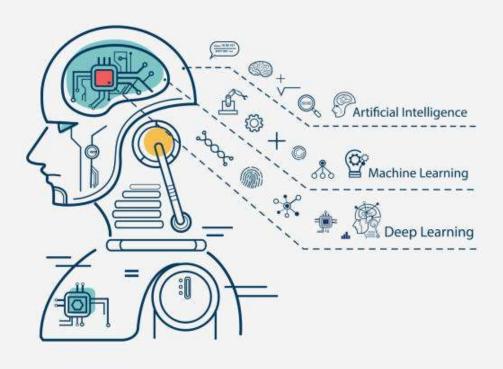
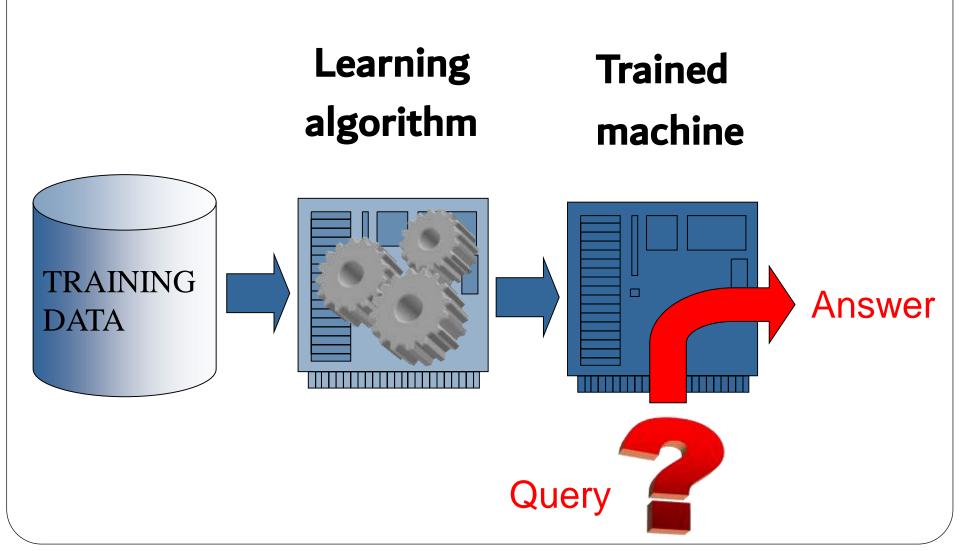
# CSE 440 Artificial Intelligence

# **Machine Learning**



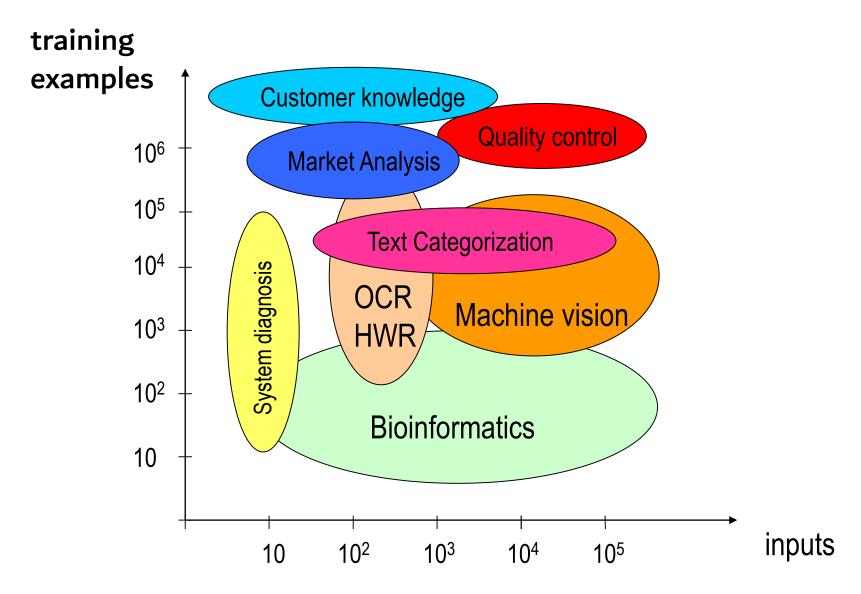
# What is Machine Learning?



