Decision Tree Learning

Patricia J Riddle

Computer Science 367

Decision Tree Learning

Discrete valued target functions - Classification problems

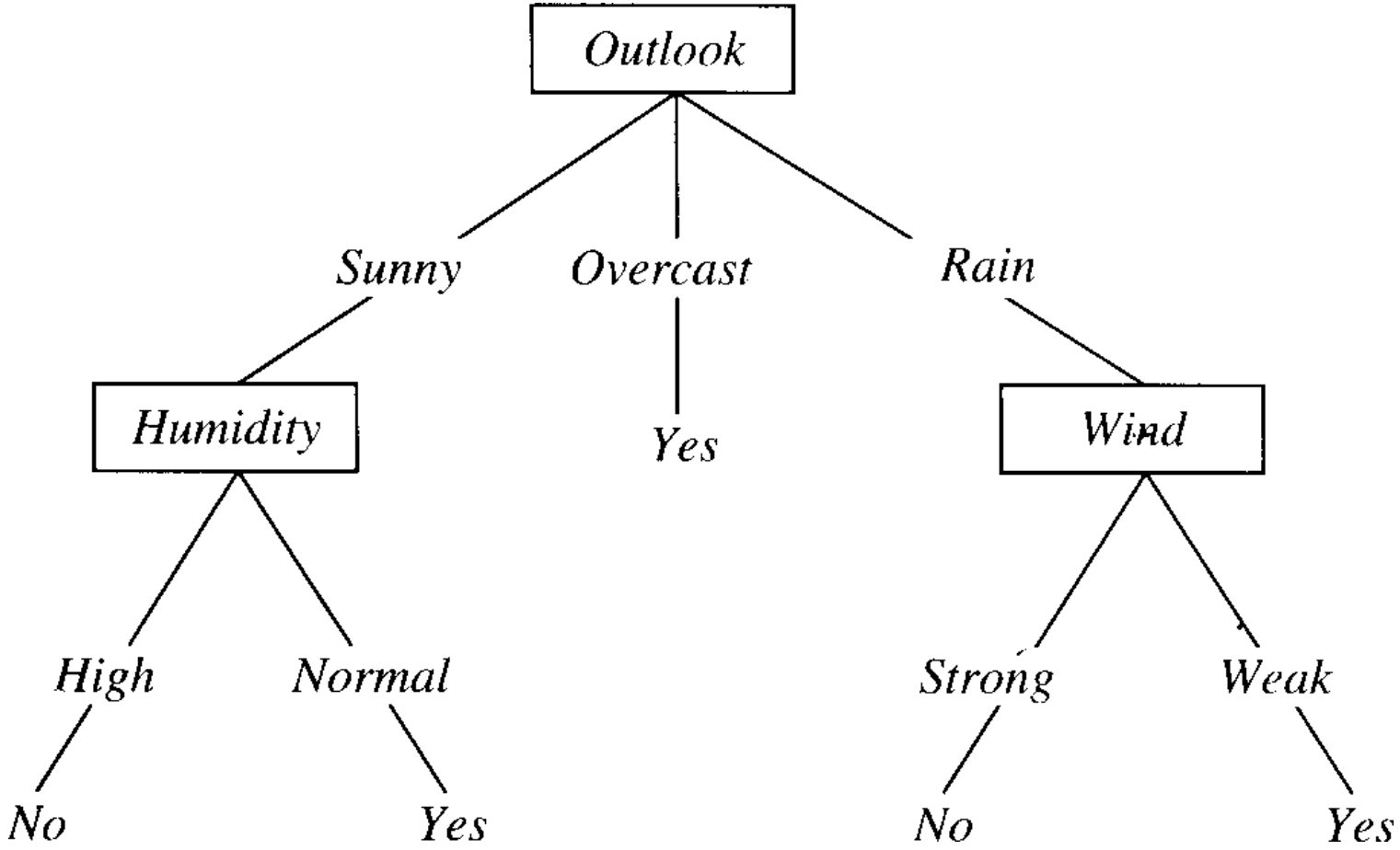
Represented as sets of if-then rules to improve human readability

Used in many success stories

Classify instances by sorting them down the tree

- Each internal node is a test on some attribute
- Each branch is one possible value for that test
- Each leaf specifies classification value

Decision tree



Learned Rules

Outlook=Sunny∧Humidity=High → PlayTennis=No

Outlook=Sunny∧Humidity=Normal → PlayTennis=Yes

Outlook=Overcast → PlayTennis=Yes

Outlook=Rain∧Wind=Strong → PlayTennis=No

Outlook=Rain∧Wind=Weak → PlayTennis=Yes

When to use Decision Tree Learning

Instances are represented by attribute value pairs (can be real valued).

The target value has discrete output values (no need to be binary, some extensions even handle real valued targets).

Disjunctive descriptions may be required

The training data

- may contain errors - errors in classification and errors in attribute values
- may contain missing attribute values

Attribute Value Pairs

attributes	Outlook	Wind	Class
Instance 1	rainy	strong	red
Instance 2	sunny	normal	red
Instance 3	sunny	normal	green
Instance 4	cloudy	strong	red
Instance 5	rainy	normal	green

ID3 Algorithm

ID3($Examples$, $Target\_attribute$, $Attributes$)

Examples are the training examples. Target_attribute is the attribute whose value is to be predicted by the tree. Attributes is a list of other attributes that may be tested by the learned decision tree. Returns a decision tree that correctly classifies the given Examples.

- Create a *Root* node for the tree
- If all $Examples$ are positive, Return the single-node tree *Root*, with label = +
- If all $Examples$ are negative, Return the single-node tree *Root*, with label = −
- If $Attributes$ is empty, Return the single-node tree *Root*, with label = most common value of $Target\_attribute$ in $Examples$
- Otherwise Begin
  - $A \leftarrow$ the attribute from $Attributes$ that best* classifies $Examples$
  - The decision attribute for *Root* $\leftarrow A$
  - For each possible value, v_i, of A,
    - Add a new tree branch below *Root*, corresponding to the test $A = v_i$
    - Let $Examples_{v_i}$ be the subset of $Examples$ that have value v_i for A
    - If $Examples_{v_i}$ is empty
      - Then below this new branch add a leaf node with label = most common value of $Target\_attribute$ in $Examples$
      - Else below this new branch add the subtree ID3($Examples_{v_i}$, $Target\_attribute$, $Attributes - \{A\}$))
- End
- Return *Root*

* The best attribute is the one with highest *information gain*, as defined in Equation (3.4).

