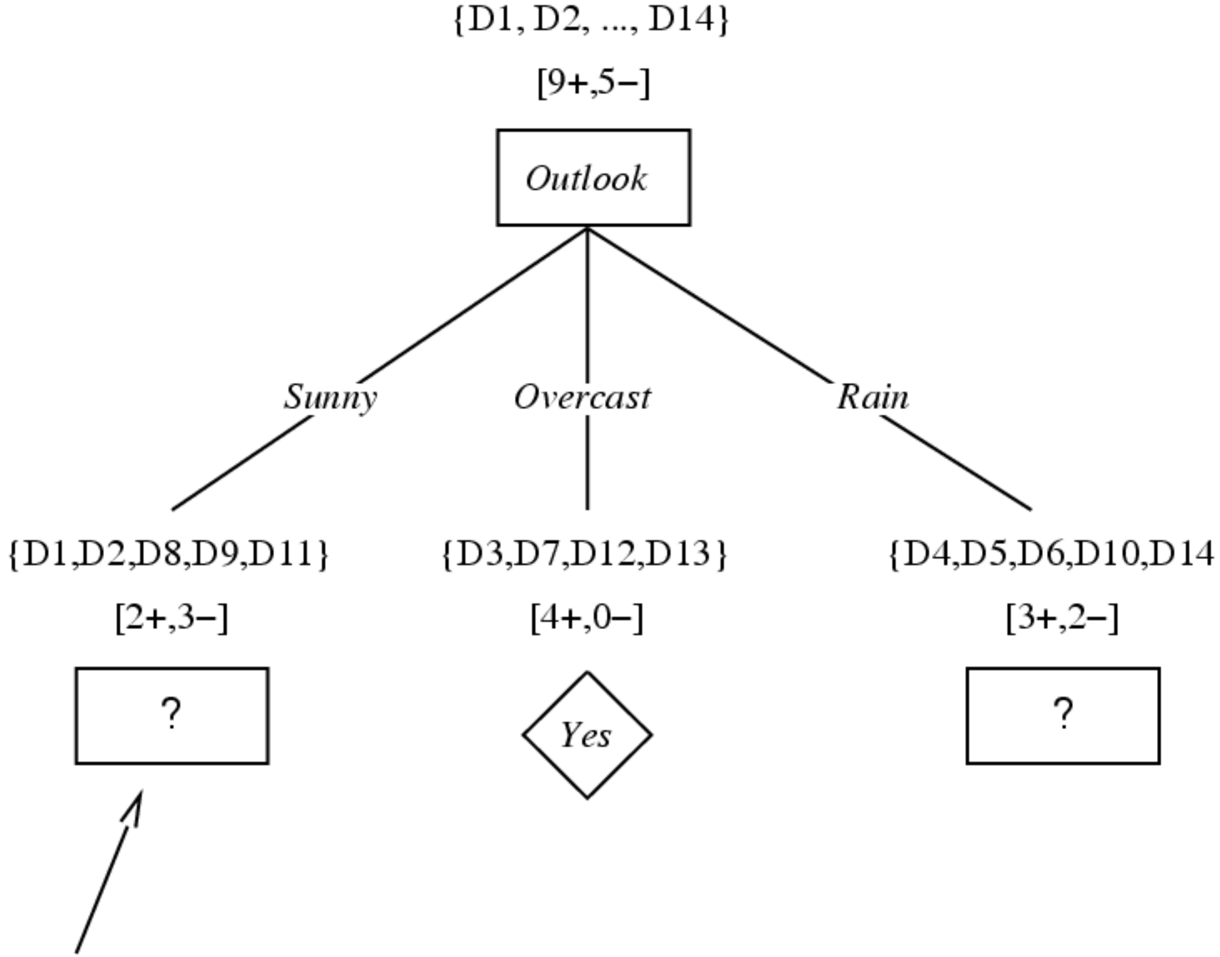
Based on slide by Pedro Domingos

Training Examples

Day	Outlook	Temperature	Humidity	Wind	PlayTenn
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Selecting the Next Attribute





Which attribute should be tested here?

