Machine Learning

Dr. Prashant Goswami Assistant Professor, BTH (DIDA) prashantgos.github.io

prashant.goswami@bth.se



What is ML?

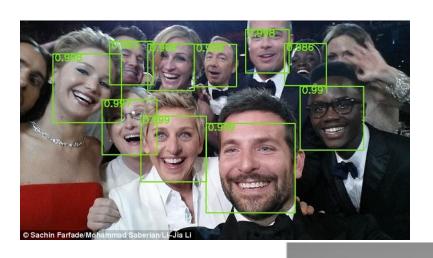
"... the construction and study of systems that can learn from data."

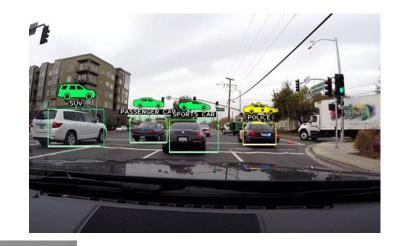
- A system that can:
 - Take known data as input.
 - Learn from the known data. Generalization.
 - Classify or draw conclusions from unseen data.

ML vs. Data Mining

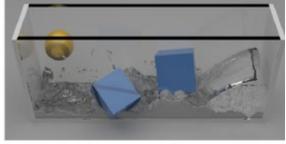
- ML focuses on prediction based on known properties learned from data.
 - Example: Facial recognition, weather predictions.
- Data Mining focuses on the discovery of previously unknown properties on the data.
 - Example: Find patterns in medical history of patients with the same disease.

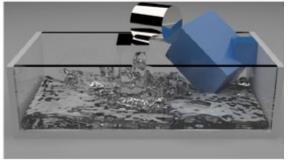
Machine Learning - Examples





$$4 \rightarrow 4$$
 $2 \rightarrow 2$ $3 \rightarrow 3$
 $4 \rightarrow 4$ $9 \rightarrow 9$ $0 \rightarrow 0$
 $5 \rightarrow 5$ $7 \rightarrow 7$ $1 \rightarrow 1$
 $9 \rightarrow 9$ $0 \rightarrow 0$ $3 \rightarrow 3$
 $6 \rightarrow 6$ $7 \rightarrow 7$ $4 \rightarrow 4$







Data Mining - Examples



Service providers

Why did the customer leave?



Crime agencies

Who could be a potential criminal?



DATA REPRESENTATION

Instance

- Useful data consists of a number of instances (examples) with input and a known output.
- Consists of a number of attributes, and one or more class attributes (target).
- A set of instances is the input to a classifier.
- The instances are used by the Classifier to form a Concept (the thing to be learned).

Attribute Types

- Nominal
 - Finite set of symbols or numbers.
- Numeric (continuous)
 - Numbers (real or integer values).
- Boolean (special case of nominal)
 - True/false
 - Yes/no
 - 1/0

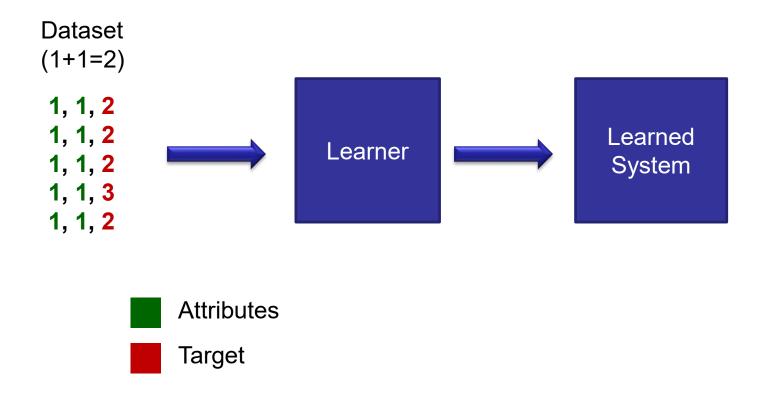
Preparing the data

- 1. Decide a suitable format for your data.
 - ARFF is a standardized data format.
- 2. Gather data and compile it into your format.
- 3. Input the data to a classifier.
 - Each classifier has pros and cons, and you should select one suitable for your type of data.

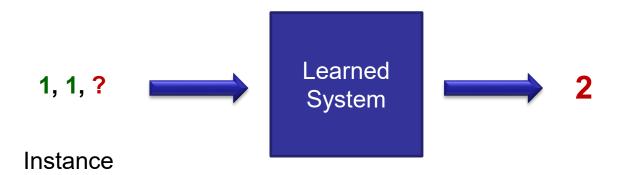
ARFF example

```
% this is a comment
@relation weather
@attribute outlook { sunny, overcast, rainy }
@attribute temperature numeric
@attribute humidity numeric
@attribute windy { true, false }
@attribute play? {yes, no }
@data
sunny, 85, 85, false, no
sunny, 80, 90, true, no
```

When we have the data, we can learn from it



When we have learned something, we can predict stuff



Knowing your data greatly simplifies the experiment design and execution!



TYPES OF CLASSIFIERS

Two main types

Supervised learning

- Learning with an instructor.
- We have some known data.
- Learn to handle the known data, and hopefully we can classify unknown data.

Unsupervised learning

- Learning without an instructor.
- Try something, and see how it works.
- Utility function to calculate how well it worked.

Two main types

- Supervised learning
 - Learning with an instructor.
 - We have some known data.
 - Learn to handle the known data, and hopefully we can classify unknown data.
- Unsupervised learning
 - Learning without an instructor.
 - Try something, and see how it works.
 - Utility function to calculate how well it worked.

Decision Trees

- Each node in the tree tests a particular attribute.
- Each leaf represents a class.

- Suitable for nominal attributes.
 - Even though we can discretize numerical attributes...
 - temp < 15 = Cold, 15-24 = Temperate, > 25 = Warm.
- Common algorithms: ID3, C45, J48.

Decision Trees

- Fast at learning and classification.
- Concept readable by humans.
- Low storage requirements.
- Bad at handling inconsistent data.
- Cannot learn some concepts:
 - Parity function: 1 if and only if an even number of inputs are 1.
 - Majority function: 1 if more than half of the inputs are 1.
 - Read more : http://www.cs.utexas.edu/~klivans/f07lec3.pdf
- Discretizing numerical attributes leads to loss of precision.

Example: Weather data

Outlook	Temperature	Humidity	Windy	Play
sunny	hot	high	false	NO
sunny	hot	high	true	NO
overcast	hot	high	false	YES
rainy	mild	high	false	YES
rainy	cool	normal	false	YES
rainy	cool	normal	true	NO
overcast	cool	normal	true	YES
sunny	mild	high	false	NO
sunny	cool	normal	false	YES
rainy	mild	normal	false	YES
sunny	mild	normal	true	YES
overcast	mild	high	true	YES
overcast	hot	normal	false	YES
rainy	mild	high	true	NO

Building the tree

- At each node, we need to find the attribute that best divides the data into Yes and No.
- To do this we calculate the information gain for each parameter and value.
- The attribute with the highest information gain is selected at each node.

$$\begin{aligned} Gain(A) &= 1 - \left(\sum_{i=1}^{v} I\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)\right) \\ I\left(\frac{p}{p+n}, \frac{n}{p+n}\right) &= \frac{p+n}{p_{tot} + n_{tot}} \left(-\frac{p}{p+n} log_2 \frac{p}{p+n} - \frac{n}{p+n} log_2 \frac{n}{p+n}\right) \end{aligned}$$

