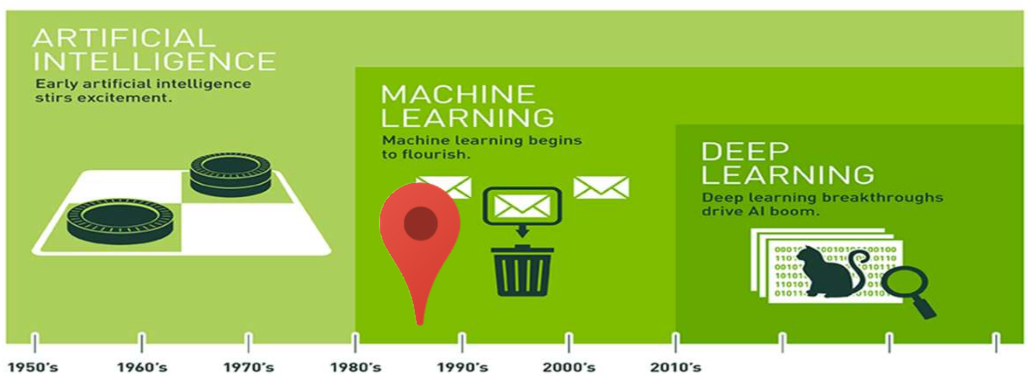
Artificial Intelligence: Machine Learning - 1

- Russell & Norvig: Sections 18.1 to 18.4

Today

1. Naïve Bayes Classifi
2. Introduction to ML

3. Decision Trees
4. (Evaluation
5. Unsupervised Learning)
6. Neural Networks



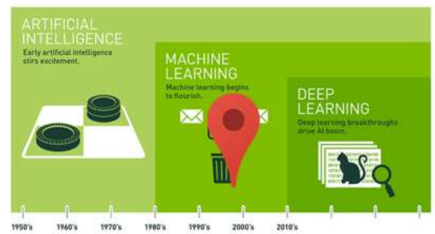
https://medium.com/machine-learning-for-humans/neural-networks-deep-learning-cdad8aeae49b

Remember this slide…

History of AI

- 1980s-2010
- The rise of Machine Learning
  - More powerful CPUs-> usable implementation of neural networks
  - Big data -> Huge data sets are available
    - document repositories for NLP (e.g. emails)
    - billions on images for image retrieval
    - billions of genomic sequences, …

😃 Rules are now learned automatically !



2011: Watson wins at Jeapardy!

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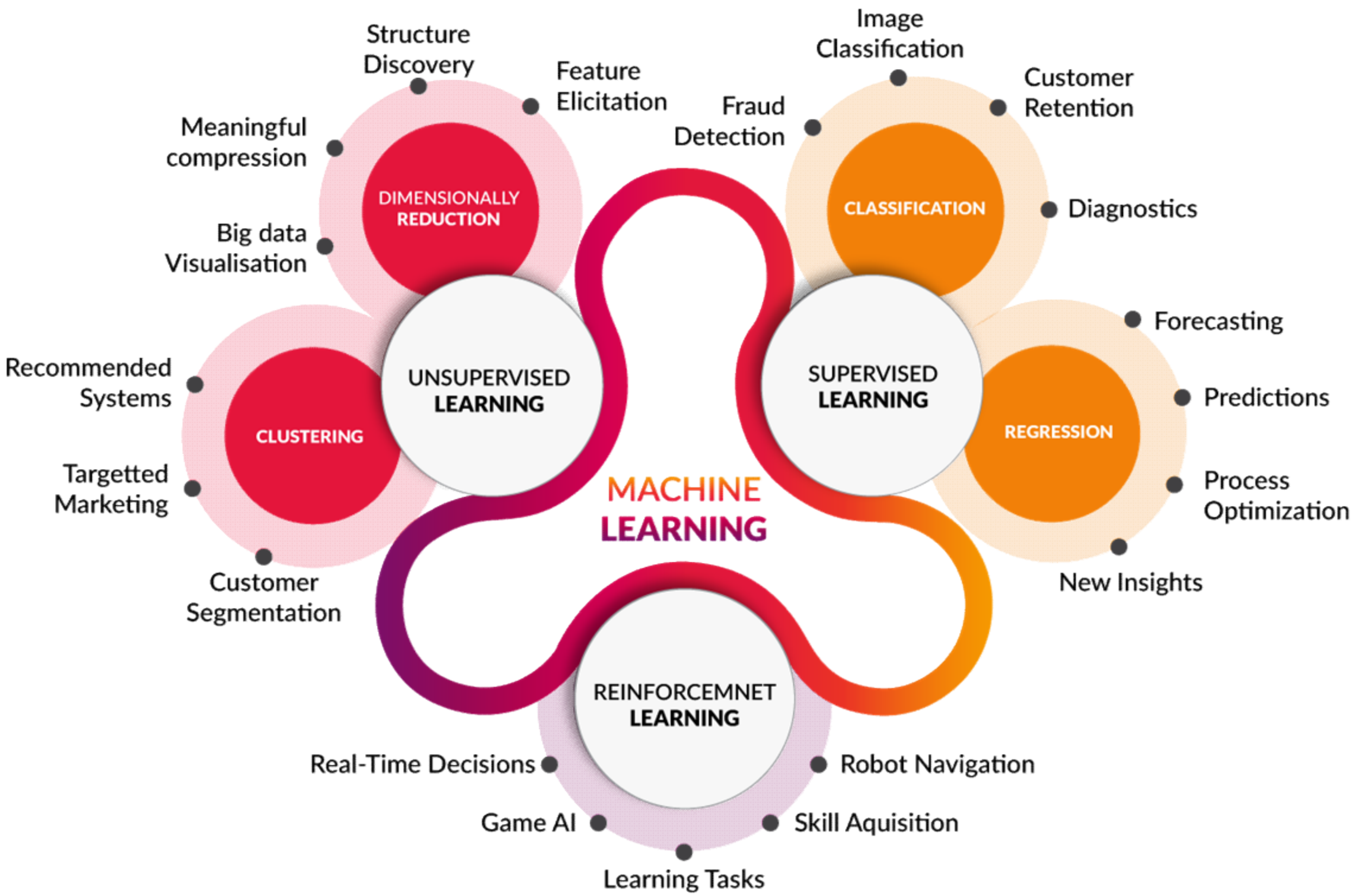
Motivation