$S_{sunny} = \{D1,D2,D8,D9,D11\}$

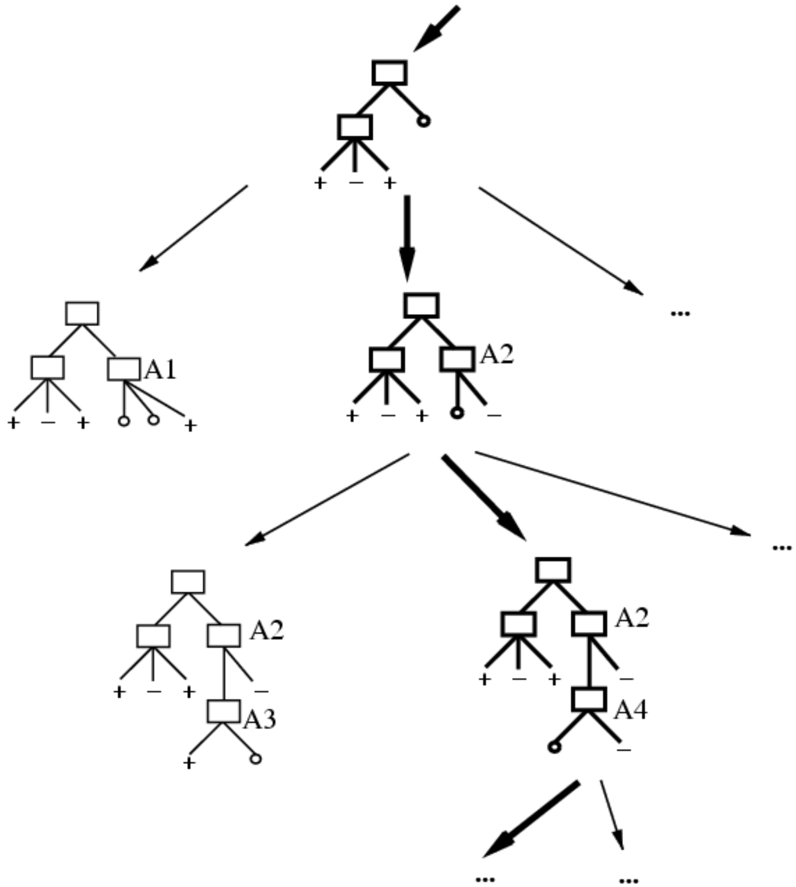
$Gain\ (S_{sunny}, Humidity) = .970 - (3/5)\ 0.0 - (2/5)\ 0.0 = .970$

$Gain\ (S_{sunny}, Temperature) = .970 - (2/5)\ 0.0 - (2/5)\ 1.0 - (1/5)\ 0.0 = .570$

$Gain\ (S_{sunny}, Wind) = .970 - (2/5)\ 1.0 - (3/5)\ .918 = .019$

Slide by Tom Mitchell

Which Tree Should We Output?



- ID3 performs heuristic search through space of decision trees
- It stops at smallest acceptable tree. Why?

Preference bias: Ockham's Razor

- Principle stated by William of Ockham (1285-1347)
  - "*non sunt multiplicanda entia praeter necessitatem*"
  - entities are not to be multiplied beyond necessity
  - AKA Occam's Razor, Law of Economy, or Law of Parsimony

Idea: The simplest consistent explanation is the best

- Therefore, the smallest decision tree that correctly classifies all of the training examples is best
  - Finding the provably smallest decision tree is NP-hard
  - ...So instead of constructing the absolute smallest tree consistent with the training examples, construct one that is pretty small

Overfitting in Decision Trees

- Many kinds of “noise” can occur in the examples:
  - Two examples have same attribute/value pairs, but different classifications
  - Some values of attributes are incorrect because of errors in the data acquisition process or the preprocessing phase
  - The instance was labeled incorrectly (+ instead of -)

- Also, some attributes are irrelevant to the decision-making process
  - e.g., color of a die is irrelevant to its outcome