Outlook	Sunny	Overcast	Rainy
Yes	2	4	3
No	3	0	2

$$I(sunny) = \frac{5}{14} \left(-\frac{2}{5}log_2 \frac{2}{5} - \frac{3}{5}log_2 \frac{3}{5} \right) \approx 0.347$$

$$I(overcast) = \frac{4}{14} \left(-\frac{4}{4} log_2 \frac{4}{4} - 0 \right) = 0$$

$$I(sunny) = \frac{5}{14} \left(-\frac{2}{5}log_2 \frac{2}{5} - \frac{3}{5}log_2 \frac{3}{5} \right) \approx 0.347$$

$$I(overcast) = \frac{4}{14} \left(-\frac{4}{4}log_2 \frac{4}{4} - 0 \right) = 0$$

$$I(rainy) = \frac{5}{14} \left(-\frac{3}{5}log_2 \frac{3}{5} - \frac{2}{5}log_2 \frac{2}{5} \right) \approx 0.347$$

$$Gain(outlook) \approx 1 - 0.347 - 0 - 0.347 = 0.306$$

$$\left[I\left(\frac{p}{p+n},\frac{n}{p+n}\right) = \frac{p+n}{p_{tot}+n_{tot}}\left(-\frac{p}{p+n}log_2\frac{p}{p+n} - \frac{n}{p+n}log_2\frac{n}{p+n}\right)\right]$$

Temperature	Hot	Mild	Cool
Yes	2	4	3
No	2	2	1

$$I(hot) = \frac{4}{14} \left(-\frac{2}{4} log_2 \frac{2}{4} - \frac{2}{4} log_2 \frac{2}{4} \right) \approx 0.286$$

$$I(mild) = \frac{6}{14} \left(-\frac{4}{6}log_2 \frac{4}{6} - \frac{2}{6}log_2 \frac{2}{6} \right) \approx 0.394$$

$$I(cool) = \frac{4}{14} \left(-\frac{3}{4} log_2 \frac{3}{4} - \frac{1}{4} log_2 \frac{1}{4} \right) \approx 0.232$$

$$Gain(temperature) \approx 1 - 0.286 - 0.394 - 0.232 = 0.088$$

Humidity	High	Normal
Yes	3	6
No	4	1

$$I(high) = \frac{7}{14} \left(-\frac{3}{7} log_2 \frac{3}{7} - \frac{4}{7} log_2 \frac{4}{7} \right) \approx 0.493$$

$$I(normal) = \frac{7}{14} \left(-\frac{6}{7} log_2 \frac{6}{7} - \frac{1}{7} log_2 \frac{1}{7} \right) \approx 0.296$$

$$Gain(humidity) \approx 1 - 0.493 - 0.296 = 0.211$$

Windy	True	False
Yes	3	6
No	3	2

$$I(true) = \frac{6}{14} \left(-\frac{3}{6}log_2\frac{3}{6} - \frac{3}{6}log_2\frac{3}{6} \right) \approx 0.429$$

$$I(false) = \frac{8}{14} \left(-\frac{6}{8}log_2 \frac{6}{8} - \frac{2}{8}log_2 \frac{2}{8} \right) \approx 0.464$$

$$Gain(windy) \approx 1 - 0.429 - 0.464 = 0.107$$

Attribute	Gain
Outlook	0.306
Temperature	0.088
Humidity	0.211
Windy	0.107

Outlook has the highest gain and is selected as root node.



Overcast has perfect gain = all instances with overcast belongs to the same class, Yes.

Let's find the sunny node!

All instances with sunny

Outlook	Temperature	Humidity	Windy	Play
sunny	hot	high	false	NO
sunny	hot	high	true	NO
sunny	mild	high	false	NO
sunny	cool	normal	false	YES
sunny	mild	normal	true	YES

5 instances left.

Temperature	Hot	Mild	Cool
Yes	0	1	1
No	2	1	0

$$I(hot) = 0$$

$$I(mild) = \frac{2}{5} \cdot 1 = 0.4$$

$$I(cool) = 0$$

$$Gain(temperature) = 1 - 0 - 0.4 - 0 = 0.6$$

Humidity	High	Normal
Yes	0	2
No	3	0

$$I(high) = 0$$

$$I(normal) = 0$$

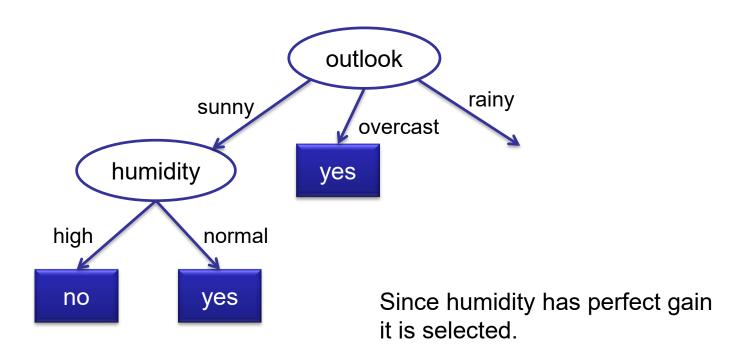
$$Gain(humidity) = 1 - 0 - 0 = 1$$

Windy	True	False
Yes	1	1
No	1	2

$$I(true) = \frac{2}{5} \cdot 1 = 0.4$$

$$I(false) = \frac{3}{5} \left(-\frac{1}{3}log_2 \frac{1}{3} - \frac{2}{3}log_2 \frac{2}{3} \right) \approx 0.551$$

$$Gain(windy) \approx 1 - 0.4 - 0.551 = 0.049$$



Let's find the rainy node!

All instances with rainy

Outlook	Temperature	Humidity	Windy	Play
rainy	mild	high	false	YES
rainy	cool	normal	false	YES
rainy	cool	normal	true	NO
rainy	mild	normal	false	YES
rainy	mild	high	true	NO

5 instances left.

Find the rainy node

Temperature	Hot	Mild	Cool
Yes	0	2	1
No	0	1	1

$$I(hot) = 0$$

$$I(mild) = \frac{3}{5} \left(-\frac{2}{3}log_2 \frac{2}{3} - \frac{1}{3}log_2 \frac{1}{3} \right) \approx 0.551$$

$$I(cool) = \frac{2}{5} \cdot 1 = 0.4$$

$$Gain(temperature) \approx 1 - 0 - 0.551 - 0.4 = 0.049$$

Find the rainy node

Humidity	High	Normal
Yes	1	2
No	1	1

$$I(high) = rac{2}{5} \cdot 1 = 0.4$$

$$I(normal) = \frac{3}{5} \left(-\frac{2}{3}log_2 \frac{2}{3} - \frac{1}{3}log_2 \frac{1}{3} \right) \approx 0.551$$

$$Gain(humidity) \approx 1 - 0.4 - 0.551 = 0.049$$

Find the rainy node

Windy	True	False
Yes	0	3
No	2	0

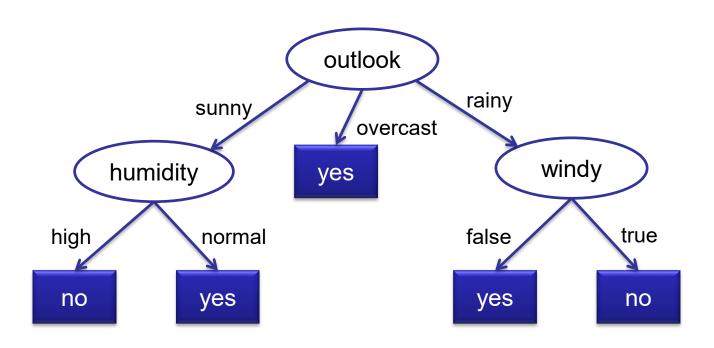
$$I(true) = 0$$

$$I(false) = 0$$

$$Gain(windy) = 1 - 0 - 0 = \boxed{1}$$

Since windy has perfect gain, it is selected.