### For which tasks?

- Classification (binary/categorical target)
- Regression and time series prediction (continuous targets)
- Clustering (targets unknown)
- Rule discovery

## For which applications?



## Banking / Telecom / Retail



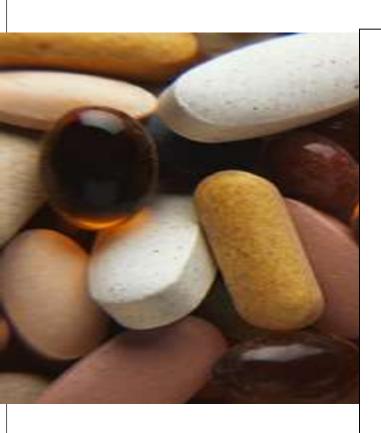
#### Identify:

- Prospective customers
- Dissatisfied customers
- Good customers
- Bad payers

#### • Obtain:

- More effective advertising
- Less credit risk
- Fewer fraud
- Decreased churn rate

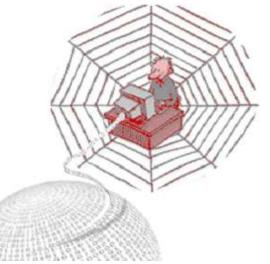
## Biomedical / Biometrics



- Medicine:
  - Screening
  - Diagnosis and prognosis
  - Drug discovery
- Security:
  - Face recognition
  - Signature / fingerprint / iris verification
  - DNA fingerprinting

## Computer / Internet





#### Computer interfaces:

- Troubleshooting wizards
- Handwriting and speech
- Brain waves

#### Internet

- Hit ranking
- Spam filtering
- Text categorization
- Text translation
- Recommendation

## ML in a Nutshell

- Tens of thousands of machine learning algorithms
- Hundreds new every year
- Every machine learning algorithm has three components:
  - Representation
  - Evaluation
  - Optimization

## Representation

- Decision trees
- Sets of rules / Logic programs
- Instances
- Graphical models (Bayes/Markov nets)
- Neural networks
- Support vector machines
- Model ensembles
- Etc.

## **Evaluation**

- Accuracy
- Precision and recall
- Squared error
- Likelihood
- Posterior probability
- Cost / Utility
- Margin
- Entropy
- K-L divergence
- Etc.

## **Optimization**

- Combinatorial optimization
  - E.g.: Greedy search
- Convex optimization
  - E.g.: Gradient descent
- Constrained optimization
  - E.g.: Linear programming

# **Types of Learning**

- Supervised (inductive) learning
  - Training data includes desired outputs
- Unsupervised learning
  - Training data does not include desired outputs
- Semi-supervised learning
  - Training data includes a few desired outputs
- Reinforcement learning
  - Rewards from sequence of actions