- Too many to list here!
  - Recommender systems (eg. Netflix)
  - Pattern Recognition (eg. Handwriting recognition)
  - Detecting credit card fraud
  - Computer vision (eg. Object recognition)
  - Discovering Genetic Causes of Diseases
  - Natural Language Processing (eg. Spam filtering)
  - Speech Recognition / Synthesis
  - Medical Diagnostics
  - Information Retrieval (eg. Image search)
  - Learning heuristics for game playing
  - …
  - *Oh… I'm out of space*

What is Machine Learning?

- Learning = crucial characteristic of an intelligent agent
- ML
  - Constructs algorithms that learn from data
  - ie perform tasks that were not explicitly programmed and improve their performance the more tasks they accomplish
  - generalize from given experiences and are able to make judgments in new situations

Types of Machine Learning

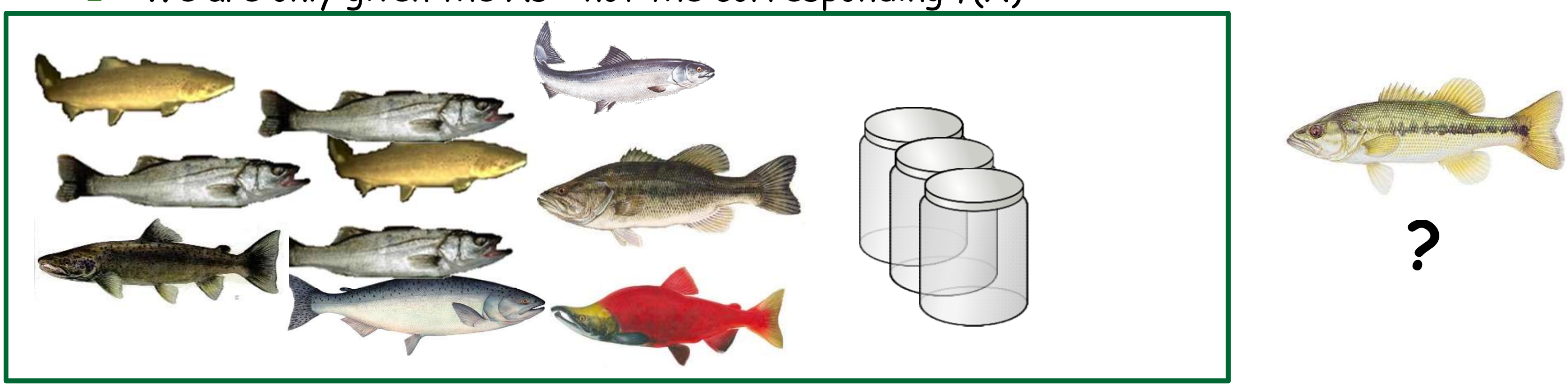


http://www.cognub.com/index.php/cognitive-platform/

Types of Machine Learning

- Supervised learning
  - We are given a training set of (X, f(X)) pairs
  - X = <color, length>

- Unsupervised learning
  - We are only given the Xs - not the corresponding f(X)



Types of Learning

- In **Supervised** learning
  - We are given a training set of (X, f(X)) pairs

big nose	big teeth	big eyes	no moustache	f(X) = not person
small nose	small teeth	small eyes	no moustache	f(X) = person

small nose	big teeth	small eyes	moustache	f(X) = ?