Final Result

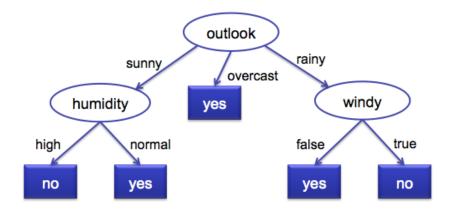


OneR vs. Decision Trees

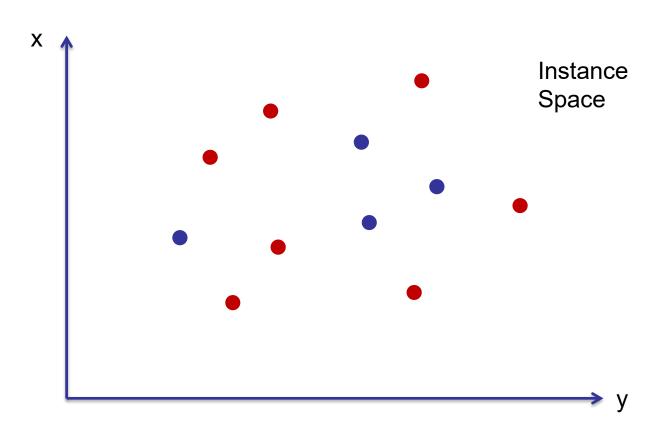
```
outlook:
    sunny -> no
    overcast -> yes
    rainy -> yes
(10/14 instances correct)
```

OneR: Learn one rule that best describes the concept

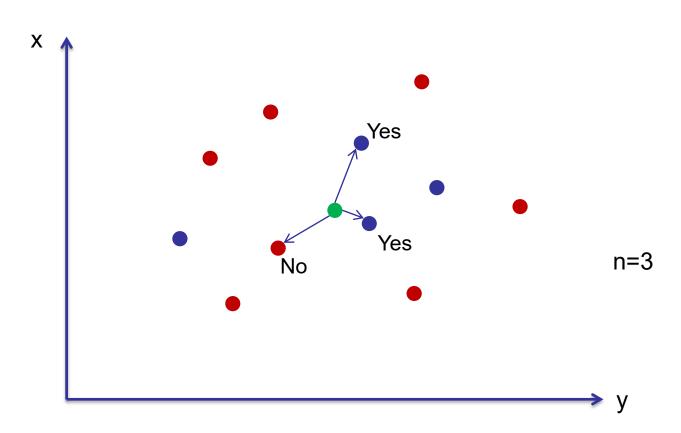
The top node in a DT is the attribute that best divides the data, which is the same as the OneR rule.



- A lazy classifier stores the training data without processing it.
- All the work is done at <u>classification</u> time.
- Calculate the n closest instances using Euclidean distance between attributes.
- K-Nearest-Neighbor.







The class of the new instance is the same as the most common class of the n=3 closest training instances = Yes!

- High storage requirements.
- No generalization is done.
- Not so good at handling missing attributes.
- Works best with numerical attributes.
 - Is A closer to B than D?
- Is often quite accurate, but the high resource demands at classification time can be a problem.

Naïve Bayes

- Based on Bayes' rule.
- Used as a Classifier
- Each attribute is independent!
- Usually not true for real-world problems, but works surprisingly well anyway!

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

Bayesian classifiers: Bayes' rule

Example:

- Is stiff neck a good sign of the disease meningitis?
- = we want to find P(m|s): probability for meningitis given a stiff neck.

Prior probabilities:

- 50% of meningitis patients have a stiff neck:
 P(s|m) = 0.5
- One in 50000 suffers from meningitis: P(m) = 1/50000
- One in 20 suffers from stiff neck:
 P(s) = 1/20
- Now we can calculate P(m|s) using Bayes' rule:

$$P(m|s) = \frac{P(s|m)P(m)}{P(s)} = \frac{0.5 \cdot 1/50000}{1/20} = 0.0002$$

Naïve Bayes Classification

- 1. Calculate frequencies of each class and each attribute value (for all attributes).
- 2. For each class,
 - a. Multiply the conditional probability of each attribute into a product, X
 - b. Multiply the class probability with X
- 3. Classify the instance as belonging to the class with the highest probability.

Lets look at an example!

Example: A limited Weather set

Outlook	Temperature	Play
sunny	hot	NO
sunny	hot	NO
overcast	hot	YES
rainy	mild	YES
rainy	cool	YES
rainy	cool	NO
overcast	cool	YES
sunny	mild	NO
sunny	cool	YES
rainy	mild	YES
sunny	mild	YES
overcast	mild	YES
overcast	hot	YES
rainy	mild	NO

Example: A limited Weather set

Outlook			Temp			Play	
	Yes	No		Yes	No	YES	NO
Sunny	3	2	Hot	2	2	9	5
Overcast	4	1	Mild	5	0		
Rainy	2	2	Cool	2	3		

Example: A limited Weather set

Outlook			Temp			Play	
	Yes	No		Yes	No	YES	NO
Sunny	3	2	Hot	2	2	9	5
Overcast	4	1	Mild	5	0		
Rainy	2	2	Cool	2	3		
P(Sunny)	3/9	2/5	P(Hot)	2/9	2/5	9/14	5/14
P(Overc)	4/9	1/5	P(Mild)	5/9	0/5		
P(Rainy)	2/9	2/5	P(Cool)	2/9	3/5		

Classifying new instances

- Do we want to go out and play if {outlook=sunny, temp=cool}?
- Now lets try the attributes against the two possible hypotheses H = YES and H = NO:
 - P(YES) * P(sunny|YES) * P(cool|YES) = 9/14 * 3/9 * 2/9 = 0.048
 - P(NO) * P(sunny|NO) * P(cool|NO) = 5/14 * 2/5 * 3/5 = 0.086
- We don't want to go out and play!
 - 1. Calculate frequencies of each class and each attribute value (for all attributes).
 - 2. For each class,
 - a. Multiply the conditional probability of each attribute into a product, X
 - b. Multiply the class probability with X
 - 3. Classify the instance as belonging to the class with the highest probability.