What Attribute is the Best Classifier?

Entropy (from information theory)

- Measures the impurity of an arbitrary collection of examples

Entropy(S)$\equiv -p_{\oplus}\log_2 p_{\oplus} - p_{\ominus}\log_2 p_{\ominus}$

- for a boolean classification where $p_{\oplus}$ is the proportion of positive examples in S and $p_{\ominus}$ is the proportion of negative examples in S.
- In all calculations involving entropy we define 0log0 to be 0

Entropy

Entropy(9+,5-)=-(9/14)$\log_2$(9/14)-(5/14)$\log_2$(5/14)=.94

- If all members of S are in the same class Entropy(S)=0
- If there is an equal number of positive and negative instances in S then Entropy(S)=1

Entropy specifies the minimum number of bits of information needed to encode the classification of an arbitrary member of S

Information Theory

A **fair coin** has an entropy of one bit.

However, if the coin is not fair, then the uncertainty is lower (if asked to bet on the next outcome, we would bet preferentially on the most frequent result), and thus the Shannon entropy is lower.

A long string of repeating characters has an entropy rate of 0, since every character is predictable.

Information Theory History

During World War II, Claude Shannon developed a model of the communication process using the earlier work of Nyquist and Hartley.

fundamental problem of communication is

reproducing at one point either exactly or approximately a message selected at another point.

How to Code

Given a source producing symbols at a rate consistent with a set of probabilities governing their frequency of occurrence, Shannon asks

> ``how much information is `produced' by such a process, or better, at what rate information is produced?"

For Shannon, the amount of self-information that is contained in or associated with a message being transmitted, when the **probability of its transmission** is **p**, is the logarithm of the inverse of the probability, or **I=log1/p**

The choice of a logarithmic base corresponds to the choice of a unit for measuring information.

If the base 2 is used the resulting units may be called binary digits, or more briefly *bits*, a word suggested by J. W. Tukey.

Deriving Entropy

A device with two stable positions . . . can store one bit of information.

N such devices can store *N* bits, since the total number of possible states is 2^N and $\log_2 2^N = N$.

The amount of information in the output of a process is proportional to the number of different values that the function might return.

Given *n* different output values, the amount of information (I) may be computed as $I = \log_2 n$.

Restaurant Example

Ordering food at a restaurant might be modeled as a channel based process.

The thoughts concerning food preference might be seen as the source, the vocalized order comes from the transmitting mouth, the waiter's ear is the receiver, and the chef is the destination.

For example, use of this model may suggest that noise effecting the channel might be examined.

Using care in the choice of codes (names for food) might help decrease the error rate in recording customer orders.

Also things ordered more often should have shorter names

English example

People have a tendency to talk, and presumably think, at the basic level of categorization

- to draw the boundary around "chairs", rather than around the more specific category "recliner", or the more general category "furniture".

People are more likely to say "You can sit in that chair" than "You can sit in that recliner" or "You can sit in that furniture".

And it is no coincidence that the word for "chair" contains fewer syllables than either "recliner" or "furniture".

In Summary

Basic-level categories, in general, tend to have short names; and nouns with **short names** tend to refer to **basic-level categories**.

Not a perfect rule, of course, but a definite tendency.

Frequent use goes along with short words; short words go along with frequent use.

Or as Douglas Hofstadter put it, there's a reason why the English language uses "the" to mean "the" and "antidisestablishmentarianism" to mean "antidisestablishmentarianism" instead of antidisestablishmentarianism other way around.

What does this have to do with ML

Machine Learning is the same as compression

Now you just have to transmit the tree and the mistakes or errors

A lot of compression algorithms are machine learning algorithms and vice versa

Information Theory is the basis of them both

General Entropy Formula

Generally, $$Entropy(S) \equiv \sum_{i=1}^{c} -p_i \log_2 p_i$$

For example if there are 4 classes and the set is split evenly, 2 bits will be needed to encode the classification of an arbitrary member of S.

If it is split less evenly an average message length of less then 2 can be used.

Just say class 1 (the frequent class and send the class for every datapoint for which that is NOT the correct class)

Entropy Intuition 1

Surprisal $\quad I(A) = -\log_2 p = \log_2(1/p)$

$$Entropy(S) \equiv \sum_{i=1}^{c} -p_i \log_2 p_i$$

Entropy, rather than being associated with a particular event, is associated with a partition of event.

Entropy Intuition 2

$$Entropy(S) \equiv \sum_{i=1}^{c} p_i I(A_i)$$

Communication engineers interpret each of the A_is as a possible transmission from an information source and thus interpret the entropy as the **average information outputted** by that source.

Entropy Function

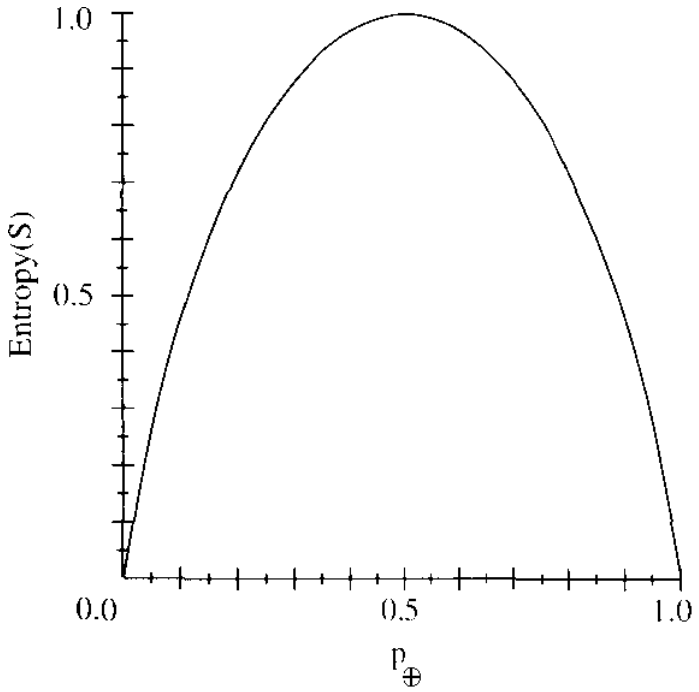


FIGURE 3.2
The entropy function relative to a boolean classification, as the proportion, $p_{\oplus}$, of positive examples varies between 0 and 1.

Information Gain

$$Gain(S,A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

Where Values(A) is the set of possible values for the attribute A and S_v is the subset of S for which attribute A has value v.

