Machine Learning

Approach based on Decision Trees

- Decision Tree Learning
  - Practical inductive inference method
  - Same goal as *Candidate-Elimination algorithm*
    - Find Boolean function of attributes
    - Decision trees can be extended to functions with more than two output values.
  - Widely used
  - Robust to noise
  - Can handle disjunctive (OR’s) expressions
  - Completely expressive hypothesis space
  - Easily interpretable (tree structure, if-then rules)

Training Examples

Object, sample, example

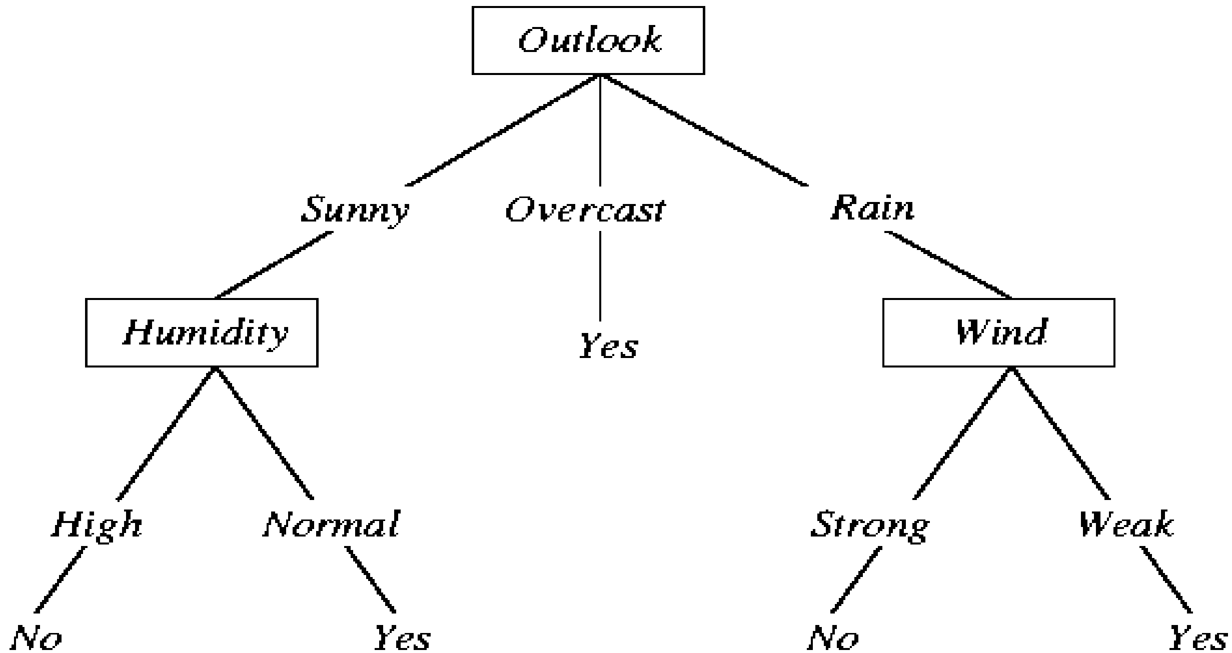
Attribute, variable, property

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
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

Shall we play tennis today?

decision

Decision Tree for *PlayTennis*



Shall we play tennis today?

- **Decision trees do classification**
  - Classifies instances into one of a discrete set of possible categories
  - **Learned function** represented by tree
  - Each ***node in tree*** is test on some attribute of an instance
  - Branches represent *values of attributes*
  - Follow the tree from root to leaves to find the output value.