Naïve Bayes

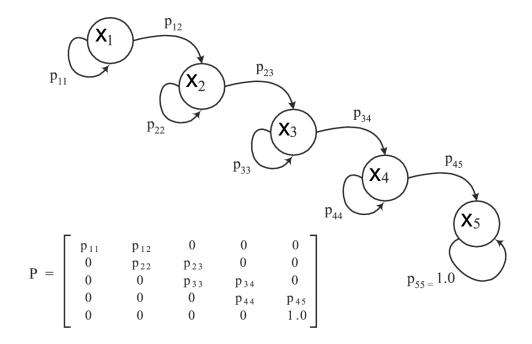
- Very good at analyzing texts.
- Texts are split into word lists:
 - "Want to buy cheap Rolex watches" → { Want, to, buy, cheap, Rolex, watches}
- Used in many email spam filters.
- Sensitive at learning the wrong thing (for example English vs. Swedish)



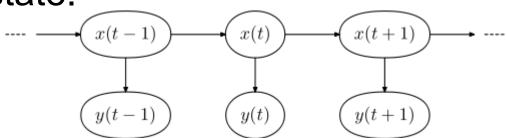
Markov Model

- Stochastic, time varying process
- Next state dependent only on current state

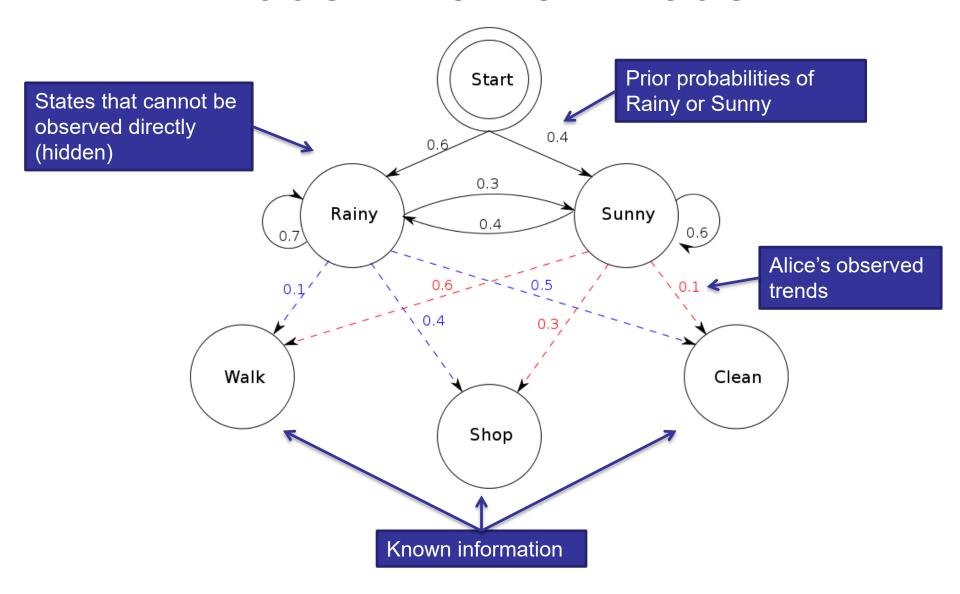
$$\Pr(X_{n+1} = x \mid X_1 = x_1, X_2 = x_2, \dots, X_n = x_n) = \Pr(X_{n+1} = x \mid X_n = x_n)$$

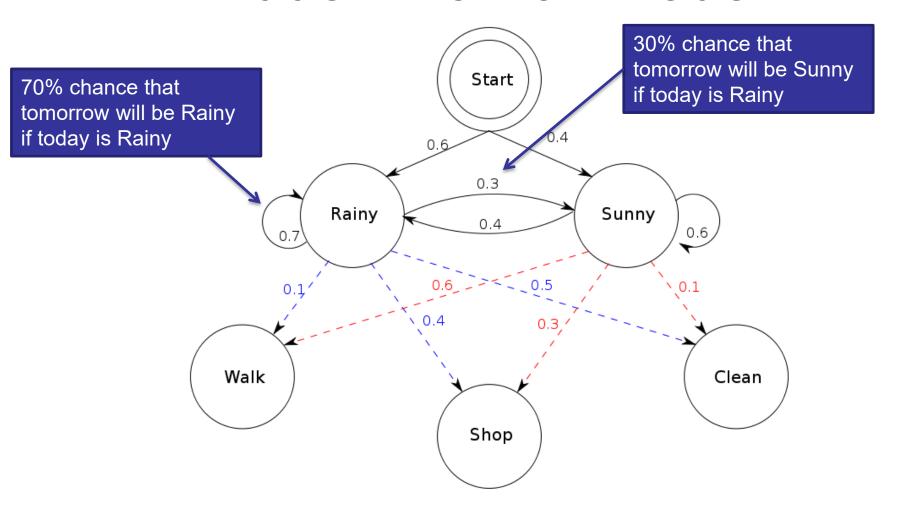


- HMM is a simplified dynamic Bayesian Network classifier.
 - We will not look into more complex Bayesian Network models.
- It contains a set of states and transition probabilities.
- Based on the input and the previous state, there
 is a probability of moving to a new state, or
 remain in the same state.

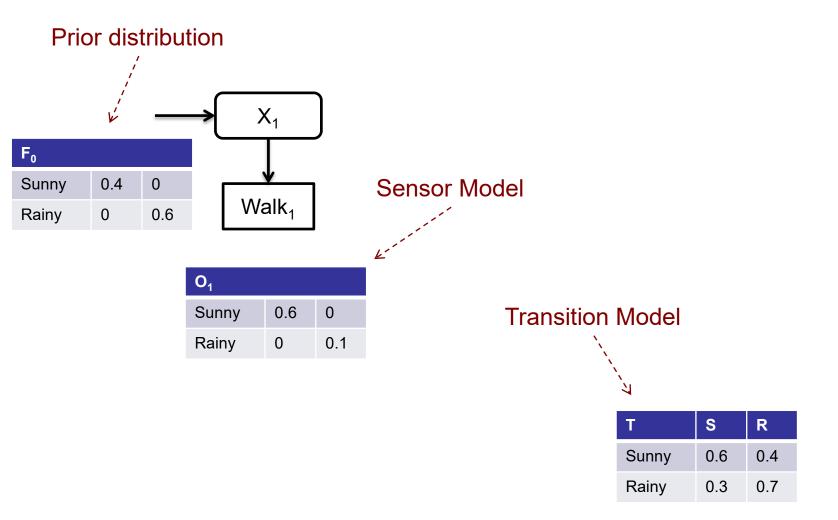


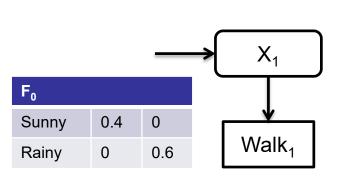
- Alice calls Bob every day.
- She knows Bob either takes a Walk, goes Shopping or Cleans the apartment.
- What Bob does is depending on the weather (Rainy, Sunny).
- Alice has observed some trends in what Bob tends to do based on the weather.
- Bob tells Alice what he did during the day, and Alice tries to guess the weather.





Transition Probabilities - based on historical data.



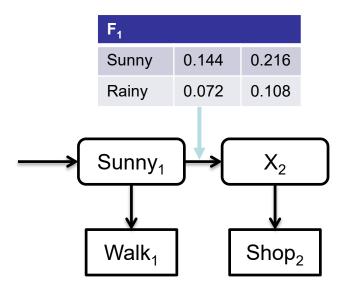


F ₁ =O ₁ *T	F ₁ =O ₁ *T*F ₀		Π (norm)
Sunny	0.144	0.216	Norm(0.144*0.216) = 0.8
Rainy	0.072	0.108	Norm(0.072*0.108) = 0.2