Information Gain is the **expected reduction in entropy** caused by knowing the value of attribute A.

Information Gain Intuition

Information Gain is the information provided about the target function value, given the value of some other attribute A.

The value of Gain(S,A) is the number of bits saved when encoding the target value of an arbitrary member S, by knowing the value of A.

Information Gain Example

Of our 14 examples suppose 6 positive and 2 negative have Wind=Weak.

Values(Wind)=Weak,Strong

S=[9+,5-]

$S_{weak} \leftarrow$[6+,2-]

$S_{strong} \leftarrow$[3+,3-]

Information Gain Example II

$$Gain(S,Wind) = Entropy(S) - \sum_{v \in \{weak,strong\}} \frac{|S_v|}{|S|} Entropy(S_v)$$

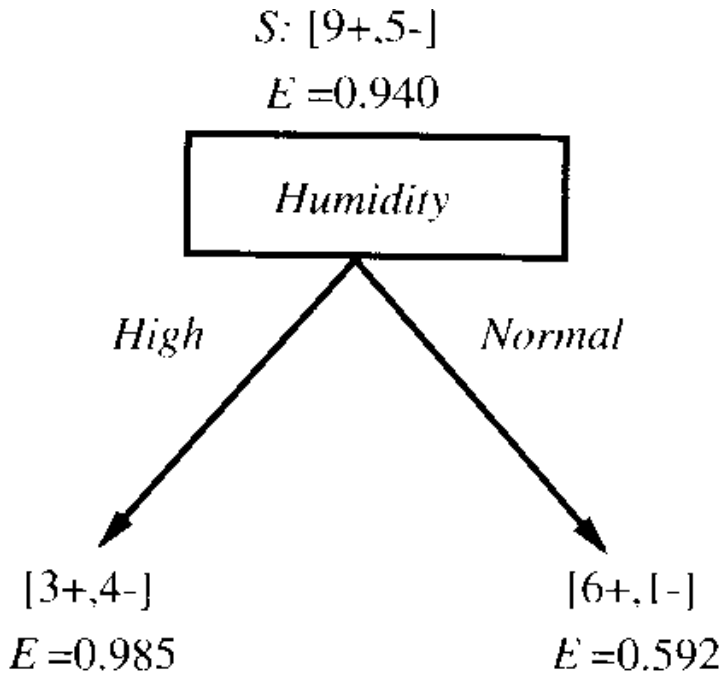
The information gain by sorting the 14 examples by Wind is:

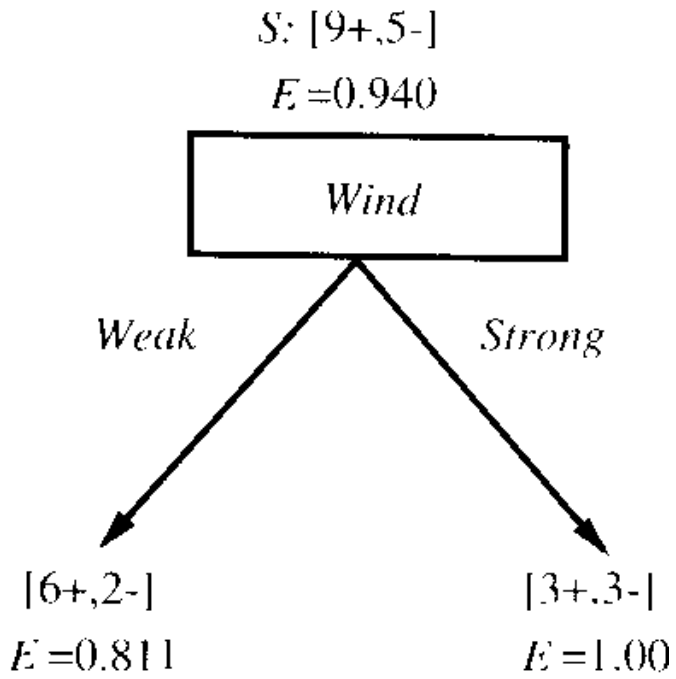
$$Entropy(S) - (8/14)\,Entropy(S_{Weak}) - (6/14)\,Entropy(S_{Strong})$$

$=0.940\text{-}(8/14)0.811\text{-}(6/14)1.00$

$=0.048$

Example Continued





Gain (S, Humidity)

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

Gain (S, Wind)

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

$$Entropy(S) \equiv \sum_{i=1}^{c} -p_i \log_2 p_i \qquad Gain(S,Wind) = Entropy(S) - \sum_{v \in \{weak,strong\}} \frac{|S_v|}{|S|} Entropy(S_v)$$

In more Detail - Humidity

S: [9+,5-]

E=-(9/14)$\log_2$(9/14)-(5/14)$\log_2$(5/14) = 0.940

S[3+,4-]

E=-(3/7)$\log_2$(3/7)-(4/7)$\log_2$(4/7) = 0.985

S[6+,1-]

E=-(6/7)$\log_2$(6/7)-(1/7)$\log_2$(1/7) = 0.592

GR=0.940-(7/14) x 0.985 - (7/14) x 0.592 = .151

$$Entropy(S) \equiv \sum_{i=1}^{c} -p_i \log_2 p_i \qquad Gain(S,Wind) = Entropy(S) - \sum_{v \in \{weak,strong\}} \frac{|S_v|}{|S|} Entropy(S_v)$$

One More Time - Wind

S: [9+,5-]

E=-(9/14)$\log_2$(9/14)-(5/14)$\log_2$(5/14) = 0.940

S[6+,2-]

E=-(6/8)$\log_2$(6/8)-(2/8)$\log_2$(2/8) = 0.811

S[3+,3-]

E=-(3/6)$\log_2$(3/6)-(3/6)$\log_2$(3/6) = 1.00

GR=0.940-(8/14) x 0.811 - (6/14) x 1.00 = .048

Decision Tree Example

ID3 uses Information Gain to select the best attribute at each step in growing the tree.