Based on Slide from M. desJardins & T. Finin

Overfitting in Decision Trees

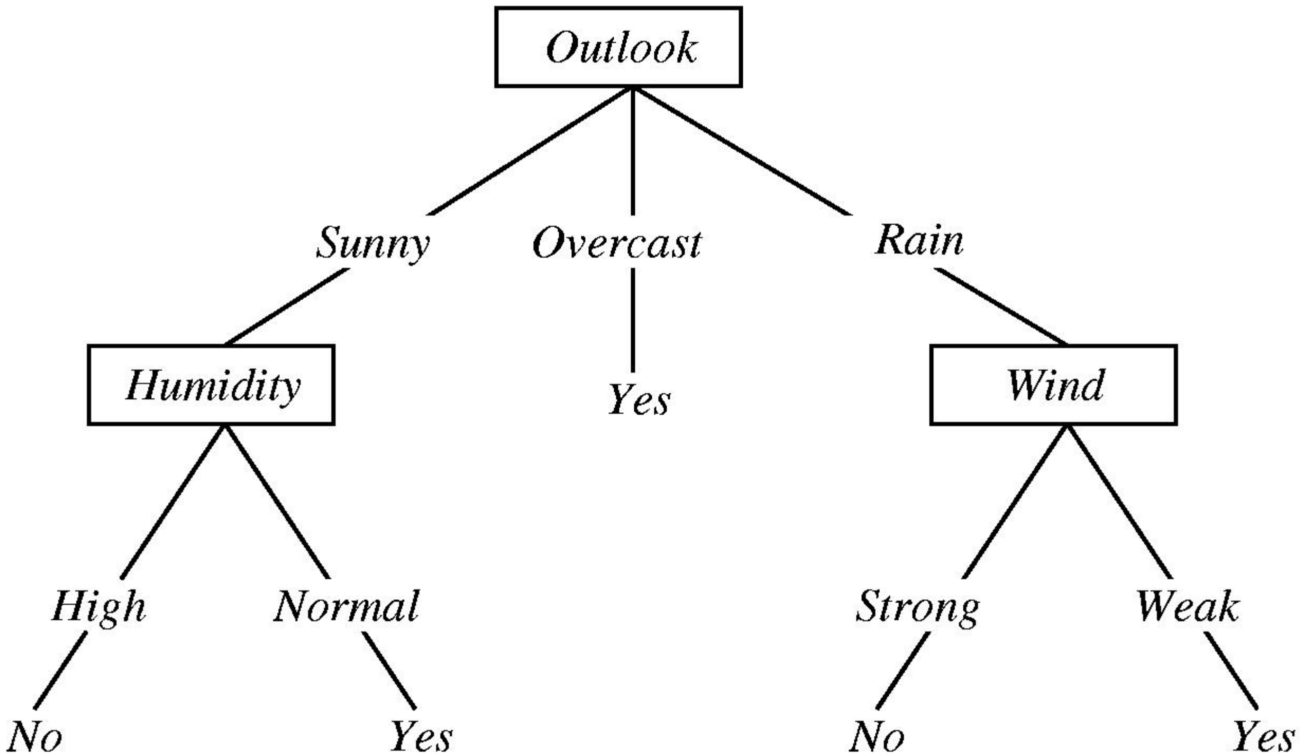
- Irrelevant attributes can result in *overfitting* the training example data
  - If hypothesis space has many dimensions (large number of attributes), we may find **meaningless regularity** in the data that is irrelevant to the true, important, distinguishing features

- If we have too little training data, even a reasonable hypothesis space will 'overfit'

Based on Slide from M. desJardins & T. Finin

Overfitting in Decision Trees

Consider adding a **noisy** training example to the following tree:



What would be the effect of adding:

<outlook=sunny, temperature=hot, humidity=normal, wind=strong, playTennis=No> ?