$$X_1 = Sunny$$

O ₁		
Sunny	0.6	0
Rainy	0	0.1

Т	S	R
Sunny	0.6	0.4
Rainy	0.3	0.7

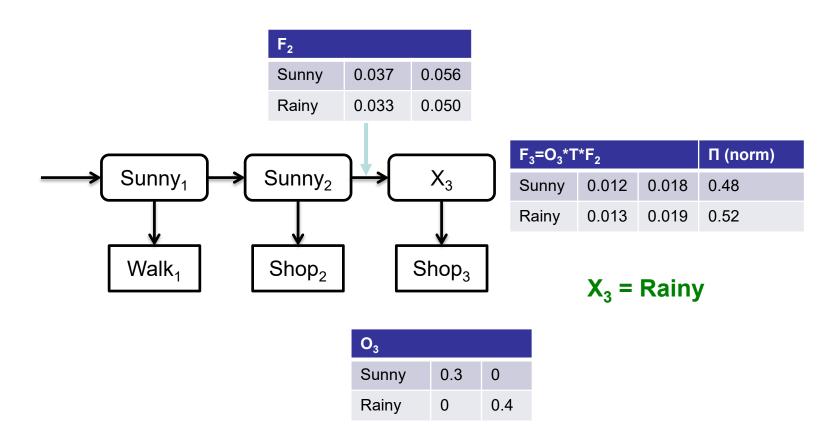


F ₂ =O ₂ *T	*F ₁		Π (norm)
Sunny	0.037	0.056	0.56
Rainy	0.033	0.050	0.44

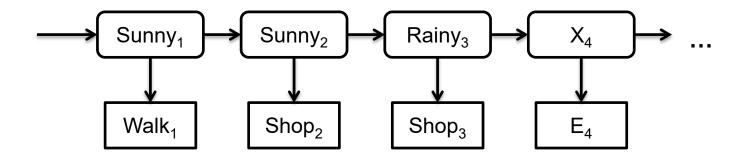
$$X_2 = Sunny$$

O ₂		
Sunny	0.3	0
Rainy	0	0.4

T	S	R
Sunny	0.6	0.4
Rainy	0.3	0.7



Т	S	R
Sunny	0.6	0.4
Rainy	0.3	0.7



- Markov Assumption: The current state depends only on a finite history of previous states.
 - First-order HMM = depends on previous state (as in the example)
 - Second-order HMM = depends on last two states.
- Finding the most likely sequence uses the Viterbi Algorithm.
 - Which we showed an example of

- Suitable for nominal attributes.
- Good at handling sequences of variable length, for example:
 - Biological data like protein sequences:

...MMNEHSIDTDNRKANNALYLFIIIGLEHSMNEMALY...



Length can vary from around 150 to 10000+

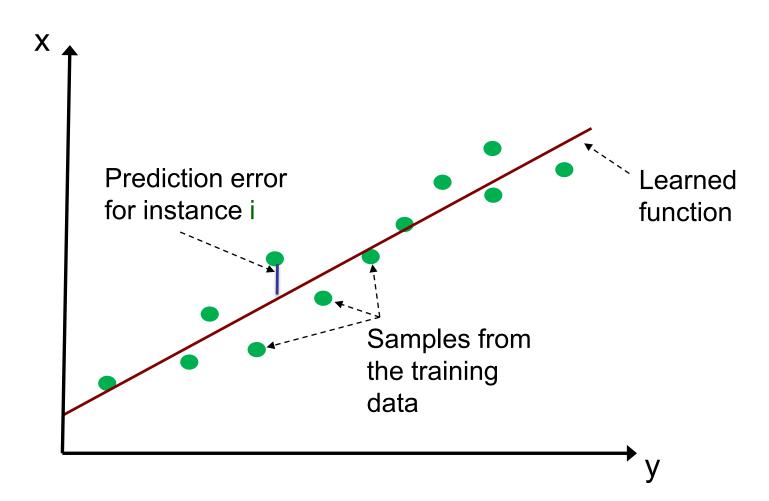
Linear Regression

- Basic idea: Express the class as a linear combination of its attributes:
 - $x = w_0 + w_1 a_1 + w_2 a_2 + ... + w_k a_k = \sum w_i a_i$
 - x = class
 - a_k = attribute values
 - w_k = weights for each attribute
- The weights are calculated (learned) from the training data.

Linear Regression

- When learning we need to minimize the prediction error over the training data.
- Let
- x⁽ⁱ⁾ = actual class value for instance i
- ∑w_ia_i⁽ⁱ⁾ = predicted class value for instance i
- $(x^{(i)} \sum w_j a_j^{(i)})^2$ = squared error for instance i
- We aim to minimize the sum of the squared error over all instances in the training data.

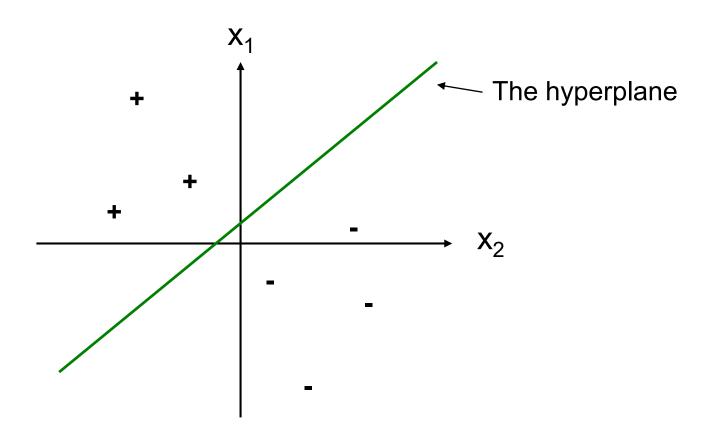
Linear Regression



The Hyperplane

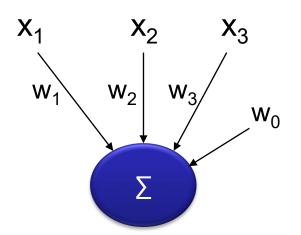
- If the data can be clearly separated into two groups, we can use the perceptron training rule.
- We learn a plane, the *hyperplane*, that separate the groups.
- Equation:
 - $w_0 + w_1 a_1 + w_2 a_2 + ... w_k a_k = 0$

The Hyperplane



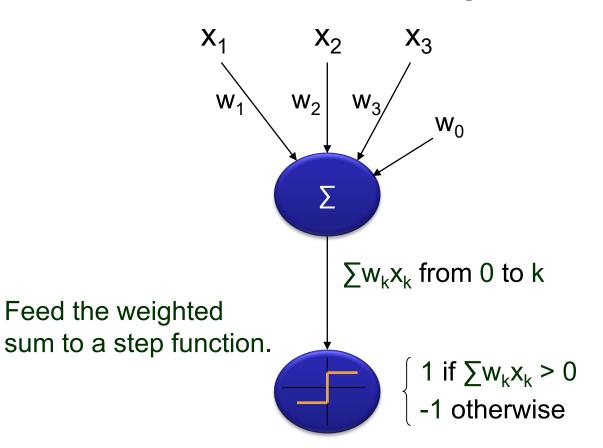
 x_1 and x_2 are attributes. + and – are the classes.

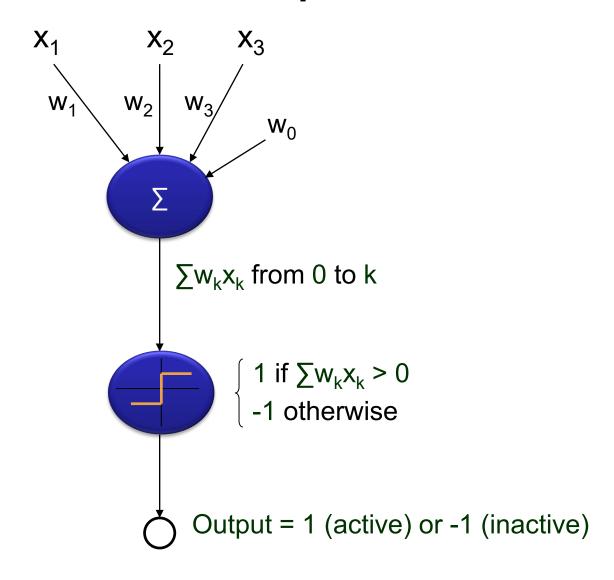
 Start with a set of attributes and weights, and a constant.