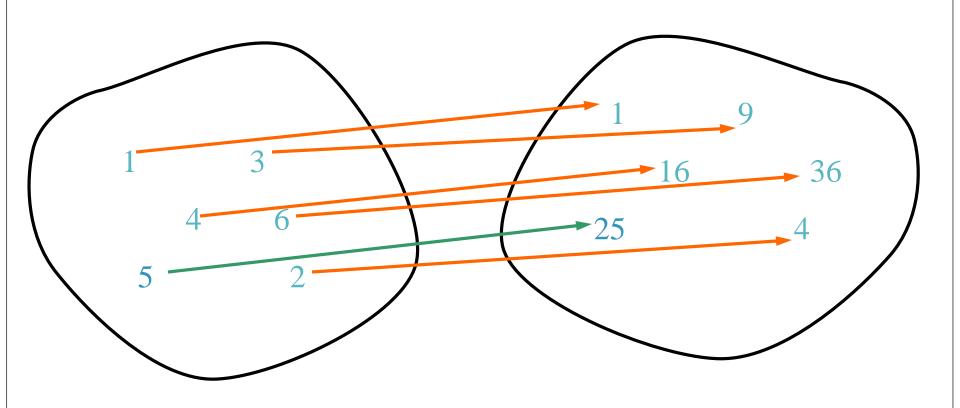
# Supervised Learning

Learning Through Examples

# **Supervised Learning**

- When a set of targets of interest is provided by an external teacher
   we say that the learning is Supervised
- The targets usually are in the form of an input output mapping that the net should learn

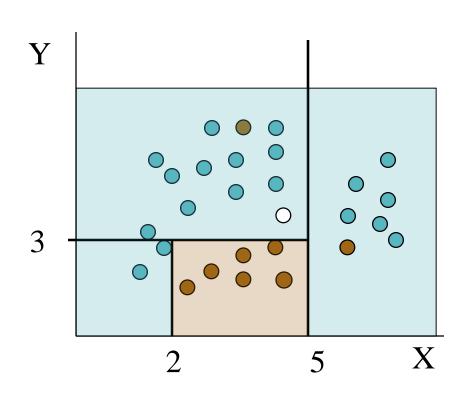
## **Learning From Examples**



## What We'll Cover

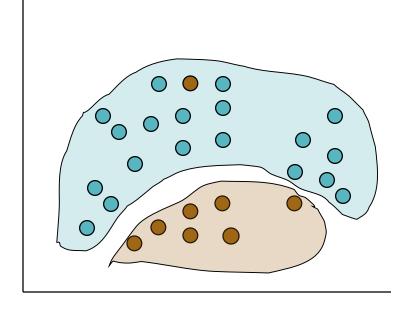
- Supervised learning
  - Decision tree induction
  - Neural networks
  - Rule induction
  - Instance-based learning
  - Bayesian learning
  - Support vector machines
  - Model ensembles
  - Learning theory

## **Classification: Decision Trees**



if X > 5 then blue else if Y > 3 then blue else if X > 2 then green else blue

## Classification: Neural Nets



- Can select more complex regions
- Can be more accurate
- Also, can overfit the data – find patterns in random noise

# **Decision Tree Learning**

Learning Through Examples

## Choosing the Best Attribute

- The key problem is 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 (fewer branches)
  - Most-Values: Choose the attribute with the largest number of possible values (smaller subsets)
  - Max-Gain: Choose the attribute that has the largest expected information gain, i.e. select attribute that will result in the smallest expected size of the subtrees rooted at its children.
- The ID3 algorithm uses the Max-Gain method of selecting the best attribute.

## ID3 (Iterative Dichotomiser 3) Algorithm

- Top-down, greedy search through space of possible decision trees
  - Remember, decision trees represent hypotheses, so this is a <u>search through hypothesis space</u>.
- 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

#### **Question?**

How do you determine which attribute best classifies data?

**Answer:** Entropy!

- Entropy is a measure of disorder or impurity
- Information gain.
  - Measures the expected reduction in entropy caused by partitioning
  - Statistical quantity measuring <u>how well an</u> <u>attribute classifies the data.</u>
    - Calculate the information gain for each attribute.
    - Choose attribute with greatest information gain.

# Information Theory Background

- If there are n equally probable possible messages, then the probability p of each is 1/n
- Information conveyed by a message is  $-\log(p) = \log(n)$
- Eg, if there are 16 messages, then log(16) = 4 and we need 4 bits to identify/send each message.
- In general, if we are given a probability distribution  $P = (p_1, p_2, ..., p_n)$
- the information conveyed by distribution (aka Entropy of P) is:

$$H(P) = -(p_1 * log(p_1) + p_2 * log(p_2) + ... + p_n * log(p_n))$$

#### **Information Gain**

Information gain is our metric for how well one attribute  $A_i$  classifies the training data.