- In **Reinforcement** learning
  - We are not given the (X, f(X)) pairs

small nose	big teeth	small eyes	moustache	f(X) = ?

  - But we get a reward when our learned f(X) is right, and we try to maximize the reward
  - Goal: maximize the nb of right answers

- In **Unsupervised** learning
  - We are only given the Xs - not the corresponding f(X)

big nose	big teeth	big eyes	no moustache	*not given*
small nose	small teeth	small eyes	no moustache	*not given*

small nose	big teeth	small eyes	moustache	f(X) = ?

  - No *teacher* involved / Goal: find regularities among the Xs (clustering)
  - Data mining

Logical Inference

- Inference: process of deriving new facts from a set of premises

- Types of logical inference:
  1. Deduction
  2. Abduction
  3. Induction

Deduction

- aka Natural Deduction
- Conclusion follows necessary from the premises.
- From $A \Rightarrow B$ and A, we conclude that B
- We conclude from the general case to a specific example of the general case
- Ex:

  All men are mortal.

  Marcus is a man.

  Marcus is mortal.

Abduction

- Conclusion is one hypothetical (most probable) explanation for the premises
- From $A \Rightarrow B$ and B, we conclude A
- Ex:

  Drunk people do not walk straight.
  John does not walk straight.
  ___
  John is drunk.

- Not sound… but may be most likely explanation for B
- Used in medicine…
  - in reality… disease $\Rightarrow$ symptoms
  - patient complains about some symptoms… doctor concludes a disease

Induction

- Conclusion about all members of a class from the examination of only a few member of the class.
- From $A \wedge C \Rightarrow B$ and $A \wedge D \Rightarrow B$, we conclude $A \Rightarrow B$
- We construct a general explanation based on a specific case.
- Ex:

  All CS students in COMP 472 are smart.

  All CS students on vacation are smart.

  All CS students are smart.
- Not sound
- But, can be seen as hypothesis construction or generalisation

Inductive Learning

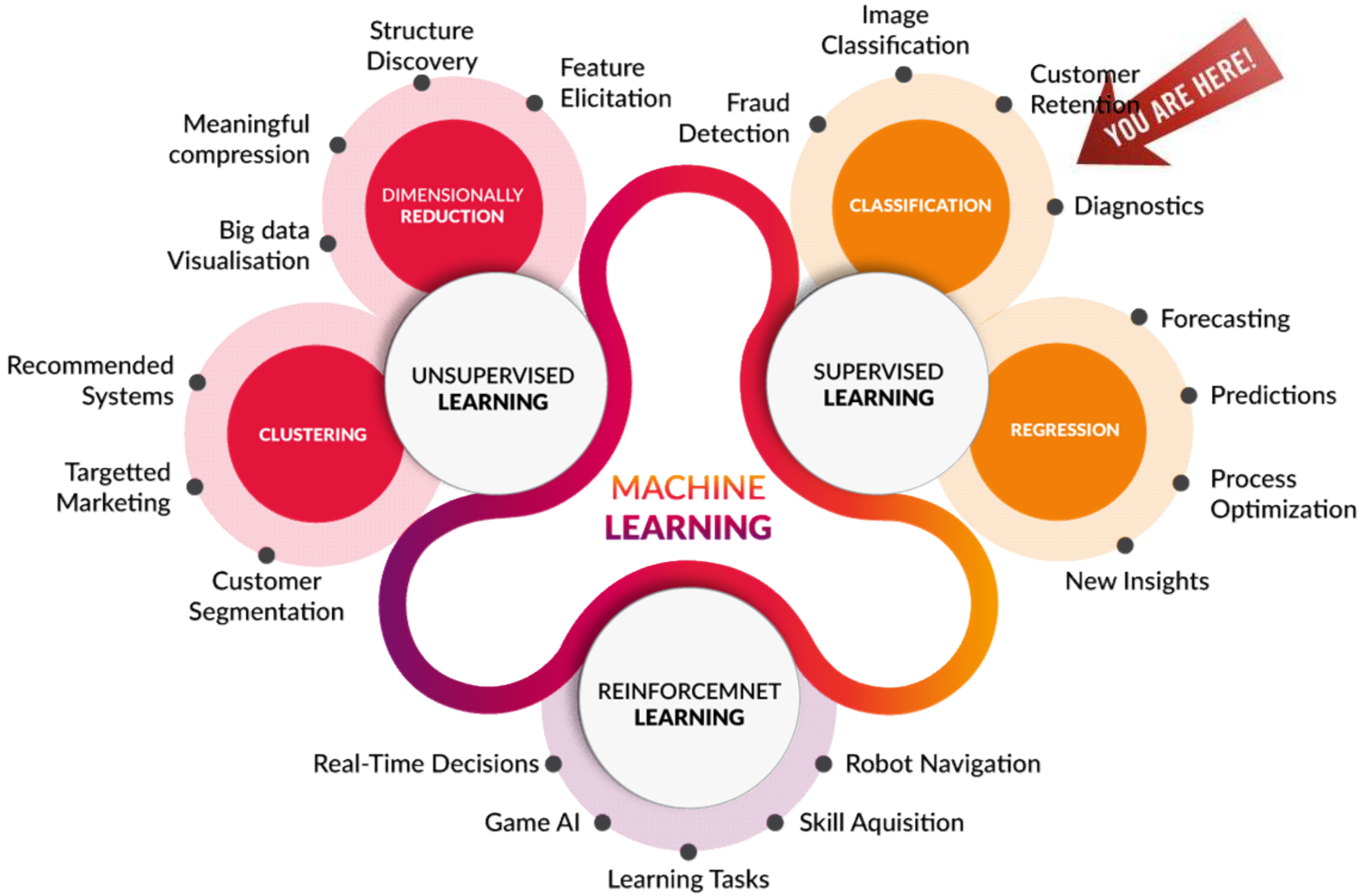
- = learning from examples
- Most work in ML
- Examples are given (positive and/or negative) to train a system in a classification (or regression) task
- Extrapolate from the training set to make accurate predictions about future examples
- Can be seen as learning a function
- Given a new instance X you have never seen
- You must find an estimate of the function f(X) where f(X) is the desired output
- Ex:

small nose	big teeth	small eyes	moustache	f(X) = ?

X

  - X = features of a face (ex. small nose, big teeth, …)
  - f(X) = function to tell if X represents a human face or not

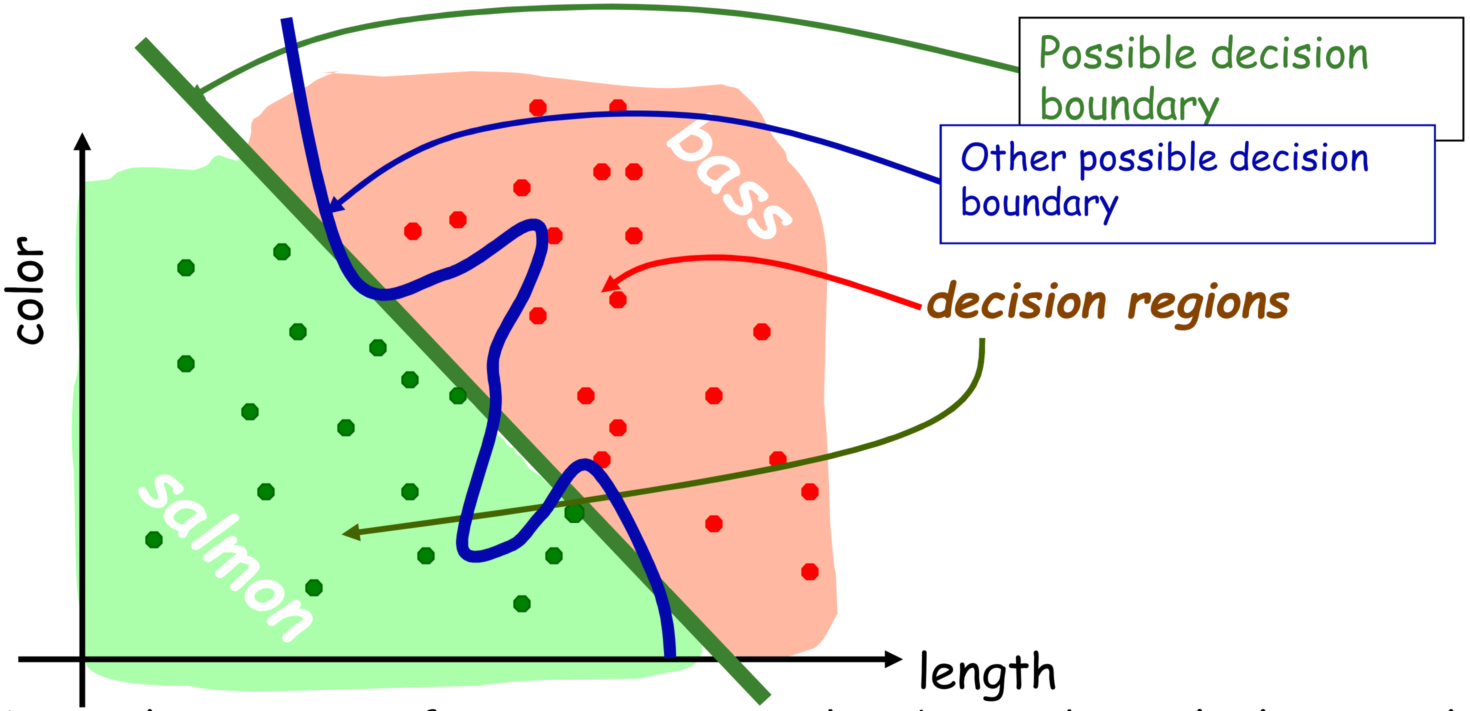
Types of Machine Learning



http://www.cognub.com/index.php/cognitive-platform/

Example

- Given pairs (X,f(X)) (the training set – the data points)
- Find a function that fits the training set well
- So that given a new X, you can predict its f(X) value



- Note: choosing one function over another beyond just looking at the training set is called **inductive bias** (eg. prefer "smoother" functions)

Inductive Learning Framework

- Input data are represented by a vector of features, X
- Each vector X is a list of (attribute, value) pairs.
  - Ex: `x = [nose:big, teeth:big, eyes:big, moustache:no]`
- The number of attributes is fixed (positive, finite)
- Each attribute has a fixed, finite number of possible values
- Each example can be interpreted as a point in a n-dimensional feature space