Feed them to a unit that calculates the weighted sum.

 $\sum w_k x_k$ from 0 to k

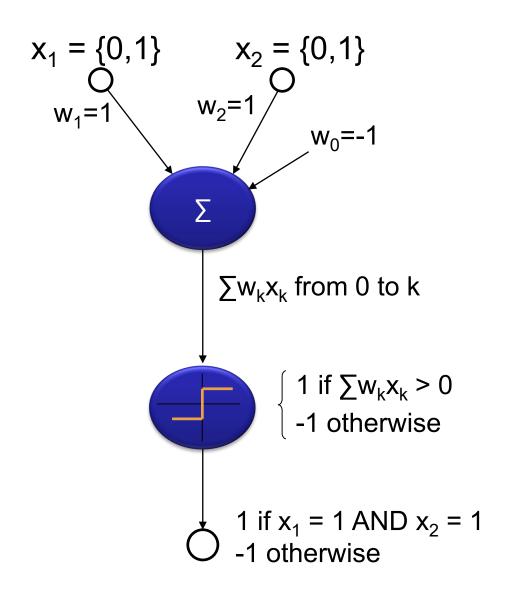




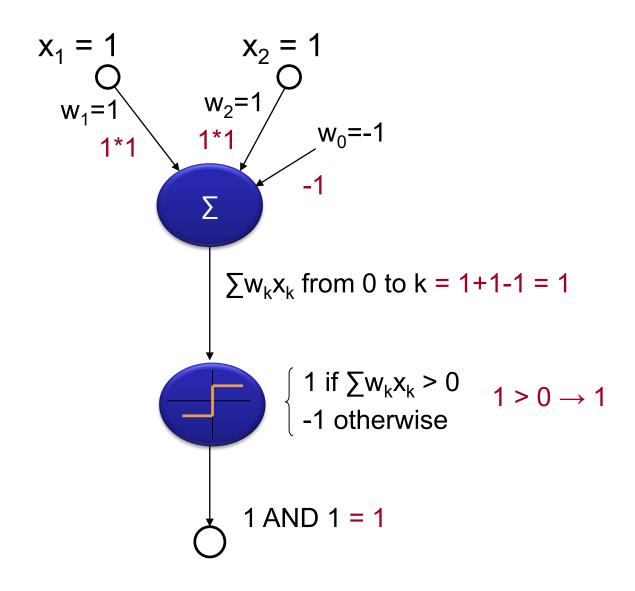
Perceptron Training

- If a misclassified instance is encountered:
 - Change parameters of the hyperplane so the instance moves closer to it.
- Each iteration goes through all training instances.
- Iteration continues until a solution is found.
- Only works if the classes can be linearly separable.

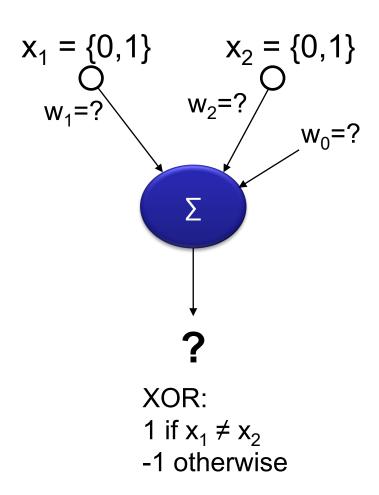
Boolean functions - AND



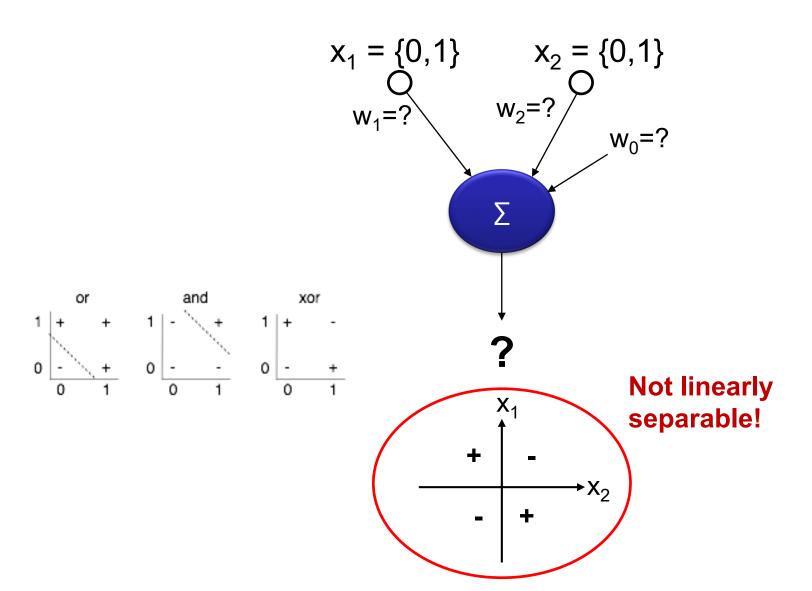
Boolean Functions - AND



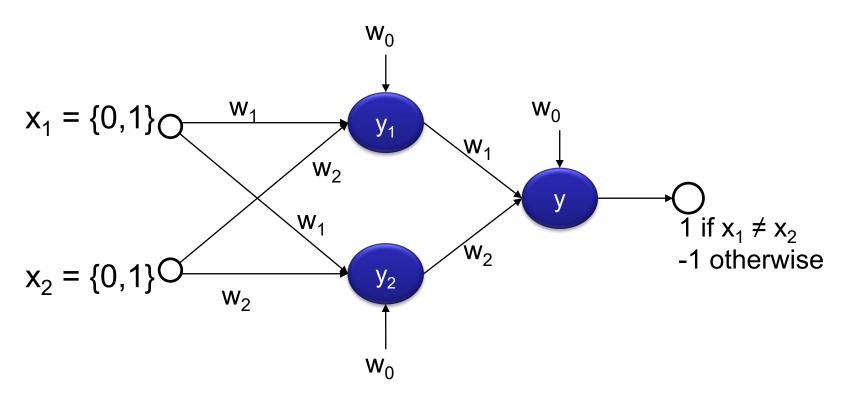
Works similarly with OR, but what about XOR?



Boolean functions - XOR



XOR - The Solution

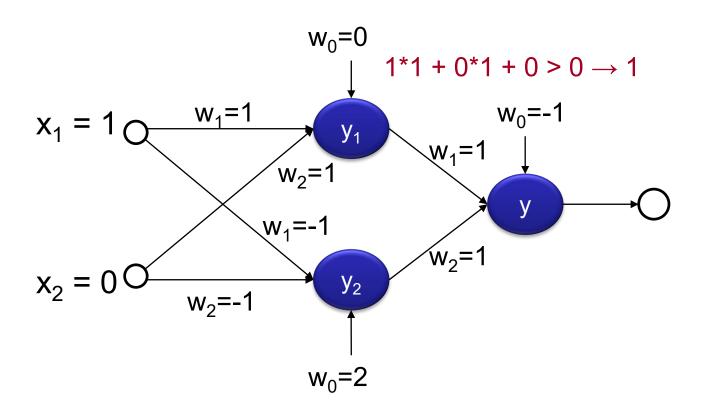


Multi-layered network! Boolean logic tells us that XOR can be expressed as:

$$y_1 = x_1 \text{ OR } x_2$$

 $y_2 = \text{NOT}(x_1 \text{ AND } x_2)$
 $y = y_1 \text{ AND } y_2$
 $y = x_1 \text{ XOR } x_2$