- Calculate the <u>entropy</u> for <u>all training examples</u>
  - positive and negative cases
  - $p_{+}$  = #pos/Tot  $p_{-}$  = #neg/Tot
  - $H(S) = -p_1 \log_2(p_1) p_1 \log_2(p_2)$
- Determine which <u>single attribute</u> best classifies the training examples using information gain.
  - For each attribute find:

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

value v

- Use <u>attribute with greatest information gain</u> as a root
- Gain (S, A) = expected reduction in entropy due to sorting on A

- 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

Examples, minterms, cases, objects, test cases,

# **Training Examples**

	Day	Outlook	Temperature	Humidity	Wind	PlayTennis
1	D1	Sunny	Hot	High	Weak	No
	D2	$\mathbf{Sunny}$	$\operatorname{Hot}$	$\mathbf{High}$	Strong	No
	D3	Overcast	$\operatorname{Hot}$	$\mathbf{High}$	Weak	Yes
	D4	$\mathbf{Rain}$	Mild	$\mathbf{High}$	Weak	Yes
	D5	$\mathbf{Rain}$	Cool	Normal	Weak	Yes
	D6	$\mathbf{Rain}$	Cool	Normal	Strong	No
	D7	Overcast	Cool	Normal	Strong	Yes
	D8	$\operatorname{Sunny}$	Mild	$\mathbf{High}$	Weak	No
	D9	$\operatorname{Sunny}$	Cool	Normal	Weak	Yes
	D10	$\mathbf{Rain}$	Mild	Normal	Weak	Yes
	D11	$\operatorname{Sunny}$	Mild	Normal	Strong	Yes
	D12	Overcast	$\mathbf{Mild}$	$\mathbf{High}$	Strong	Yes
	D13	Overcast	$\operatorname{Hot}$	Normal	Weak	Yes
	D14	$\operatorname{Rain}$	Mild	$\mathbf{High}$	Strong	No

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	$\mathbf{Sunny}$	$\operatorname{Hot}$	$\mathbf{High}$	Strong	No
D3	Overcast	$\operatorname{Hot}$	$\mathbf{High}$	Weak	Yes
D4	$\mathbf{Rain}$	Mild	$\mathbf{High}$	$\mathbf{Weak}$	Yes
D5	$\mathbf{Rain}$	Cool	Normal	$\mathbf{Weak}$	Yes
D6	$\mathbf{Rain}$	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	$\operatorname{Sunny}$	Mild	$\mathbf{High}$	Weak	No
D9	$\operatorname{Sunny}$	Cool	Normal	$\mathbf{Weak}$	Yes
D10	$\mathbf{Rain}$	Mild	Normal	Weak	Yes
D11	$\operatorname{Sunny}$	Mild	Normal	Strong	Yes
D12	Overcast	Mild	$\mathbf{High}$	Strong	Yes
D13	Overcast	$\operatorname{Hot}$	Normal	Weak	Yes
D14	$\mathbf{Rain}$	Mild	$\mathbf{High}$	Strong	No

14 cases

9 positive cases

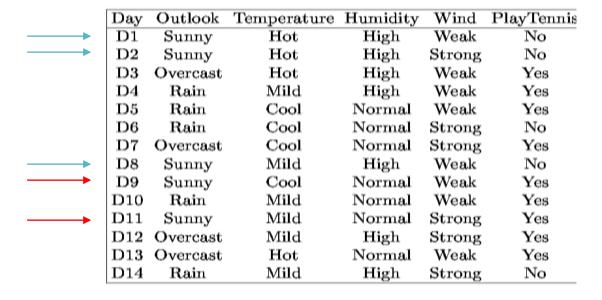
Step 1: <u>Calculate entropy</u> for all cases:

$$N_{Pos} = 9$$
  $N_{Neg} = 5$   $N_{Tot} = 14$   
 $H(S) = -(9/14)*log_2(9/14) - (5/14)*log_2(5/14) = 0.940$ 

entropy

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

$$N_{Pos} = 2$$
  $N_{Neg} = 3$   $N_{Tot} = 5$   
 $H(Sunny) = -(2/5)*log_2(2/5) - (3/5)*log_2(3/5) = 0.971$   
 $Outlook = Overcast$   
 $N_{Pos} = 4$   $N_{Neg} = 0$   $N_{Tot} = 4$   
 $H(Overcast) = -(4/4)*log_24/4) - (0/4)*log_2(0/4) = 0.00$ 



#### Outlook = Rain

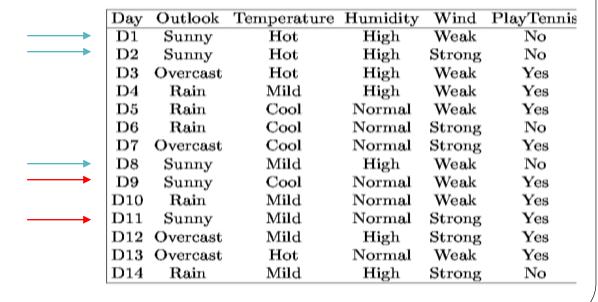
$$N_{Pos} = 3$$
  $N_{Neg} = 2$   $N_{Tot} = 5$   
H(Rain) = -(3/5)\*log<sub>2</sub>(3/5) - (2/5)\*log<sub>2</sub>(2/5) = 0.971

Calculate Information Gain for attribute Outlook

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

$$Gain(S, Outlook) = 0.940 - (5/14)*0.971 - (4/14)*0 - (5/14)*0.971$$

Gain(S, Outlook) = 0.246

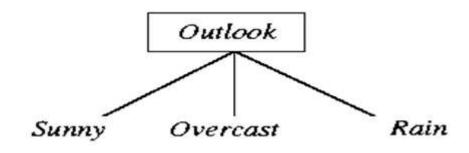


- Attribute = *Temperature* 
  - (Repeat process looping over {Hot, Mild, Cool})
     Gain(S, Temperature) = 0.029
- Attribute = *Humidity* 
  - (Repeat process looping over {High, Normal})Gain(S, Humidity) = 0.029
- Attribute = Wind
  - (Repeat process looping over {Weak, Strong})Gain(S, Wind) = 0.048

## 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

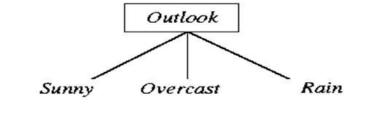
#### .: Outlook is root node of tree



- Iterate algorithm to find attributes which best classify training examples under the values of the root node
- Example continued
  - Take three subsets:

Outlook = Overcast  $(N_{Tot} = 4)$ 

• Outlook = Rainy  $(N_{Tot} = 5)$ 



 For each subset, repeat the above calculation looping over all attributes other than *Outlook*

 $(N_{Tot} = 5)$ 

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes

	Day	Outlook	Temperature	Humidity	$\mathbf{Wind}$	PlayTennis
	D1	Sunny	Hot	High	Weak	No
	D2	Sunny	$\mathbf{Hot}$	$\operatorname{High}$	Strong	No
	$D_3$	Overcast	$\operatorname{Hot}$	$\mathbf{High}$	Weak	Yes
	D4	$\mathbf{Rain}$	$\mathbf{Mild}$	$\mathbf{High}$	Weak	Yes
	$D_5$	$\mathbf{Rain}$	Cool	Normal	Weak	Yes
	D6	$\mathbf{Rain}$	Cool	Normal	Strong	No
	D7	Overcast	Cool	Normal	Strong	Yes
	D8	$\operatorname{Sunny}$	$\mathbf{Mild}$	$\mathbf{High}$	Weak	No
	D9	Sunny	Cool	Normal	Weak	Yes
e.	D10	$\mathbf{Rain}$	$\mathbf{Mild}$	Normal	Weak	Yes
	D11	$\operatorname{Sunny}$	$\mathbf{Mild}$	Normal	Strong	Yes
	D12	Overcast	$\mathbf{Mild}$	$\mathbf{High}$	Strong	Yes
	D13	Overcast	$\mathbf{Hot}$	Normal	Weak	Yes
	D14	Rain	Mild	High	Strong	No