  - where n is the number of attributes

Note: *attribute == feature*

Example

has-hair?	has-scales?	has-feathers?	flies?	lives in water?	lays eggs?	
1	0	0	0	0	0	Dog
1	0	0	0	0	0	Cat
1	0	0	1	0	0	Bat
1	0	0	0	1	0	Whale
0	0	1	1	0	1	Canary
0	0	1	1	0	1	Robin
0	0	1	1	0	1	Ostrich
0	1	0	0	0	1	Snake
0	1	0	0	0	1	Lizard
0	1	0	0	1	1	Alligator

Real ML applications typically require hundreds, thousands or millions of examples

source: Alison Cawsey: The Essence of AI (1997).

Techniques in ML

- Probabilistic Methods
  - ex: Naïve Bayes Classifier
- Decision Trees
  - Use only discriminating features as questions in a big if-then-else tree
- Neural networks
  - Also called parallel distributed processing or connectionist systems
  - Intelligence arise from having a large number of simple computational units
- …

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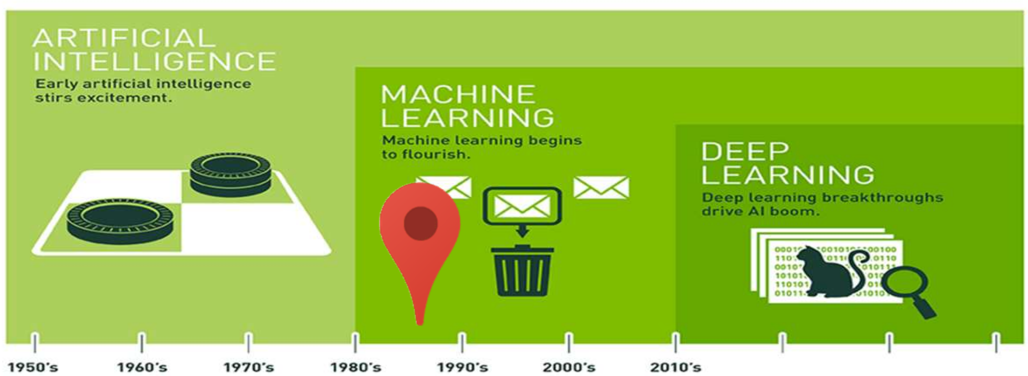


https://medium.com/machine-learning-for-humans/neural-networks-deep-learning-cdad8aeae49b

Guess Who?