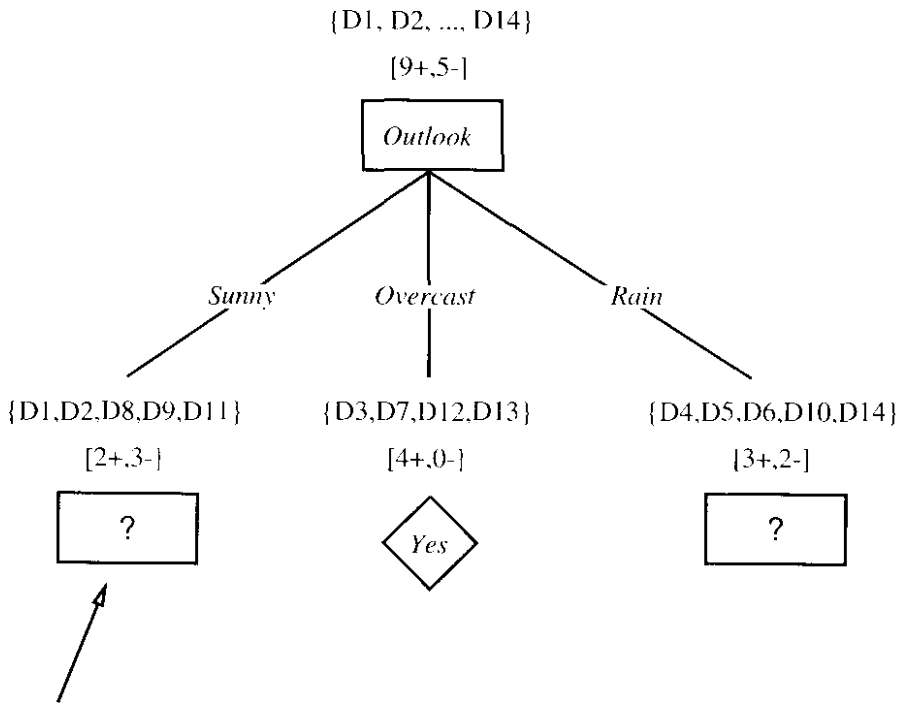
Gain(S,Outlook)=0.246

Gain(S,Humidity)=0.151

Gain(S,Wind)=0.048

Gain(S,Temperature)=0.029

Partially Grown Tree



Which attribute should be tested here?

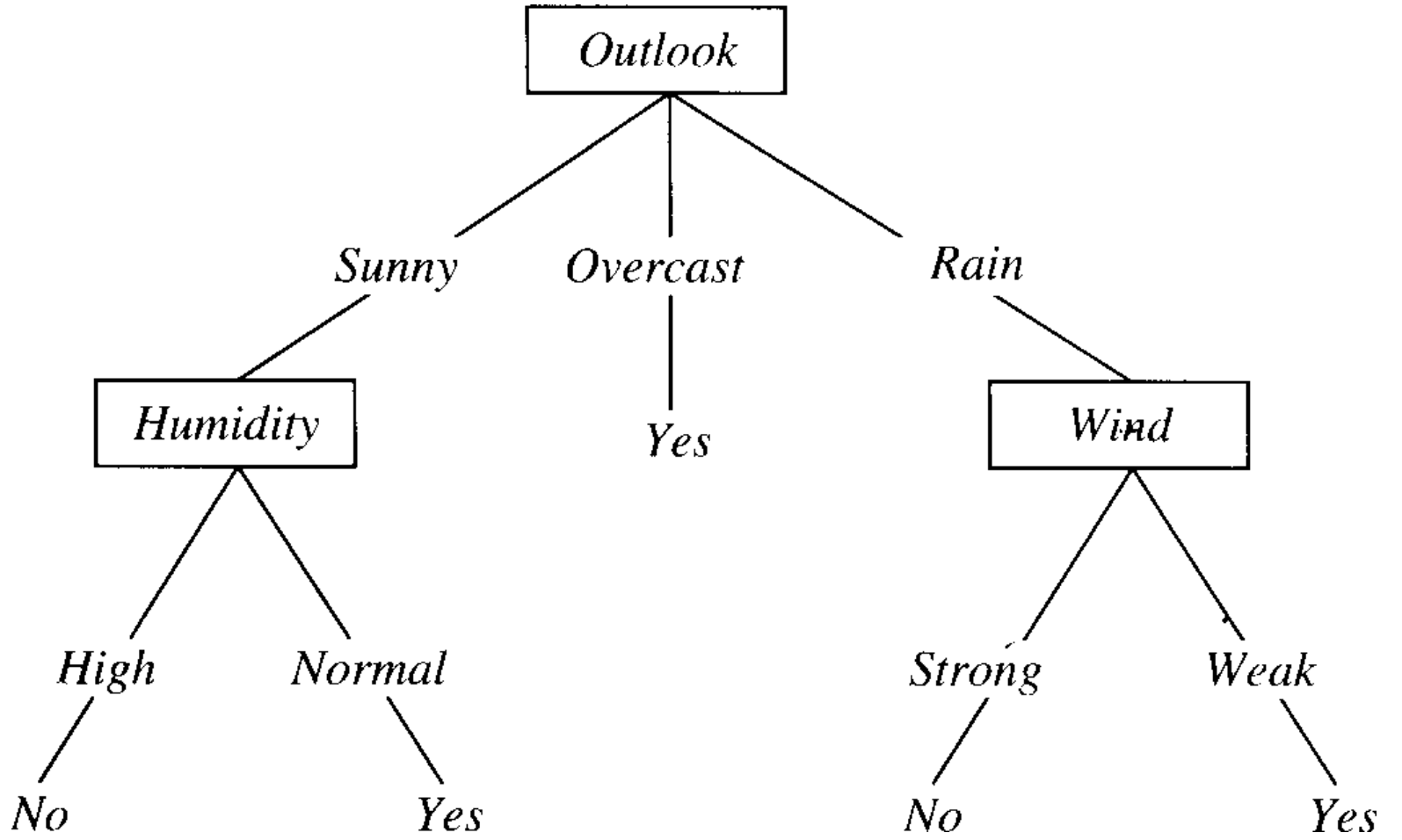
S_{sunny} = {D1,D2,D8,D9,D11}

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

Final Tree


Outlook
Sunny
Overcast
Rain
Humidity
Yes
Wind
High
Normal
Strong
Weak
No
Yes
No
Yes

Searching in Decision Trees

ID3 can be seen as searching the space of possible decision trees:

Simple to complex hill-climbing search

Complete hypothesis space of finite discrete-valued functions

ID3 maintains only a single current hypothesis

Greedy Search (no backtracking)

Searching II

Can’t tell how many alternative decision trees are consistent with the available training data

Can’t pose queries for new instances that optimally resolve the competing hypothesis

Pure ID3 performs no backtracking - can converge to local optimum - greedy search

ID3 not incremental - less sensitive to errors in individual training instances - easily extended to handle noisy data