Based on Slide by Pedro Domingos

Overfitting in Decision Trees

Consider error of hypothesis h over

- training data: $error_{train}(h)$
- entire distribution $\mathcal{D}$ of data: $error_{\mathcal{D}}(h)$

Hypothesis $h \in H$ **overfits** training data if there is an alternative hypothesis $h' \in H$ such that

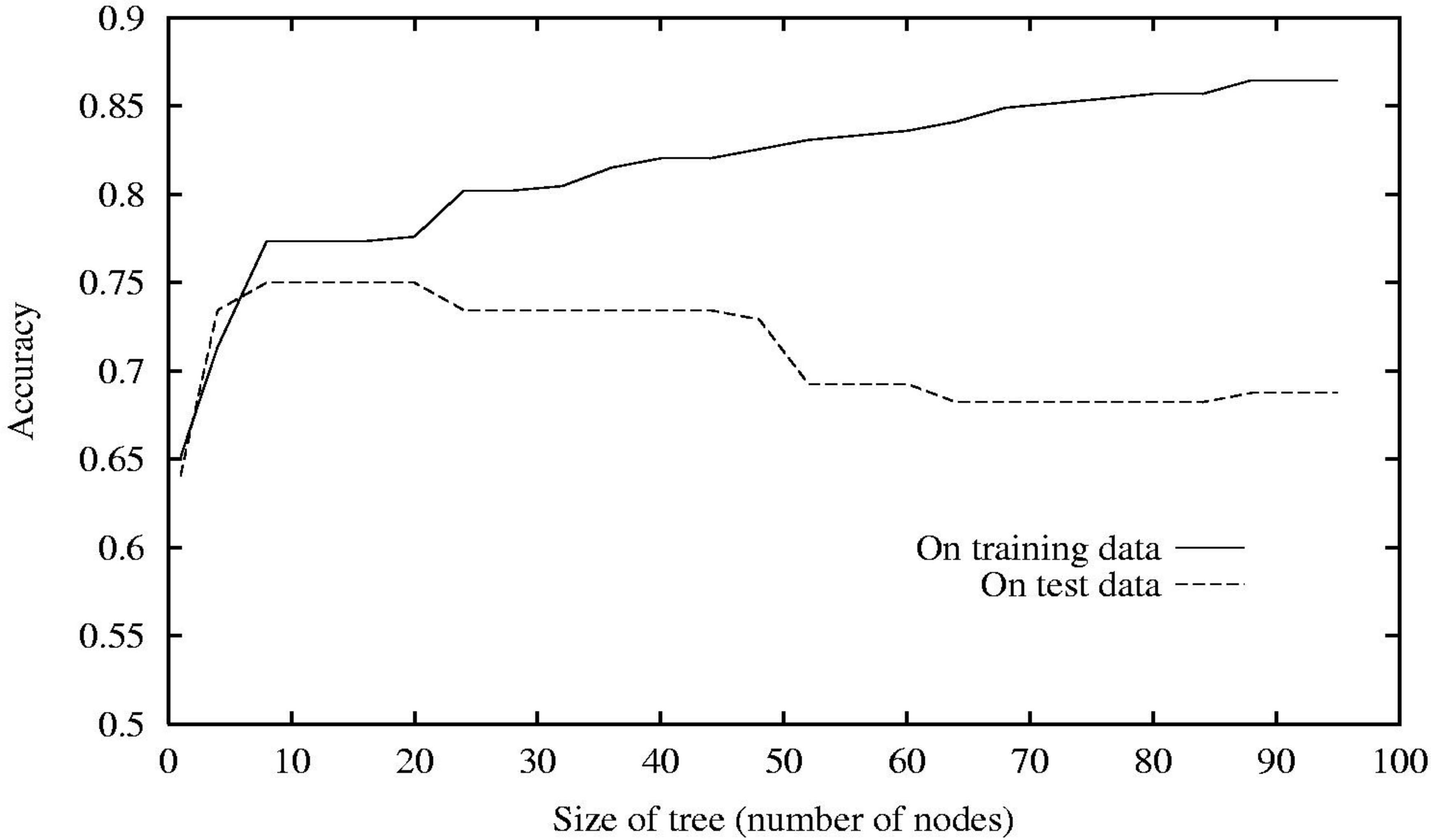
$$error_{train}(h) < error_{train}(h')$$

and

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

Slide by Pedro Domingos

Overfitting in Decision Trees



Slide by Pedro Domingos

Avoiding Overfitting in Decision Trees

How can we avoid overfitting?