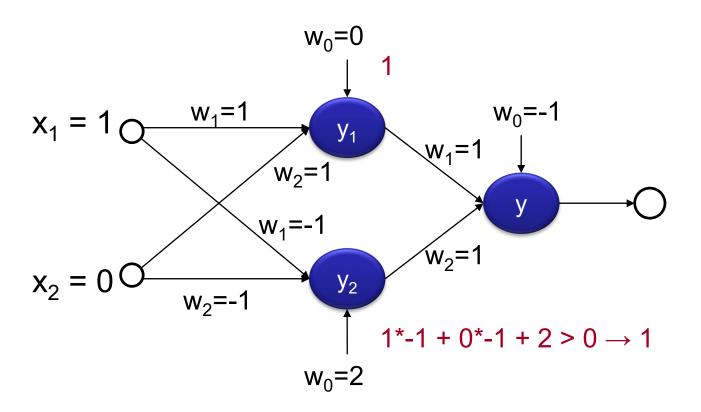
XOR - True



$$y_1 = x_1 \text{ OR } x_2$$

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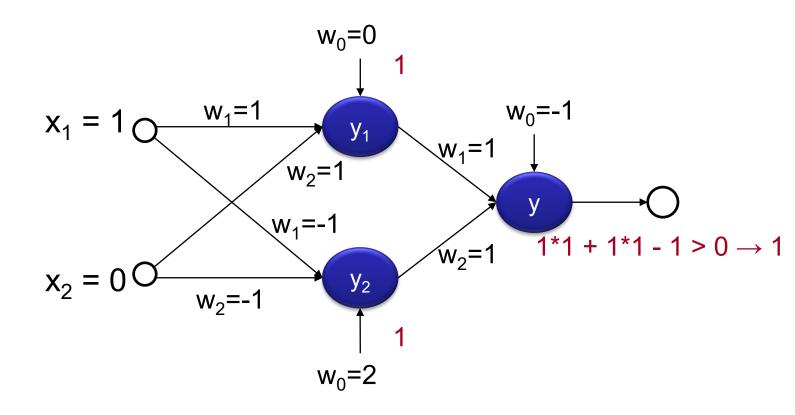
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XOR – True



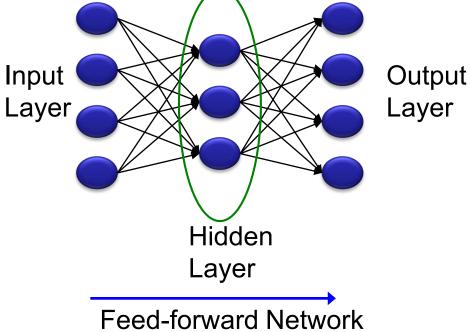
$$y_1 = x_1 \text{ OR } x_2$$

 $y_2 = \text{NOT}(x_1 \text{ AND } x_2)$
 $y = y_1 \text{ AND } y_2$

1 XOR 0 = 1

A *linearly inseparable* function, like XOR, can be expressed in a multilayered perceptron network!

Also known as an Artificial Neural Network (ANN).

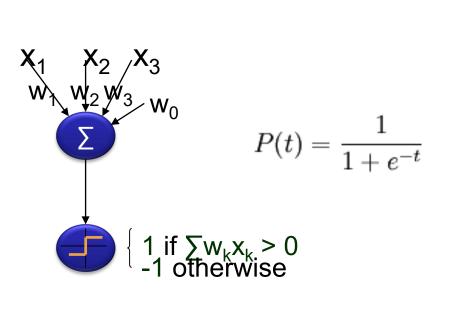


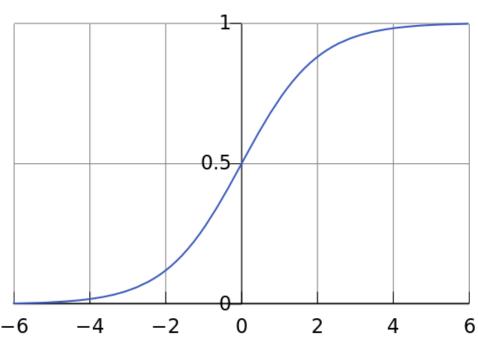
How do we learn the weights?

- Feed an instance through the network.
- If not correctly classified, calculate the squared error.
- Propagate the error backwards through the network and modify the weights.
- Continue for all training instances and until the total error is below a threshold.
- Backpropagation is a common algorithm for training ANNs.

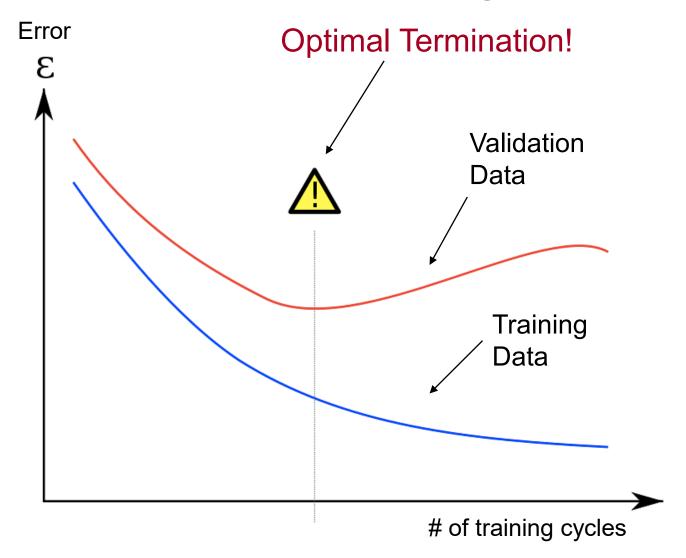
Backpropagation

- BP does however require that the activation functions is differentiable for all x.
- A step function (-1 if below threshold, +1 if equal or above threshold) is not differentiable.
- Instead we use a sigmoid function.





Overfitting

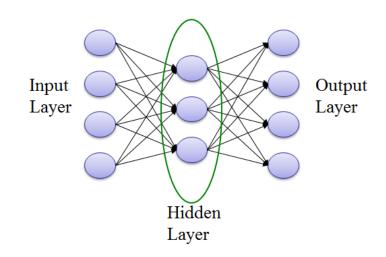


Properties of ANNs

- Good at handling inconsistent, noisy data.
 - Good at handling missing or unimportant attributes.
- Learning is usually <u>very</u> slow.
- Risk of overfitting.
- Not understandable by humans.
- Requires lots of diverse data.
- Image classification is a problem very well suited for ANNs.

ANN design

- No general rules for designing the layers.
- Start with one input node for each attribute, and enough output nodes to represent all classes.
- Try with a small number (3-5) of hidden nodes and see how it works. Increase if needed.
- Larger networks are slower to train, but does not have to be better at classifying your data!



Support Vector Machines

- Linear Models can only represent Linearly Separable classes.
- For many applications this is too simple.
 - The XOR problem

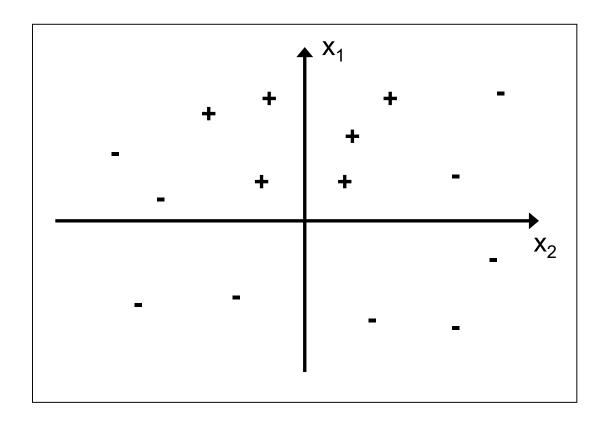
 What if we somehow can transform a nonlinear problem to a linear problem?