ID3 Hypothesis Space

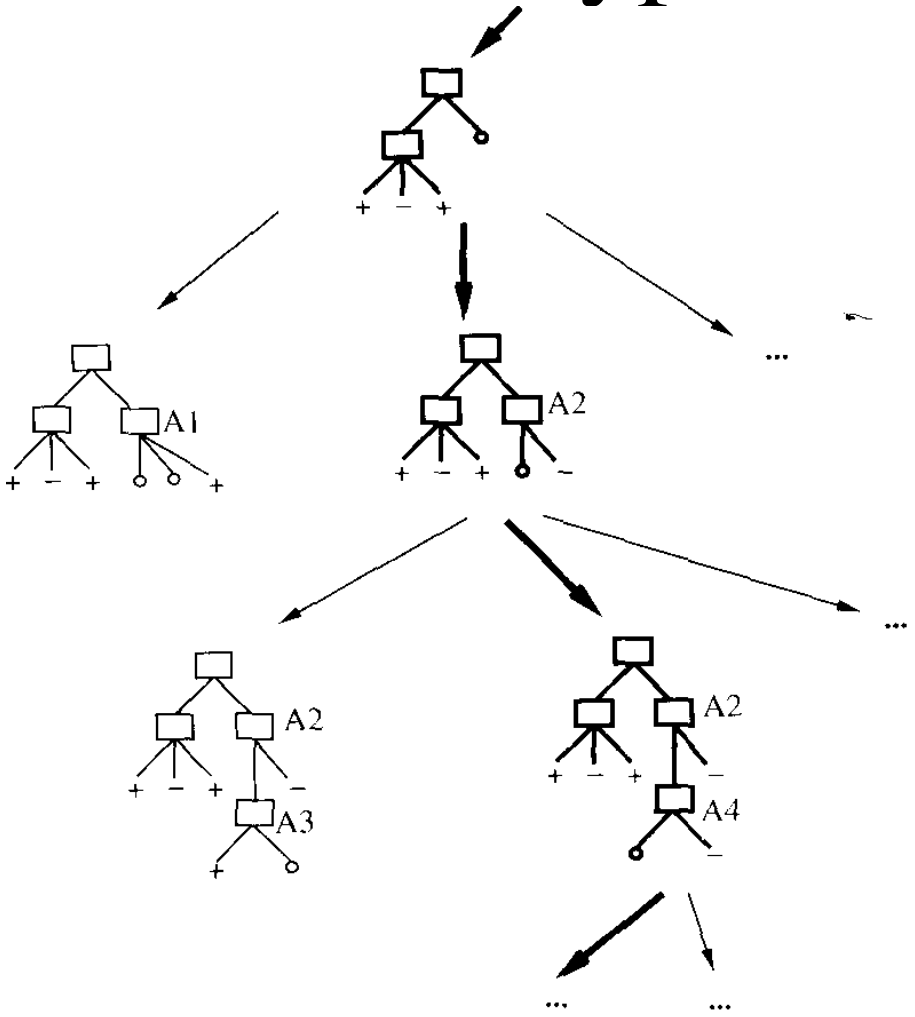


FIGURE 3.5
Hypothesis space search by ID3. ID3 searches through the space of possible decision trees from simplest to increasingly complex, guided by the information gain heuristic.

Inductive Bias in Decision Tree Learning

Much harder to define because of heuristic search

Shorter trees are preferred over long ones.

Trees that place high information gain attributes close to the root are preferred over those that do not.

Restriction Biases and Preference Biases

ID3 ***incompletely searches a complete hypothesis space*** from simple to complex hypothesis. Its bias is solely a consequence of the ordering of hypothesis searched. Its hypothesis space introduces no additional bias - ***preference or search bias***.

Candidate-Elimination ***completely searches an incomplete hypothesis space.*** Its bias is solely a consequence of the expressive power of its hypothesis representation. Its search strategy introduces no additional bias - ***restriction or language bias.***

What is the Best Bias?

A preference bias is more desirable

First learner

- restriction bias (linear function),
- preference bias (LMS algorithm for parameter tuning)

Occam's razor

Prefer the simplest hypothesis that fits the data.

Why?

Fewer short hypothesis then long ones - it is less likely that one will find a short hypothesis that coincidently fits the training data

This is really rubbish!!!!

Occam's razor is Slashed

Prefer decision trees containing exactly 17 leaf nodes with 11 nonleaf nodes, that use the decision attribute A1 at the root and test attributes A2 through A11, in numerical order.

There are relatively few such trees and we might argue (by the same reasoning above) that our a priori chance of finding one consistent with an arbitrary set of data is therefore small.

Another problem - based on internal learner's representation

Different Representations

	outlook	humidity	wind	temp
	rainy	high	normal	low

	Outlook & humidity	Wind & temp
	Rainy-high	Normal-low

Overfitting Definition

Given a hypothesis space H, a hypothesis $h \in H$ is said to overfit the training data if there exists some alternative hypothesis $h' \in H$, such that h has a smaller error than h' over the training examples, but h' has a smaller error than h over the entire distribution of instances.