- Stop growing when data split is not statistically significant
- Acquire more training data
- Remove irrelevant attributes (manual process – not always possible)
- **Grow full tree, then post-prune**

How to select "best" tree:

- Measure performance over training data
- Measure performance over separate validation data set
- Add complexity penalty to performance measure
  (heuristic: simpler is better)

Based on Slide by Pedro Domingos

Reduced-Error Pruning

Split training data further into *training* and *validation* sets

Grow tree based on *training set*

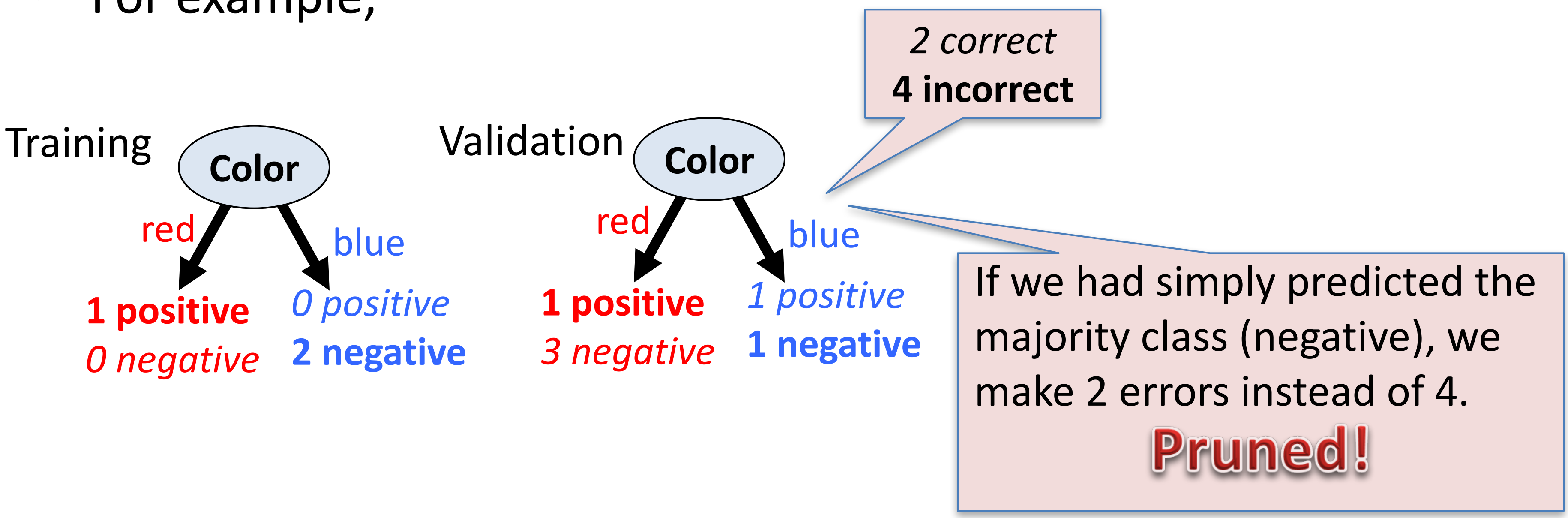
Do until further pruning is harmful:

1. Evaluate impact on validation set of pruning each possible node (plus those below it)
2. Greedily remove the node that most improves *validation set* accuracy