#### • For example:

• 
$$Outlook$$
 = Sunny (N<sub>Pos</sub> = 2, N<sub>Neg</sub> = 3, N<sub>Tot</sub> = 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(
$$S_{Supple}$$
, Temperature) = 0.971 - (2/5)\*0 - (2/5)\*1 - (1/5)\*0

$$Gain(S_{Sunnv}, Temperature) = 0.571$$

#### Similarly:

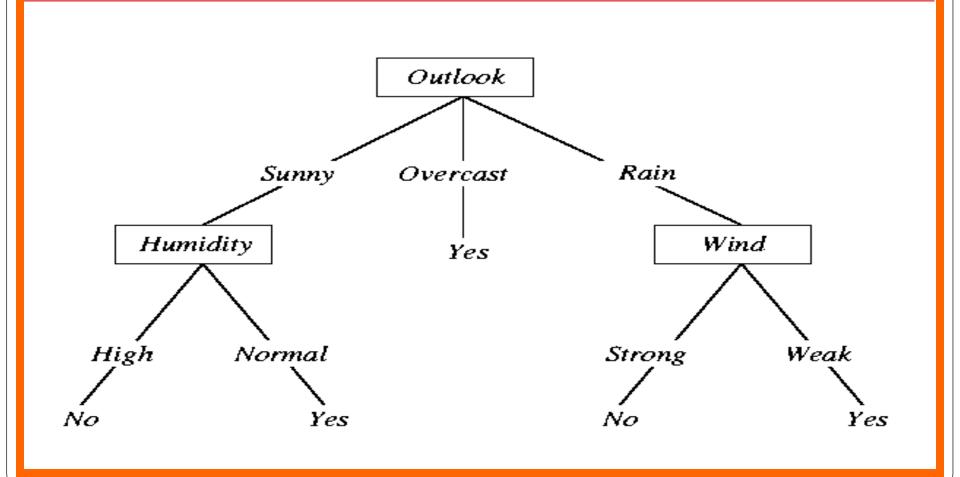
Gain(
$$S_{Sunny}$$
, Humidity) = 0.971  
Gain( $S_{Sunny}$ , Wind) = 0.020

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes

- : Humidity classifies Outlook = Sunny instances best and is placed as the node under Sunny outcome.
- Repeat this process for Outlook = Overcast & Rainy

• End up with tree:

#### Decision Tree for PlayTennis



## •Important:

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

#### or

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

- Note: In this example data were perfect.
  - No contradictions
  - Branches led to unambiguous <u>Yes, No decisions</u>
  - 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 <u>handle noisy data.</u>

# **About Entropy and Information Gain**

**Decision Tree Learning** 

## **Entropy**

# "characterizes the impurity of an arbitrary collection of examples" [Mitchell, 1997]

- So if the impurity or randomness of a collection (with respect to the target classifier) is high then the entropy is high
- But if there is no randomness (complete uniformity with respect to the target classifier) then the entropy is zero

Entropy(S) 
$$\equiv -p_+\log_2 p_+ - p_-\log_2 p_-$$

Where target classification is boolean

- p. :the proportion of positive examples in collection S
- p. :the proportion of negative examples in collection S

## Entropy Example 1...

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

Entropy([2+,0-]) = 
$$-(2/2)\log_2(2/2) - (0/2)\log_2(0/2)$$
  
=  $-1\log_2(1) - (0/2)\log_2(0/2)$   
=  $-1*0 - 0*0$   
=  $0 - 0$   
=  $0 - 0$   
=  $0 - 0$   
Rain Weak Yes  
Sunny Strong Yes