- The tree itself forms hypothesis
  - Disjunction (OR's) of conjunctions (AND's)
  - Each path from root to leaf forms conjunction of constraints on attributes
  - Separate branches are disjunctions
- Example from *PlayTennis* decision tree:

(Outlook=Sunny $\wedge$ Humidity=Normal)

$\vee$

(Outlook=Overcast)

$\vee$

(Outlook=Rain $\wedge$ Wind=Weak)

- **Types of problems decision tree learning is good for:**
  - Instances represented by attribute-value pairs
    - For algorithm in book, attributes take on a small number of discrete values
    - Can be extended to real-valued attributes
      - (numerical data)
    - Target function has **discrete output values**
    - Algorithm in book assumes Boolean functions
    - Can be extended to multiple output values

- Hypothesis space can include disjunctive expressions.
  - In fact, hypothesis space is complete space of finite discrete-valued functions
- Robust to imperfect training data
  - classification errors
  - errors in attribute values
  - missing attribute values

• Examples:
- Equipment diagnosis
- Medical diagnosis
- Credit card risk analysis
- Robot movement
- Pattern Recognition
  - face recognition
  - hexapod walking gates

- **Algorithms used:**
  - ID3 Quinlan (1986)
  - C4.5 Quinlan(1993)
  - C5.0 Quinlan
  - Cubist Quinlan
  - CART Classification and regression trees Breiman (1984)
  - ASSISTANT Kononenco (1984) & Cestnik (1987)
- ID3 is algorithm discussed in textbook
  - Simple, but representative
  - Source code publicly available

- **ID3 Algorithm**
  - Top-down, greedy search through space of possible decision trees
    - Remember, decision trees represent hypotheses, so this is a search through hypothesis space.
  - What is top-down?
    - How to start tree?
      - What attribute should represent the root?
    - As you proceed down tree, choose attribute for each successive node.
    - ***No backtracking***:
      - So, algorithm proceeds from top to bottom

- What is a **greedy search**?
  - At each step, make decision which makes greatest improvement in whatever you are trying optimize.
  - Do not backtrack (unless you hit a dead end)
  - This type of search is likely not to be a globally optimum solution, but generally works well.
- What are we really doing here?
  - At each node of tree, make decision on which **attribute** best classifies training data at that point.
  - Never backtrack (in ID3)
  - Do this for each branch of tree.
  - End result will be tree structure representing a ***hypothesis which works best for the training data***.

Question?

How do you determine *which attribute best classifies data*?

Answer: **Entropy!**

- ***Information gain:***
  - Statistical quantity measuring how well an attribute classifies the data.
    - Calculate the information gain for each attribute.
    - Choose attribute with greatest information gain.

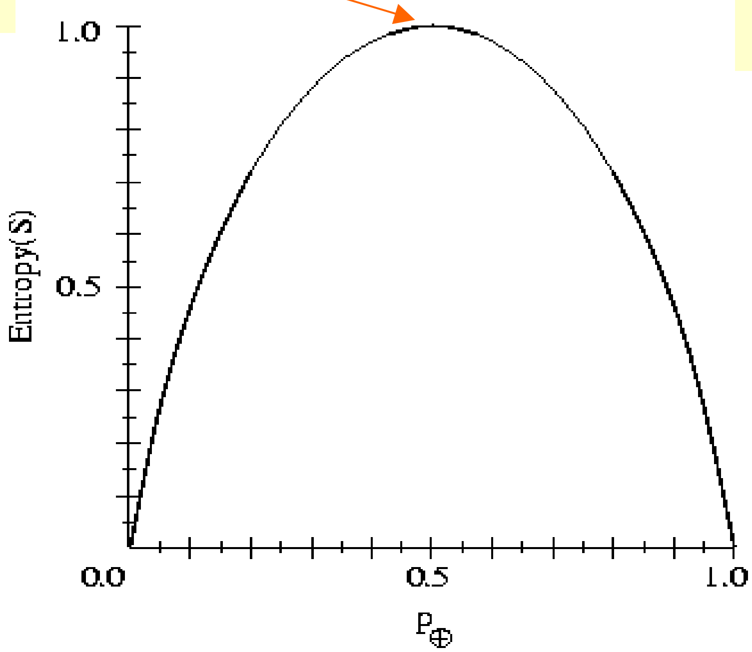
- **But how do you measure information?**
  - **Claude Shannon in 1948 at Bell Labs established the field of information theory.**
  - **Mathematical function, *Entropy*, measures** information content **of *random process*:**
    - **Takes on largest value when events are equiprobable.**
    - **Takes on smallest value when only one event has non-zero probability.**
  - **For two states:**
    - **Positive examples and Negative examples from set S:**

$$H(S) = -p_{+}\log_2(p_{+}) - p_{-}\log_2(p_{-})$$

Entropy of set S denoted by H(S)