Slide by Pedro Domingos

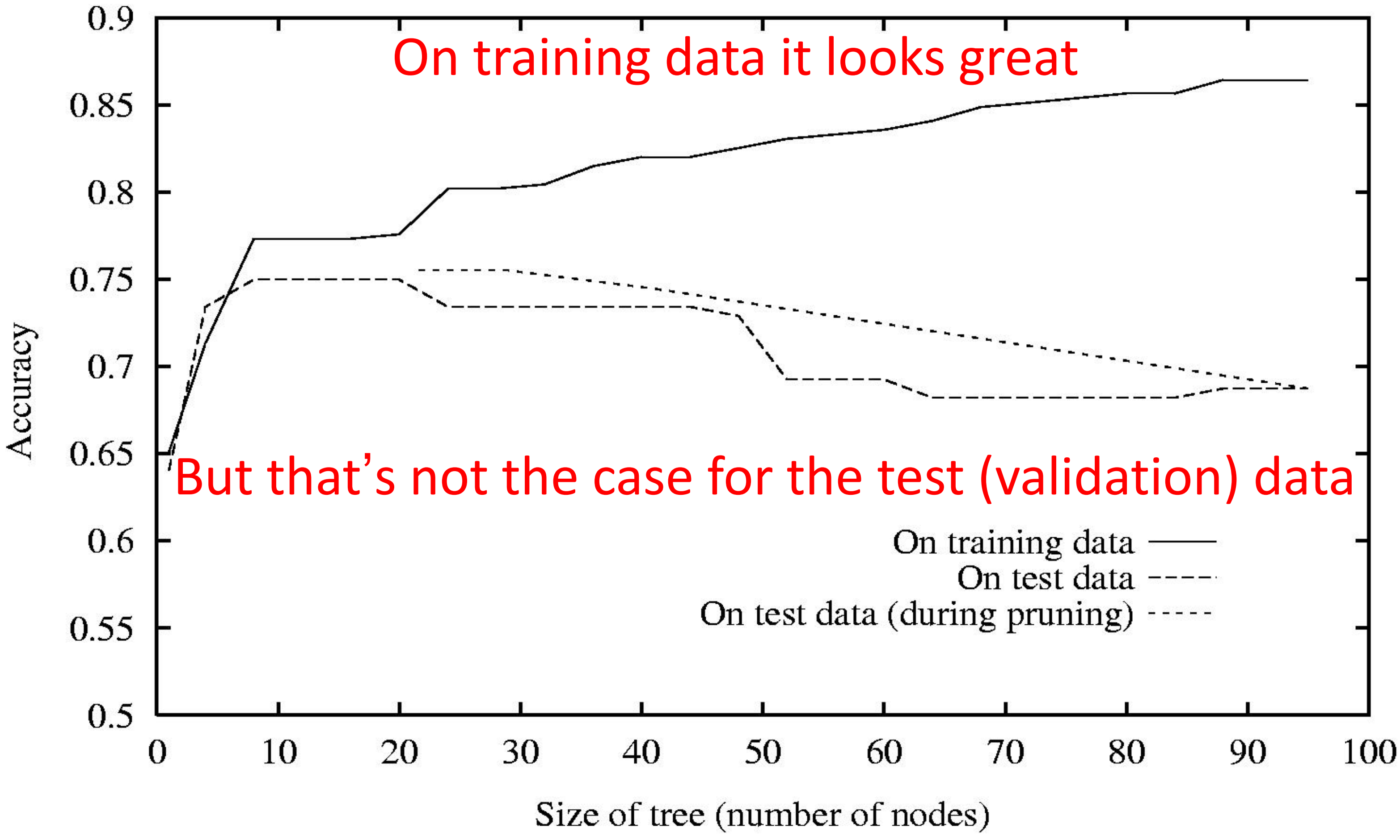
Pruning Decision Trees

- Pruning of the decision tree is done by replacing a whole subtree by a leaf node.
- The replacement takes place if a decision rule establishes that the expected error rate in the subtree is greater than in the single leaf.
- For example,