Decision Trees

- Simplest, but most successful form of learning algorithm
- Very well-know algorithm is ID3 (Quinlan, 1987) and its successor C4.5
- Look for features that are very good indicators of the result, place these features (as questions) in nodes of the tree
- Split the examples so that those with different values for the chosen feature are in a different set
- Repeat the same process with another feature

ID3 / C4.5 Algorithm

- Top-down construction of the decision tree
- Recursive selection of the "best feature" to use at the current node in the tree
  - Once the feature is selected for the current node, generate children nodes, one for each possible value of the selected attribute
  - Partition the examples using the possible values of this attribute, and assign these subsets of the examples to the appropriate child node
  - Repeat for each child node until all examples associated with a node are classified

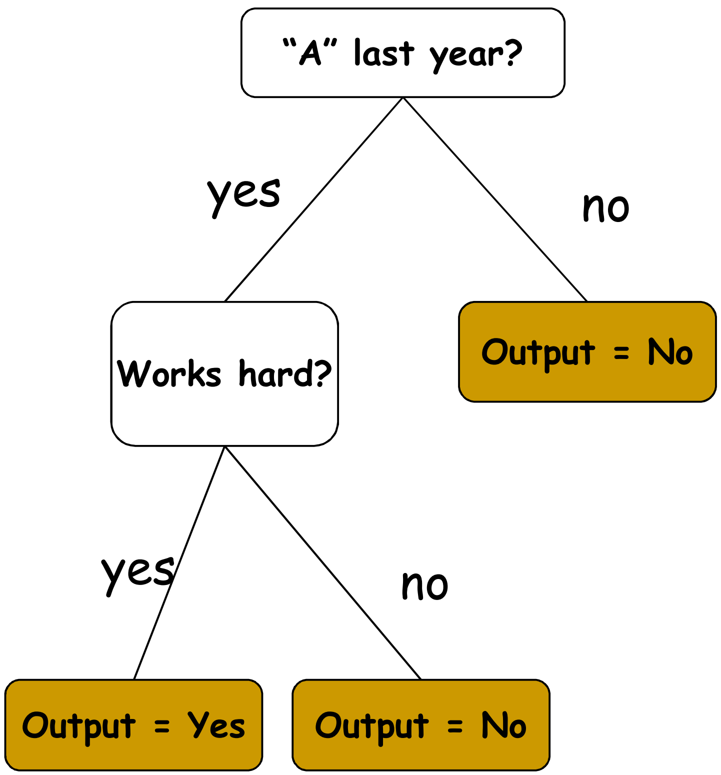
http://www.rulequest.com/Personal/

Example

Info on last year's students to determine if a student will get an 'A' this year

	Features (X)				Output f(X)
Student	**'A' last year?**	**Black hair?**	**Works hard?**	**Drinks?**	**'A' this year?**
X1: Richard	Yes	Yes	No	Yes	**No**
X2: Alan	Yes	Yes	Yes	No	**Yes**
X3: Alison	No	No	Yes	No	**No**
X4: Jeff	No	Yes	No	Yes	**No**
X5: Gail	Yes	No	Yes	Yes	**Yes**
X6: Simon	No	Yes	Yes	Yes	**No**

Example



	Features				Output f(X)
Student	'A' last year?	Black hair?	Works hard?	Drinks ?	**'A' this year?**
Richard	Yes	Yes	No	Yes	**No**
Alan	Yes	Yes	Yes	No	**Yes**
Alison	No	No	Yes	No	**No**
Jeff	No	Yes	No	Yes	**No**
Gail	Yes	No	Yes	Yes	**Yes**
Simon	No	Yes	Yes	Yes	**No**

Example 2: The Restaurant

- Goal: learn whether one should wait for a table
- Attributes
  - Alternate: another suitable restaurant nearby
  - Bar: comfortable bar for waiting
  - Fri/Sat: true on Fridays and Saturdays
  - Hungry: whether one is hungry
  - Patrons: how many people are present (none, some, full)
  - Price: price range ($, $$, $$$)
  - Raining: raining outside
  - Reservation: reservation made
  - Type: kind of restaurant (French, Italian, Thai, Burger)
  - WaitEstimate: estimated wait by host (0-10 mins, 10-30, 30-60, >60)