Entropy

Largest entropy



Boolean functions with the same number of ones and zeros have largest 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

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

- In general:
  - For an <u>ensemble</u> of random events: $\{A_1, A_2, \ldots, A_n\}$, occurring with probabilities: $\mathbf{z} = \{P(A_1), P(A_2), \ldots, P(A_n)\}$

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

(Note: $1 = \sum_{i=1}^{n} P(A_i)$ and $0 \le P(A_i) \le 1$)

If you consider the self-information of event, *i*, to be: $-\log_2(P(A_i))$
Entropy is weighted average of information carried by each event.

Does this make sense?

- If an event conveys information, that means it's a surprise.
- If an event always occurs, $P(A_i)=1$, then it carries no information. $-log_2(1) = 0$
- If an event rarely occurs (e.g. $P(A_i)=0.001$), it carries a lot of info. $-log_2(0.001) = 9.97$
- **The less likely the event, the more the information it carries** since, for $0 \leq P(A_i) \leq 1$, $-log_2(P(A_i))$ increases as $P(A_i)$ goes from 1 to 0.
- (Note: ignore events with $P(A_i)=0$ since they never occur.)

- What about entropy?
  - Is it a good measure of the information carried by an ensemble of events?
  - If the events are equally probable, the entropy is maximum.

1) For N events, each occurring with probability *1/N*.

$$H = -\sum(1/N)\log_2(1/N) = -\log_2(1/N)$$

This is the maximum value.

(e.g. For N=256 (ascii characters) $-\log_2(1/256) = 8$
number of bits needed for characters.
Base 2 logs measure information in bits.)

This is a good thing since an ensemble of equally probable events is as uncertain as it gets.

(Remember, **information corresponds to surprise** - ***uncertainty***.)

– **2)** *H* is a continuous function of the probabilities.

- That is always a good thing.

– **3)** If you sub-group events into compound events, the entropy calculated for these compound groups is the same.

- That is good since the uncertainty is the same.

- ***It is a remarkable fact that the equation for entropy shown above (up to a multiplicative constant) <u>is the only function</u> which satisfies these three conditions.***

- **Choice of base 2 log corresponds to choosing units of information.(BIT's)**
- ***Another remarkable thing:***
  - ***This is the same definition of entropy used in statistical mechanics for the measure of disorder.***
  - ***Corresponds to macroscopic thermodynamic quantity of Second Law of Thermodynamics.***

- The concept of a quantitative measure for information content plays an important role in many areas:
- For example,
  - Data communications (channel capacity)
  - Data compression (limits on error-free encoding)
- Entropy in a message corresponds to ***minimum number of bits needed to encode that message***.
- In our case, for a set of training data, the entropy measures the number of bits needed to encode classification for an instance.
  - Use probabilities found from entire set of training data.
  - **Prob(Class=Pos) = Num. of positive cases / Total case**
  - **Prob(Class=Neg) = Num. of negative cases / Total cases**

(Back to the story of ID3)

- *Information* ***gain*** is our metric for how well one attribute **A_i** classifies the training data.
- Information gain for a particular attribute =

  Information about target function,

  given the value of that attribute.