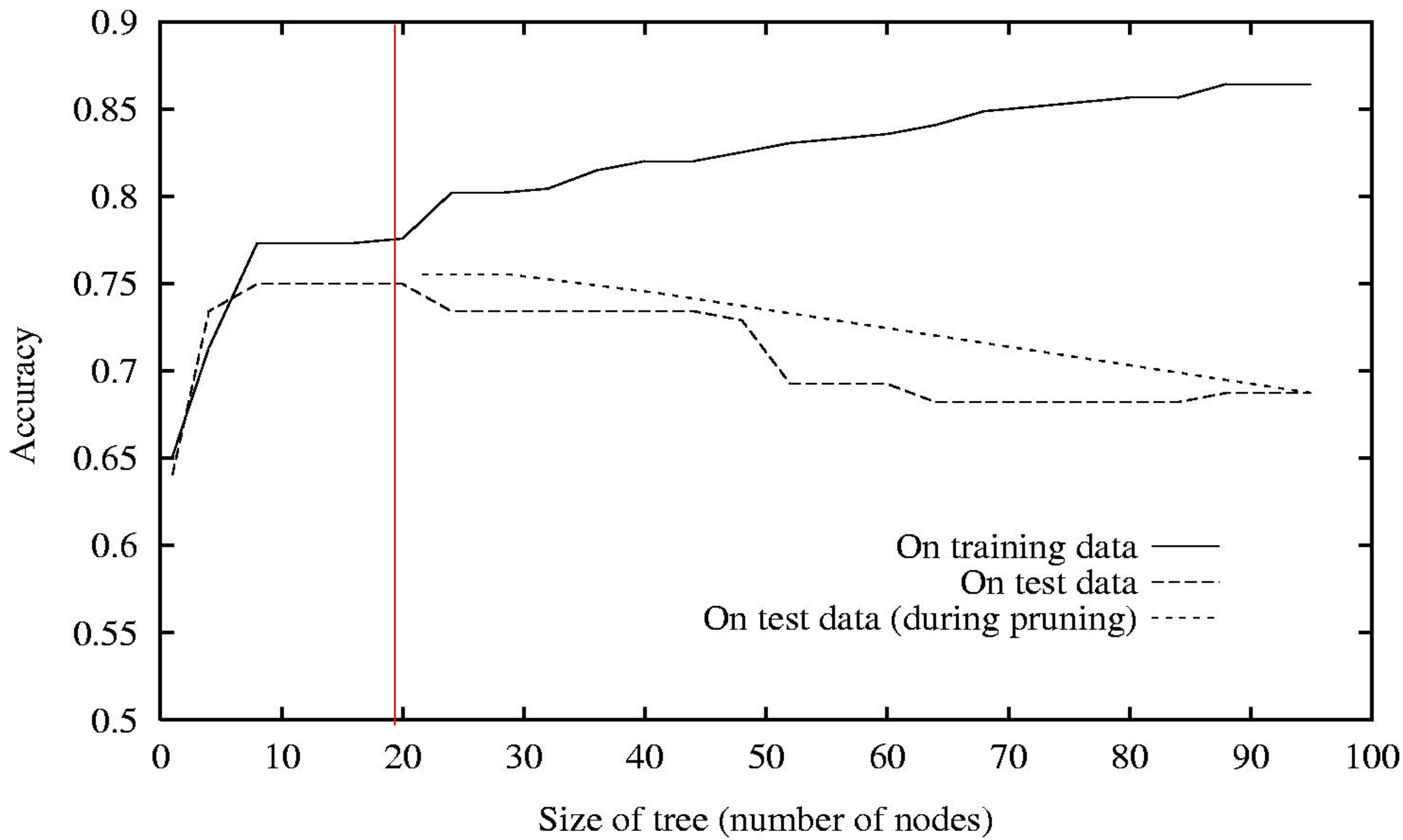
Based on Example from M. desJardins & T. Finin

Effect of Reduced-Error Pruning



Based on Slide by Pedro Domingos

Effect of Reduced-Error Pruning



The tree is pruned back to the red line where it gives more accurate results on the test data

Based on Slide by Pedro Domingos

Summary: Decision Tree Learning

- Widely used in practice
- Strengths include
  - Fast and simple to implement
  - Can convert to rules
  - Handles noisy data
- Weaknesses include
  - Univariate splits/partitioning using only one attribute at a time --- limits types of possible trees
  - Large decision trees may be hard to understand
  - Requires fixed-length feature vectors
  - Non-incremental (i.e., batch method)

Summary: Decision Tree Learning

• Representation:	decision trees
• Bias:	prefer small decision trees
• Search algorithm:	greedy
• Heuristic function:	information gain or information content or others

- Overfitting / pruning

Slide by Pedro Domingos