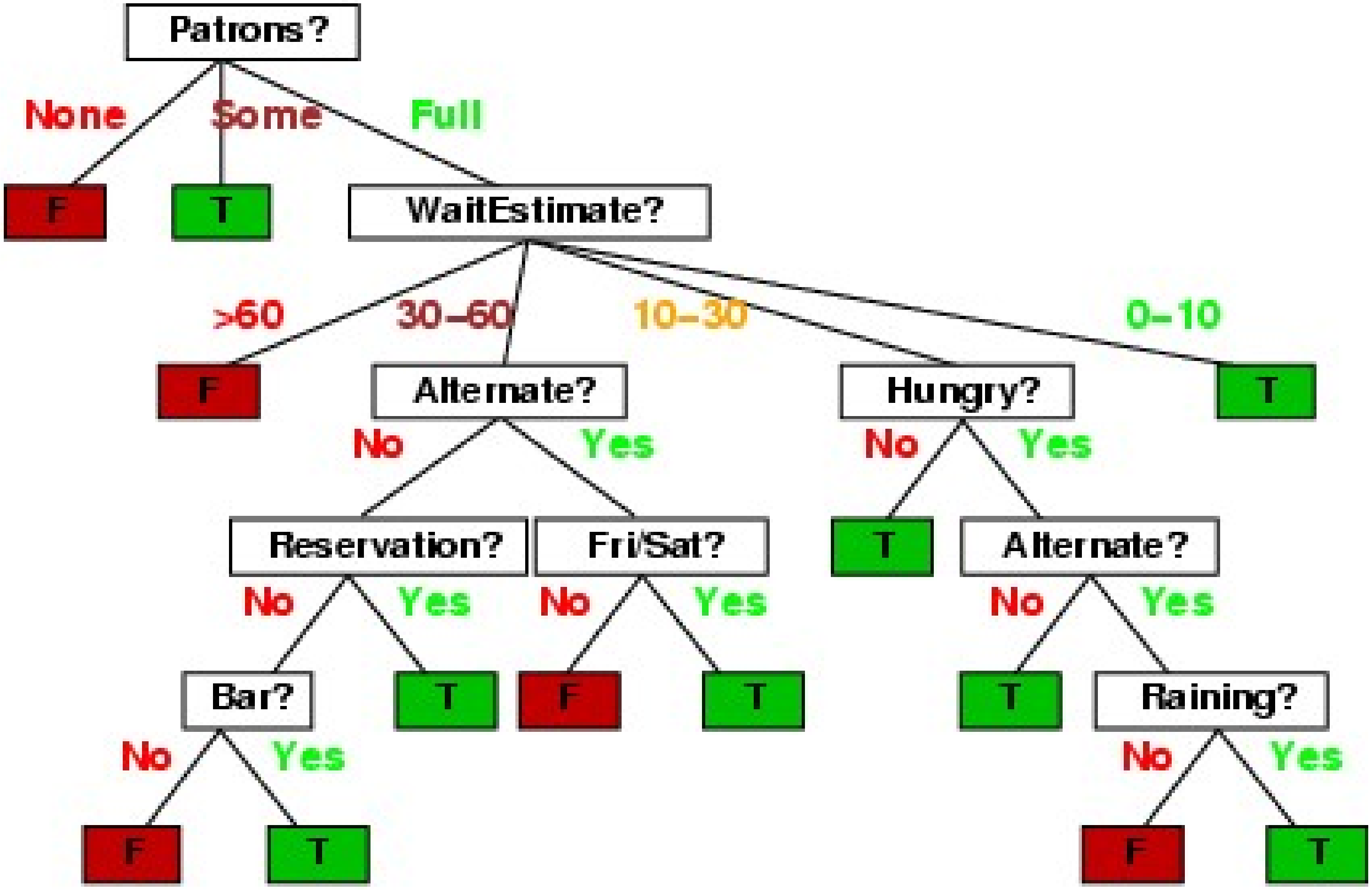
Example 2: The Restaurant

- Training data:

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

source: Norvig (2003)

A First Decision Tree



- But is it the best decision tree we can build?

source: Norvig (2003)

Ockham's Razor Principle

It is vain to do more than can be done with less… Entities should not be multiplied beyond necessity. [Ockham, 1324]

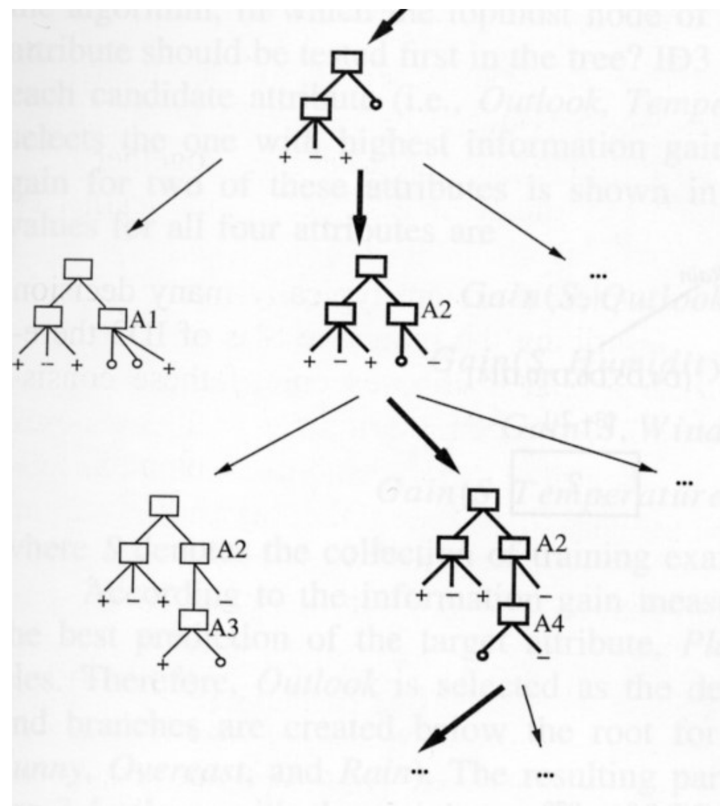
- In other words… always favor the simplest answer that correctly fits the training data
- i.e. the smallest tree on average