  (conditional entropy)
- Mathematical expression:

Entropy

$$Gain(S, A_i) = H(S) - \sum_{v \in Values(A_i)} P(A_i = v) H(S_v)$$

Information gain

- **ID3 algorithm (for boolean-valued function)**
  - Calculate the entropy for all training examples
    - positive and negative cases
    - p_+ = #pos/Tot $\qquad$ p_- = #neg/Tot
    - $H(S) = -p_+ \log_2(p_+) - p_- \log_2(p_-)$
  - Determine which ***single* attribute** best classifies the training examples using information gain.
    - For each attribute find:

$$Gain(S, A_i) = H(S) - \sum_{v \in Values(A_i)} P(A_i = v) H(S_v)$$

    - Use attribute with greatest information gain **as a root**

- **Example:** *PlayTennis*
  - Four attributes used for classification:
    - *Outlook* = {Sunny,Overcast,Rain}
    - *Temperature* = {Hot, Mild, Cool}
    - *Humidity* = {High, Normal}
    - *Wind* = {Weak, Strong}
  - One predicted (target) attribute (binary)
    - *PlayTennis* = {Yes,No}
  - Given 14 Training examples
    - 9 positive
    - 5 negative

Training Examples

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14 cases

9 positive cases

- Step 1: *Calculate* ***entropy*** for all cases:

$N_{Pos} = 9$ $N_{Neg} = 5$ $N_{Tot} = 14$

$H(S) = -(9/14)*\log_2(9/14) - (5/14)*\log_2(5/14) = 0.940$

entropy

- Step 2: Loop over all attributes, calculate gain:
  - **Attribute = *Outlook***
    - Loop over values of *Outlook*

      Outlook = Sunny

      $N_{Pos} = 2$ $N_{Neg} = 3$ $N_{Tot} = 5$

      H(Sunny) = $-(2/5)*\log_2(2/5) - (3/5)*\log_2(3/5) = 0.971$

      Outlook = Overcast

      $N_{Pos} = 4$ $N_{Neg} = 0$ $N_{Tot} = 4$

      H(Sunny) = $-(4/4)*\log_2 4/4 - (0/4)*\log_2(0/4) = 0.00$

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D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Outlook = Rain

$N_{Pos} = 3$ $N_{Neg} = 2$ $N_{Tot} = 5$

$H(Sunny) = -(3/5)*\log_2(3/5) - (2/5)*\log_2(2/5) = 0.971$

- Calculate **Information Gain** for attribute Outlook

$$Gain(S,Outlook) = H(S) - N_{Sunny}/N_{Tot}*H(Sunny) - N_{Over}/N_{Tot}*H(Overcast) - N_{Rain}/N_{Tot}*H(Rainy)$$

$$Gain(S,Outlook) = 9.40 - (5/14)*0.971 - (4/14)*0 - (5/14)*0.971$$

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

– **Attribute = *Temperature***

- (Repeat process looping over {Hot, Mild, Cool})

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

– Attribute = *Humidity*

- (Repeat process looping over {High, Normal})

  Gain(S,*Humidity*) = 0.029

– Attribute = *Wind*

- (Repeat process looping over {Weak, Strong})

  Gain(S,*Wind*) = 0.048

Find attribute with greatest information gain:

Gain(S,*Outlook*) = 0.246, Gain(S,*Temperature*) = 0.029

Gain(S,*Humidity*) = 0.029, Gain(S,*Wind*) = 0.048

∴ Outlook is root node of tree

- **Iterate algorithm to find attributes which best classify training examples under the values of the root node**
- **Example continued**
  - **Take three subsets:**
    - ***Outlook* = Sunny** **(N_{Tot} = 5)**
    - ***Outlook* = Overcast** **(N_{Tot} = 4)**
    - ***Outlook* = Rainy** **(N_{Tot} = 5)**
  - **For each subset, repeat the above calculation looping over all attributes <u>other than *Outlook*</u>**

– For example:

- *Outlook* = Sunny (N_{Pos} = 2, N_{Neg}=3, N_{Tot} = 5) H=0.971
  - *Temp* = Hot (N_{Pos} = 0, N_{Neg}=2, N_{Tot} = 2) H = 0.0
  - *Temp* = Mild (N_{Pos} = 1, N_{Neg}=1, N_{Tot} = 2) H = 1.0
  - *Temp* = Cool (N_{Pos} = 1, N_{Neg}=0, N_{Tot} = 1) H = 0.0

  Gain(S_{Sunny},*Temperature*) = 0.971 - (2/5)*0 - (2/5)*1 - (1/5)*0

  Gain(S_{Sunny},*Temperature*) = 0.571

  Similarly:

  Gain(S_{Sunny},*Humidity*) = 0.971

  Gain(S_{Sunny},*Wind*) = 0.020

  ∴ Humidity classifies *Outlook*=Sunny instances best and is placed as the node under Sunny outcome.