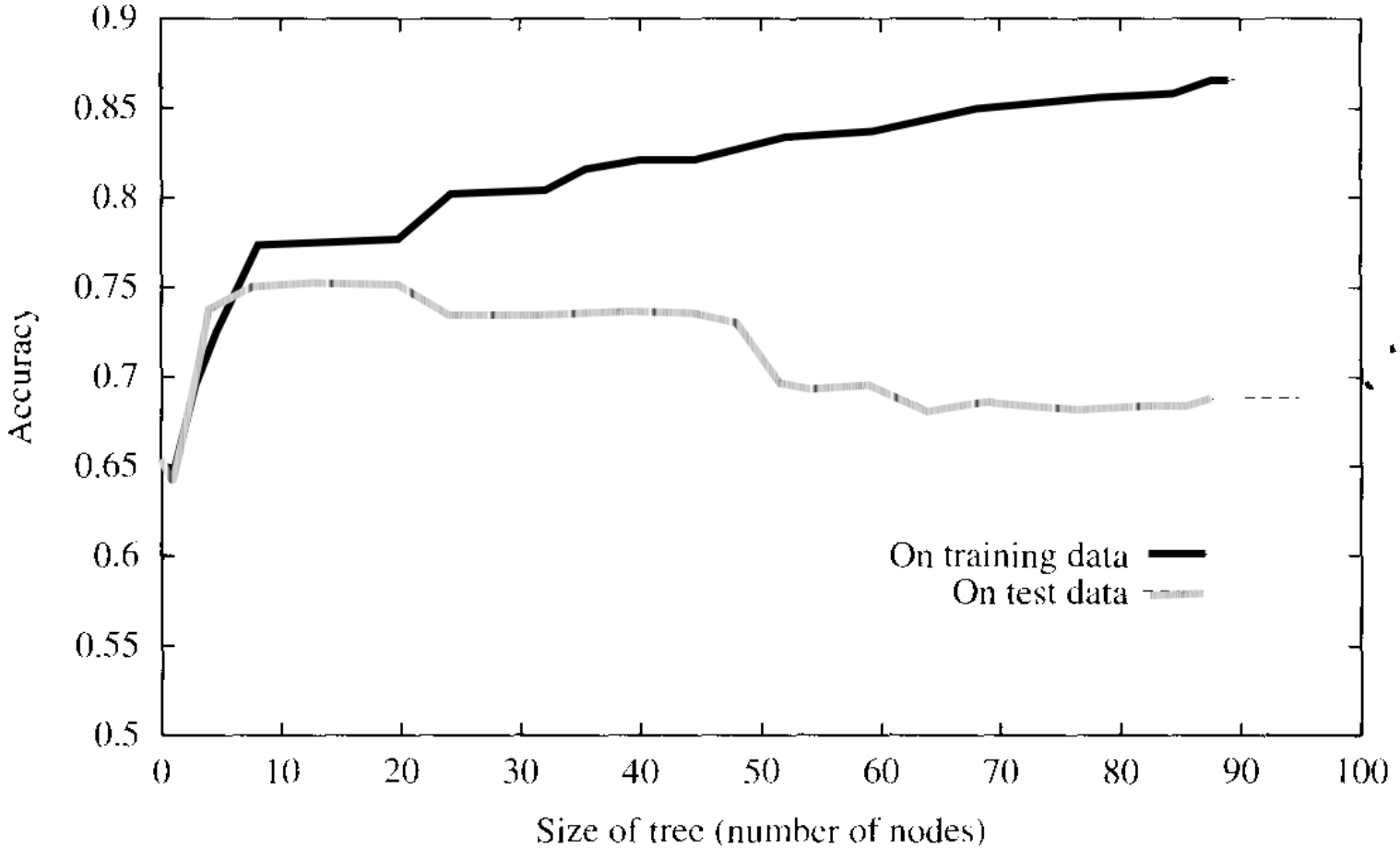
Pretty useless definition - not causal

What Increases Overfitting

Noise (errors) in the data,

Number of training instances too small

Overfitting in Decision Trees



Approaches to Overfitting

Stop growing tree earlier

Post-prune the tree

Separate set of examples -

training and validation set approach - even if the training set is mislead by random errors the validation set is unlikely to exhibit the same random fluctuations - 2/3 training, 1/3 validation

Statistical test

What is Overfitting really?

Given a hypothesis space H, a hypothesis h∈H is said to **overfit** the training data if there exists some alternative hypothesis h´∈H, such that h has a smaller error than h´ over the training examples, but h´ has a smaller error that h over the entire distribution of instances.

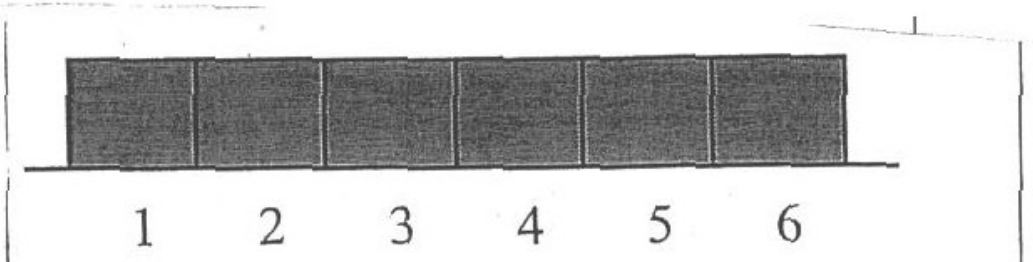
Not a very useful definition!

What causes Overfitting?

Why would complexity cause overfitting???

What about multiple comparisons?

Sampling Distributions for 1 die and 10 dice?

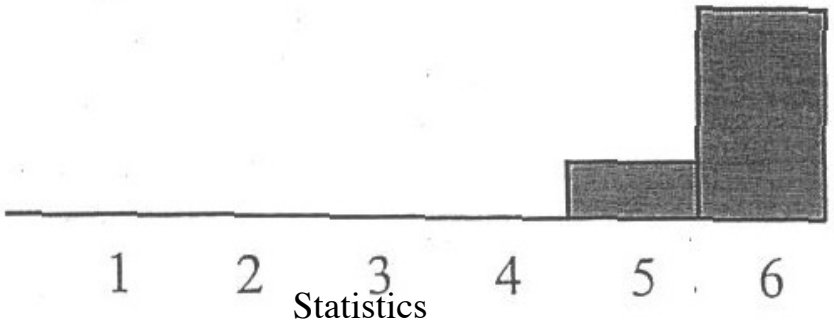


$E(X_i|H_0) = 3.5$

$p(X_i>5|H_0) = 0.167$

(a)

ampling distributions for one die and ten dice



Multiple Comparisons

Cause overfitting, oversearching, feature selection problems

Solutions

New test data

Bonferroni & Sidak (mathematical adjustment, assumes independence)

Cross validation - biased if k is to large because then the training sets are virtually the same - leave one out

Randomization tests - my favorite - drawback is cpu intensive- but to estimate p-values between .1 and .01 usually requires no more than 100-1000 trials

Multiple Comparisons Problem Increases

Number of attributes goes up

Number of Data Points does down

Random Error Goes up

Signal is more complex

Randomisation Test

A permutation test (also called a randomization test, re-randomization test, or an exact test) is a type of statistical significance test in which a **reference distribution is obtained by calculating all possible values** of the test statistic under rearrangements of the labels on the observed data points.

Parametric versus Non-parametric

Parametric tests, such as those described in exact statistics, are exact tests when the **parametric assumptions are fully met**, but in practice the use of the term exact (significance) test is reserved for those tests that do not rest on parametric assumptions – non-parametric tests.

However, in practice most implementations of **non-parametric** test software use **asymptotical algorithms** for obtaining the significance value, which makes the implementation of the test non-exact.