(Max Uniformity, Min Randomness)

### Entropy Example 2...

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

```
Entropy([1+,1-]) = -(1/2)\log_2(1/2) - (1/2)\log_2(1/2)
= -0.5 * \log_2(0.5) - 0.5 * \log_2(0.5)
= (-0.5 * -1) - (0.5 * -1)
= 0.5 - (-0.5)
= 1
```

Outlook	Wind	WearCoat
Rain	Weak	Yes
Sunny	Weak	No

(Max Randomness)

## Entropy Example 3...

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

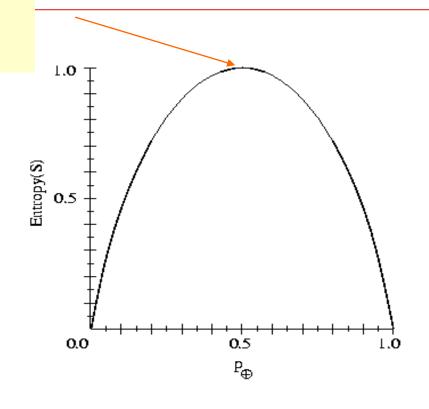
Entropy([2+,1-]) = 
$$-(2/3)\log_2(2/3) - (1/3)\log_2(1/3)$$
  
=  $-0.67 * \log_2(0.67) - (0.33) * \log_2(0.33)$   
=  $-(0.67 * -0.58) - (0.33 * -1.6)$   
=  $0.39 - (-0.53)$   
=  $0.92$ 

N.B. For reasons of speed/brevity, I'm just working to 2 decimal places!

Outlook	Wind	WearCoat
Rain	Weak	Yes
Sunny	Strong	Yes
Sunny	Weak	No

Largest entropy

### **Entropy**



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

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

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

#### Information Gain

- Measures the expected reduction in entropy caused by partitioning
- Statistical quantity measuring how well an attribute classifies the data.

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

$$entropy$$

$$Entropy for value v$$

 Maximum gain means minimum entropy for attribute Ai, meaning Ai has less randomness in classifying

## **Extensions of Decision Tree Learning**

#### **Extensions** of the Decision Tree Learning

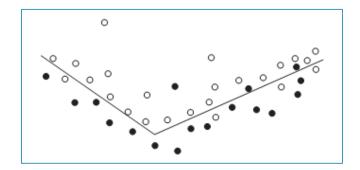
- Noisy data and Overfitting
- Cross-Validation for Experimental Validation of Performance
- Pruning Decision Trees
- Real-valued data
- Using gain ratios
- Generation of rules
- Setting Parameters
- Incremental learning

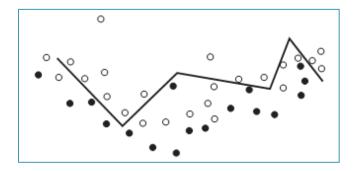
#### Noisy data and Overfitting

- Many kinds of "noise" that could 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
    - Errors in the preprocessing phase
  - The classification is wrong (e.g., + instead of -) because of some error
- Some attributes are irrelevant to the decision-making process,
  - e.g., color of a die is irrelevant to its outcome.
  - Irrelevant attributes can result in overfitting the training data.

#### Noisy data and Overfitting

- Black dots are positive, others negative
- Two lines represent two hypothesis
- Thick line is complex hypothesis correctly classifies all data
- Thin line is simple hypothesis but incorrectly classifies some data
- The simple hypothesis makes some errors but reasonably closely represents the trend in the data
- The complex solution does not at all represent the full set of data
- Fix overfitting /overlearning problem
  - By cross validation
  - By pruning lower nodes in the decision tree.