Non-linear Mapping

- A non-straight line in one space, can in fact be straight in another space.
- So by transforming the class boundary to another space, the problem can be linearly separable.

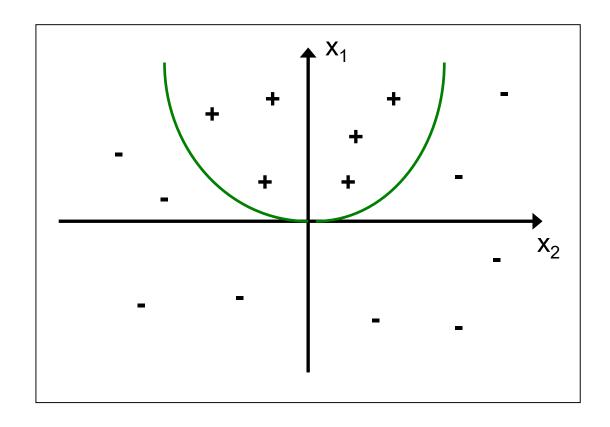
Better understood with an example!

Non-linear Mapping - Example



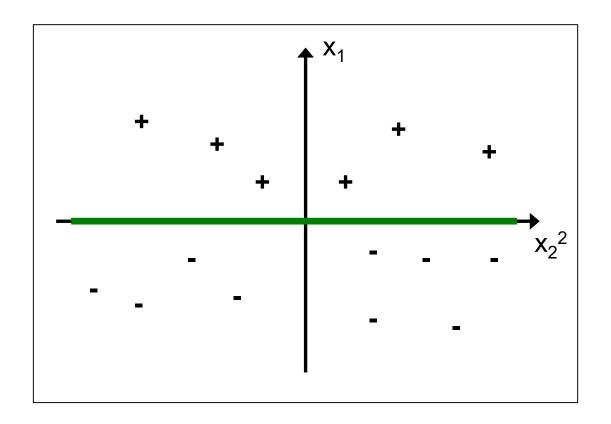
Not linearly separable in the (x_1,x_2) plane

Non-linear Mapping - Example



Separable, but not a straight line $(x_1=x_2^2)$

Non-linear Mapping - Example



Separable in the (x_1, x_2^2) plane!

Non-linear Mapping

- In fact, polynomials of sufficiently high degree can represent any function accurately:
 - $x=w_1x_1^3+w_2x_1^2a_2+w_3x_1x_2^2+...$
- In a linear model, weights are learned to find a plane that separate the classes.
- In a non-linear model, weights and coefficients are learned to find a plane that separate the classes in some space.



EVALUATION

Evaluation

- Evaluation is a key element in successful machine learning experiments.
- We need to know how different methods work and compare them with each other.
 - Is ANN better than KNN on my data?
- Accuracy = how many instances correctly classified.
 - 9/14 = 64.3%

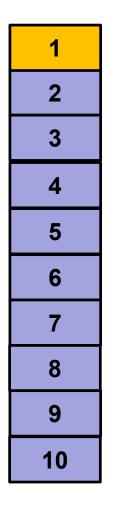
Data usage

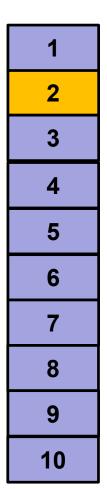
- All known data can be used for training and validation.
- Not a very good idea, since we don't test the generalization capabilities of the classifier.
- = does not prove that our system works on new data!

Data usage

- The data can be divided into a training set and a validation set.
 - Use the training set to train the classifier.
 - Use the validation set to see how well it worked.
- Better, but very sensitive to how we divide the data!

Data usage - Cross Validation





	1
	2
	3
	4
	5
	6
	7
	8
	9
•	10
	7 8 9

1
2
3
4
5
6
7
8
9
10

10-fold Cross Validation = divide data into 10 parts.

9 parts are used for training,1 part for validation.

Iterate until all parts have been used for validation.

Data usage – Cross Validation

- More accurate than using one training set and one validation set.
- Drawback is increased training time.
- Still sensitive to how we divide the data, especially for small datasets.

Is Accuracy a good metric?

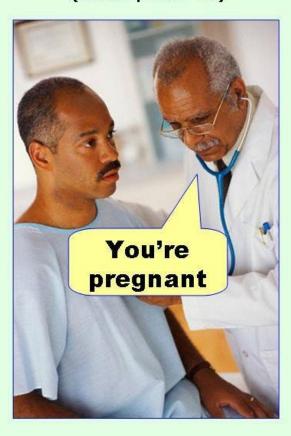
Simple to calculate, but is often overly optimistic.

- TP = true positives
- FP = false positives
- TN = true negatives
- FN = false negatives

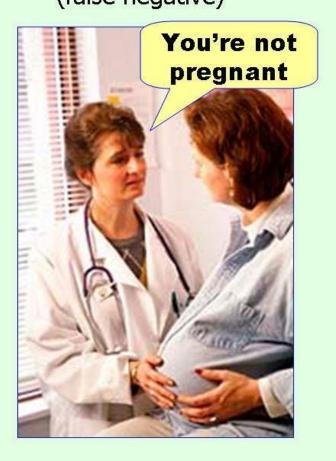
A more complete description of the learner.

A good way to put it...

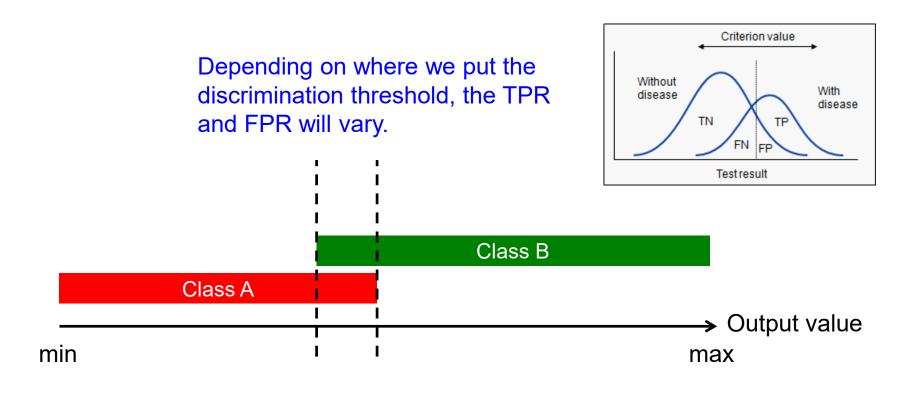
Type I error (false positive)



Type II error (false negative)



Discrimination Threshold



TPR = TP / (TP + FN)

FPR = FP / (FP + TN)



- Weka is a free project containing a large number of machine learning algorithms.
- It can be used with a GUI or through a Java API.
- It supports data in csv or arff format.
- Website:
 - http://www.cs.waikato.ac.nz/ml/weka/

That was all for this lecture



http://etc.ch/45Cv

Acknowledgements

Dr. Johan Hagelbäck Linnæus University



johan.hagelback@lnu.se



http://aiguy.org