ML Randomisation Test

1. Run your ML algorithm and get a value (error, accuracy)
2. Remove the class column, randomly shuffle, and reattach the column (the class should now be random)
3. Run your ML algorithm and get a value (error, accuracy)
4. Repeat line 3 and 4 until 100-1000 values are calculated.
5. Plot these numbers. (These numbers will be a normal distribution.)
6. Find out the confidence interval that your original value (line 1) gives you.

Why does Pruning Decision Trees Work?

By pruning decision trees we are making the hypothesis space smaller (only small decision trees are allowed) so the effect of the multiple comparison's problem is reduced.

Do I believe this? – maybe – but also a validation set

Reduced Error Pruning

Consider each node for pruning

Pruning = removing the subtree at that node, make it a leaf and assign the most common class at that node

A node is removed if the resulting tree performs no worse then the original on the validation set - removes coincidences and errors

Reduced Error Pruning II

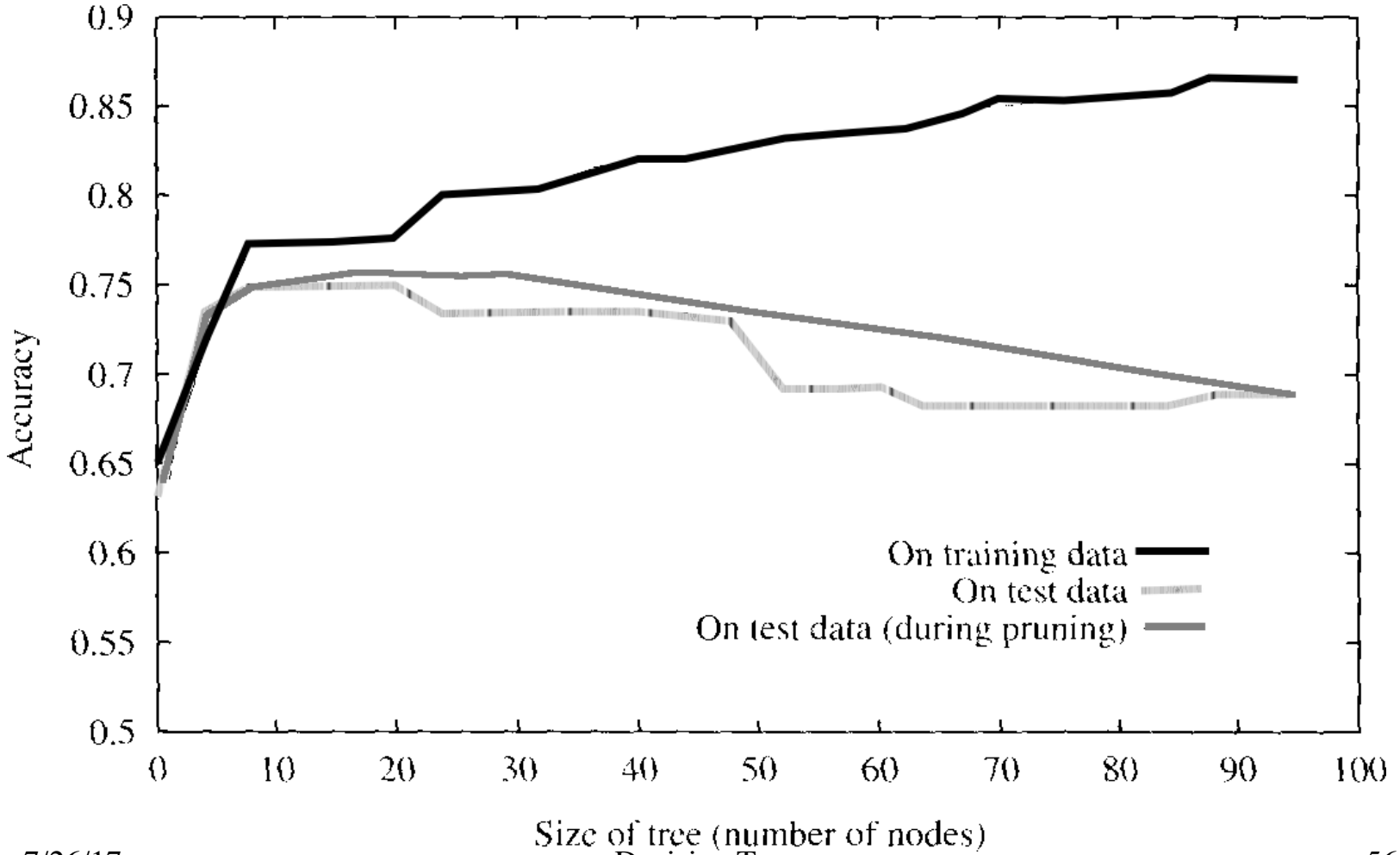
Nodes are removed iteratively choosing the node whose removal most increases the decision tree accuracy on the graph.

Pruning continues until further pruning is harmful.

Uses training, validation & test sets

effective approach if a large amount of data is available

Impact of Reduced Error Pruning



Rule Post Pruning

1. Infer decision tree from training set

2. Convert tree to rules - one rule per branch

3. Prune each rule by removing preconditions that result in improved estimated accuracy

4. Sort the pruned rules by their estimated accuracy and consider them in this sequence when classifying unseen instances

Why Convert to Rules?