#### **Cross Validation: An Evaluation Methodology**

- Standard methodology: cross validation
  - 1. Collect a large set of examples (all with correct classifications!).
  - 2. Randomly divide collection into two disjoint sets: training and test.
  - 3. Apply learning algorithm to training set giving hypothesis H
  - 4. Measure performance of H w.r.t. test set
- Important: keep the training and test sets disjoint!
- Learning is not to minimize training error (wrt data) but the error for test/cross-validation: a way to fix overfitting
- To study the efficiency and robustness of an algorithm, repeat steps 2-4 for different training sets and sizes of training sets.
- If you improve your algorithm, start again with step 1 to avoid evolving the algorithm to work well on just this collection.

#### **Pruning Decision Trees**

- Pre Pruning: Stop growing before a fully grown tree
- Post Pruning: Trim fully grown tree from the bottom
  - Reduced Error Pruning
  - Rule post pruning



#### Real-valued data

- Select a set of thresholds defining intervals;
  - each interval becomes a discrete value of the attribute
- We can use some simple heuristics
  - always divide into quartiles
- We can use domain knowledge
  - divide age into infant (0-2), toddler (3 5), and school aged (5-8)
- or treat this as another learning problem
  - try a <u>range of ways to discretize</u> the continuous variable
  - Find out which yield "better results" with respect to some metric.

#### **Performance Evaluation**

**Decision Tree Learning** 

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	TP	FN
	Class=No	FP	TN

TP (true positive)

FN (false negative)

FP (false positive)

TN (true negative)

- TP: predicted to be in YES, and is actually in it
- FP: predicted to be in YES, but is not actually in it
- TN: predicted not to be in YES, and is not actually in it
- FN: predicted not to be in YES, but is actually in it

#### Accuracy

	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	TP	FN
	Class=No	FP	TN

#### Most widely-used metric:

Accuracy = 
$$\frac{TP + TN}{TP + TN + FP + FN}$$

#### Class imbalance problem

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10
- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

#### Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	Yes	No	
Yes	TP	FN	Р
No	FP	TN	N
	P'	N'	All

 Classifier Accuracy, or recognition rate: percentage of test set tuples that are correctly classified

Accuracy = (TP + TN)/AII

Error rate: 1 - accuracy, orError rate = (FP + FN)/All

- Sensitivity: True Positive recognition rate
  - Sensitivity = TP/P
- Specificity: True Negative recognition rate
  - Specificity = TN/N

# Classifier Evaluation Metrics: Precision and Recall, and F-measures

Precision: exactness – what % of tuples that the classifier labeled as positive are actually positive

precision = 
$$\frac{TP}{TP + FP}$$

- Recall: completeness what % of positive tuples did the classifier label as positive?
  - Perfect score is 1.0

$$recall = \frac{TP}{TP + FN}$$

- F-measure (F<sub>1</sub> score or F-score)
  - harmonic mean of precision and recall,

$$F = \frac{2 \times precision \times recall}{precision + recall}$$

- Precision is biased towards TP & FP
- Recall is biased towards TP & FN
- F-measure is biased towards all except TN

#### Classifier Evaluation Metrics: Matthews correlation coefficient (MCC)

- MCC takes into account true and false positives and negatives.
- Generally regarded as a balanced measure which can be used even if the classes are of very different sizes.
- It returns a value between -1 and +1.
  - 1 represents a perfect prediction
  - 0 no better than random prediction
  - -1 indicates total disagreement between prediction and observation

#### Classifier Evaluation Metrics: Matthews correlation coefficient (MCC)

$$N = TN + TP + FN + FP$$

$$S = \frac{TP + FN}{N}$$

$$P = \frac{TP + FP}{N}$$

$$MCC = \frac{TP / N - S \times P}{PS(1 - S)(1 - P)}$$

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

#### References

- Chapter 18 of "Artificial Intelligence: A modern approach" by Stuart Russell, Peter Norvig.
- Chapter 10 of "Al Illuminated" by Ben Coppin.