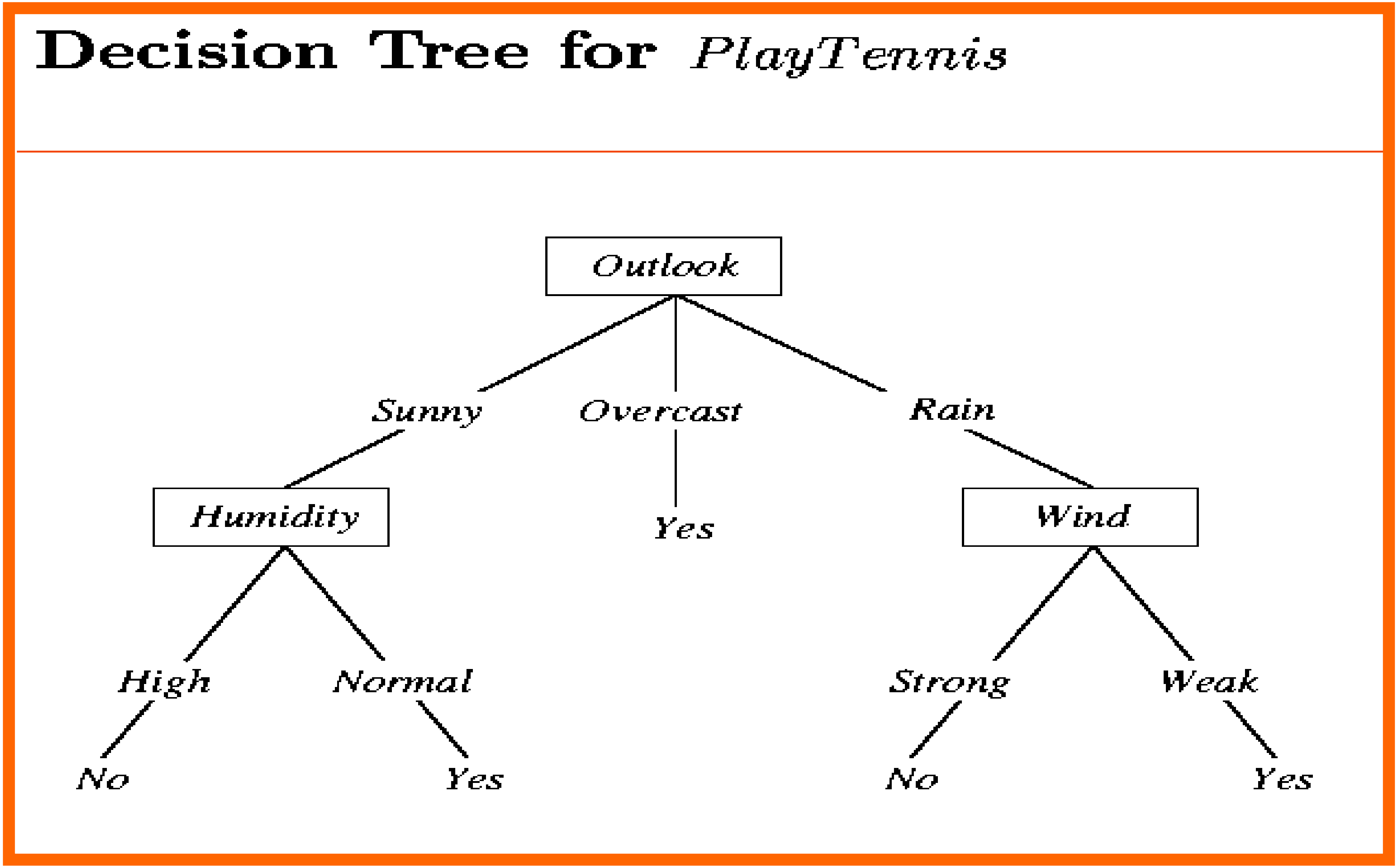
– Repeat this process for *Outlook* = Overcast &Rainy