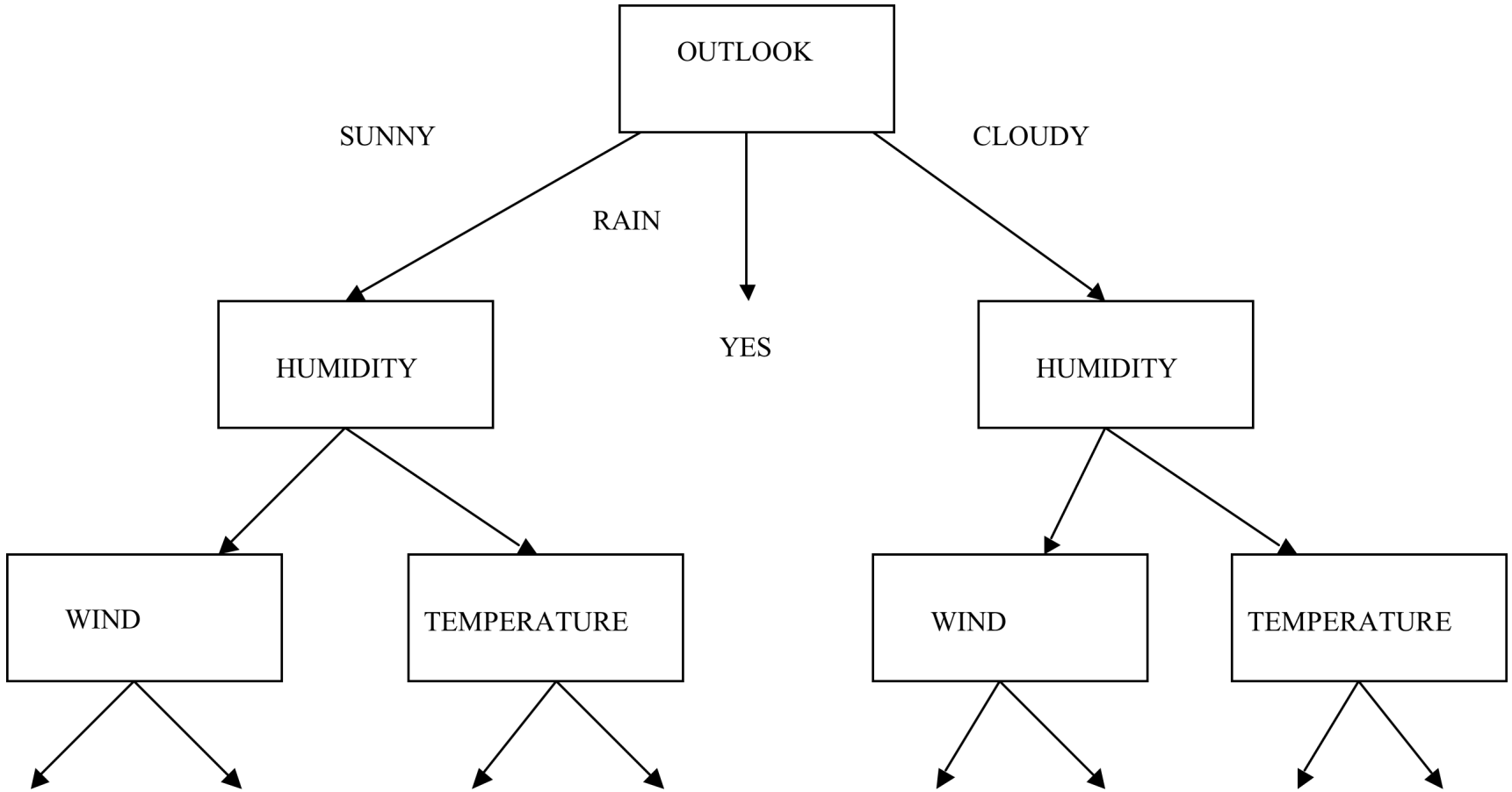
Allows distinguishing among different contexts in which a node might be used

Removes distinction between attribute tests near the root versus leafs

- no messy bookkeeping

Easier for people to understand

Tree With Redundancies



Continuous Valued Attributes?

Dynamically creating new discrete valued attributes A_c that is true if $A < c$

1. Sort examples according to the continuous attribute value
2. Identify adjacent examples that differ in their target classifications
3. Generate candidate threshold midway between these points
4. Calculate the information gain of each candidate and pick best
5. Dynamically created boolean attributes to compete with others to appear in tree

The value of c that maximizes information gain must be one of these points

Example

Temperature	40	48	60	72	80	90
PlayTennis	No	No	Yes	Yes	Yes	No

(48+60)/2 = 54

(80+90)/2 = 85

$Temperature_{>54}$, $Temperature_{>85}$

Other Measures for Picking Attributes

- Information Gain has natural bias towards attributes with many values over ones with few
  - For instance Date attribute has highest information gain (or Student ID)

- Use Gain Ratio

Gain Ratio

Entropy of S with respect to the values of A

$$GainRatio(S,A) \equiv \frac{Gain(S,A)}{SplitInfo(S,A)}$$

$$SplitInfo(S,A) \equiv -\sum_{i=1}^{c} \frac{|S_i|}{|S|} \log_2 \frac{|S_i|}{|S|}$$

Gain Ratio Intuition

If attribute A splits the examples each into separate unique values (Date), SplitInfo = $\log_2 n$

If attribute B splits the examples in half, SpiltInfo=1

Then if attributes A and B have the same Gain then B will clearly score higher

Problems with Gain Ratio

If $|S_i| \approx |S|$, then GainRatio is undefined or very large

To avoid selecting attributes on this basis

1. Calculate Gain of each attribute
2. Calculate GainRatio only on attributes with above average Gain
3. Choose best GainRatio

Other Evaluation Functions

Many other evaluation functions

Distance metric Lopez de Mantaras, 1991

- Distance between our partition and the perfect partition
- Not biased by number of values for an attribute

Missing Attribute Values in Training Examples

Blood-Test_Result

1. Standard methodology from Statistics is to throw away data
2. Assign missing value to the most common value at node n
3. Alternatively, assign missing value to the most common value at node n for examples with the same target value
4. Assign probability to each possible value, estimated by frequencies at node n

Missing Attribute II

Latter tack, can be subdivided again later in the tree

Same approach can be used to classify examples

Attributes with Differing Costs

Temperature, BiopsyResult, Pulse, BloodTestResults

Prefer decision trees that use low-cost attributes where possible

Divide Gain by the cost of the attribute

Do not guarantee optimal cost-senstive decision tree, but bias the search in favor of low cost attributes

Differing Costs II

Robot domain - $\frac{Gain^2(S,A)}{Cost(A)}$

Medical Domain $\frac{2^{Gain(S,A)}-1}{(Cost(A)+1)^w}$

Where $w \in \{0,1\}$ is a constant that determines the relative important of cost versus information gain

Summary

Decision Trees are practical for discrete-valued functions, grows tree from root down, selecting next best attribute at each new node added to tree.

ID3 searches complete hypothesis space. It can represent any discrete-valued function defined over discrete values instances, therefore it avoids the problem of the target function not being in the hypothesis space.

Inductive Bias implicit in ID3 is ***preference*** for smaller trees, only grows as large as needed to classify training examples.

Summary continued

Overfitting data is an important issue.

Very large variety of extensions: post-pruning, handling real-valued attributes, accommodating missing attribute values, incrementally refining decision trees, other attribute selection measures, considering costs associated with instance attributes (or target values).

Questions you should be able to answer - 1

- What does information theory have to do with Machine Learning?
- What is the difference between a preference bias and a restriction bias?
- Is an algorithm that has a larger inductive bias better or worse?

Questions you should be able to answer - 2

- What is overfitting? What really causes it?
- What is the multiple comparison's problem?
- What is a randomization test?