- **Important:**
  - Attributes are excluded from consideration if they appear higher in the tree
- Process continues for each new leaf node until:
  - Every attribute has already been included along path through the tree

  or

  - Training examples associated with this leaf all have same target attribute value.

– End up with tree:



- **Note:** In this example data was perfect.
  - No contradictions
  - Branches led to unambiguous *Yes*, *No* decisions
  - If there are contradictions take the majority vote
    - This handles noisy data.
- **Another note:**
  - Attributes are eliminated when they are assigned to a node and never reconsidered.
    - e.g. You would not go back and reconsider *Outlook* under *Humidity*
- **ID3 uses all of the training data at once**
  - Contrast to Candidate-Elimination
  - Can handle noisy data.

- What is the **hypothesis space** for decision tree learning?
  - Search through space of all possible decision trees
    - from simple to more complex guided by a heuristic: *information gain*
  - The space searched is complete space of finite, discrete-valued functions.
    - Includes disjunctive and conjunctive expressions
  - Method only maintains one current hypothesis
    - In contrast to Candidate-Elimination
  - Not necessarily global optimum
    - attributes eliminated when assigned to a node
    - No backtracking
    - Different trees are possible

- **Inductive Bias:** (restriction vs. preference)
  - ID3
    - searches *complete hypothesis space*
    - But, *incomplete search* through this space looking for simplest tree
    - This is called a **preference** (or search) bias
  - Candidate-Elimination
    - Searches an *incomplete hypothesis space*
    - But, does a *complete search* finding all valid hypotheses
    - This is called a **restriction** (or language) bias
  - Typically, preference bias is better since you do not limit your search up-front by restricting hypothesis space considered.

- **Summary of ID3 Inductive Bias**
  - **Short trees** are preferred over long trees
    - It accepts the first tree it finds
  - Information gain heuristic
    - Places high information gain attributes near root
    - Greedy search method is an approximation to finding the shortest tree
  - Why would short trees be preferred?
    - Example of **Occam's Razor:**

      Prefer simplest hypothesis consistent with the data.

      (Like Copernican vs. Ptolemic view of Earth's motion)

– Homework Assignment

- Tom Mitchell's software

See:

- http://www.cs.cmu.edu/afs/cs.cmu.edu/project/theo-3/www/ml.html
- Assignment #2 (on decision trees)
- Software is at: http://www.cs.cmu.edu/afs/cs/project/theo-3/mlc/hw2/
  - Compiles with gcc compiler
  - Unfortunately, README is not there, but it's easy to figure out:
    - » After compiling, to run:

      dt [-s <random seed>] <train %> <prune %> <test %> <SSV-format data file>
    - » %train, %prune, & %test are percent of data to be used for training, pruning & testing. These are given as decimal fractions. To train on all data, use 1.0 0.0 0.0
  - Data sets for PlayTennis and Vote are include with code.
  - Also try the Restaurant example from Russell & Norvig
  - Also look at www.kdnuggets.com/ (Data Sets)

    Machine Learning Database Repository at UC Irvine - (try "zoo" for fun)

Questions and Problems

- 1. Think how the method of finding best variable order for decision trees that we discussed here be adopted for:
  - ordering variables in binary and multi-valued decision diagrams
  - finding the bound set of variables for Ashenhurst and other functional decompositions
- 2. Find a more precise method for variable ordering in trees, that takes into account special function patterns recognized in data
- 3. Write a Lisp program for creating decision trees with entropy based variable selection.

- Sources
  - Tom Mitchell
  - Machine Learning, Mc Graw Hill 1997
  - Allan Moser