- This type of assumption is called inductive bias
  - inductive bias = making a choice beyond what the training instances contain

Finding the Best Tree

- can be seen as searching the space of all possible decision trees
- Inductive bias: prefer shorter trees on average
- how?
- search the space of all decision trees
  - always pick the next attribute to split the data based on its "discriminating power" (information gain)
  - in effect, steepest ascent hill-climbing search where heuristic is information gain

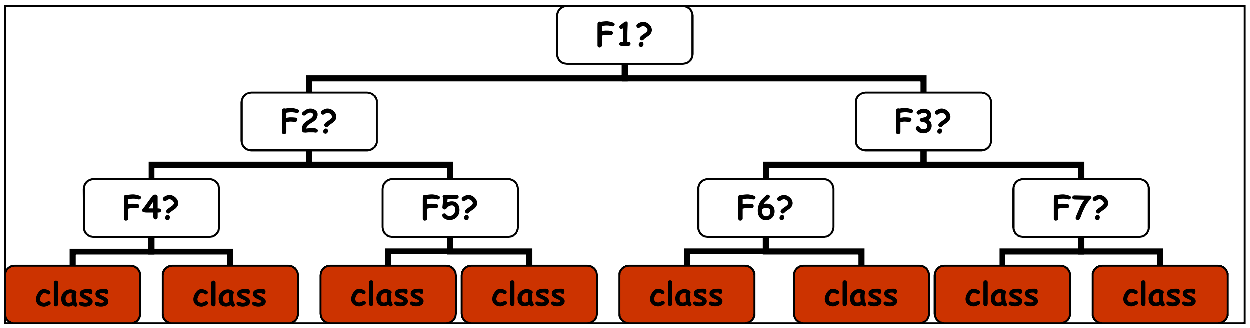
empty tree

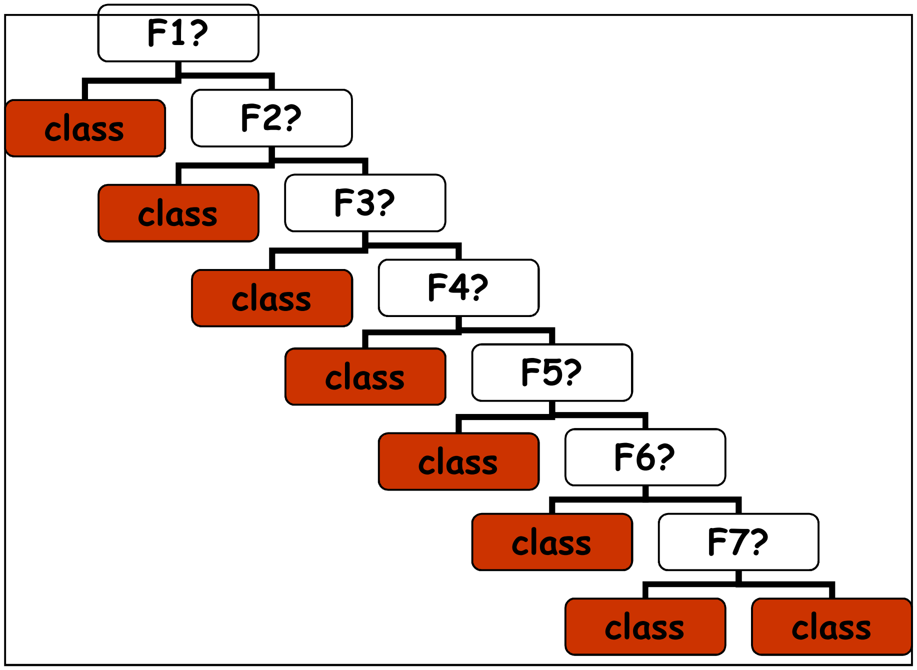


complete tree

source: Tom Mitchell, Machine Learning (1997)

Which Tree is Best?





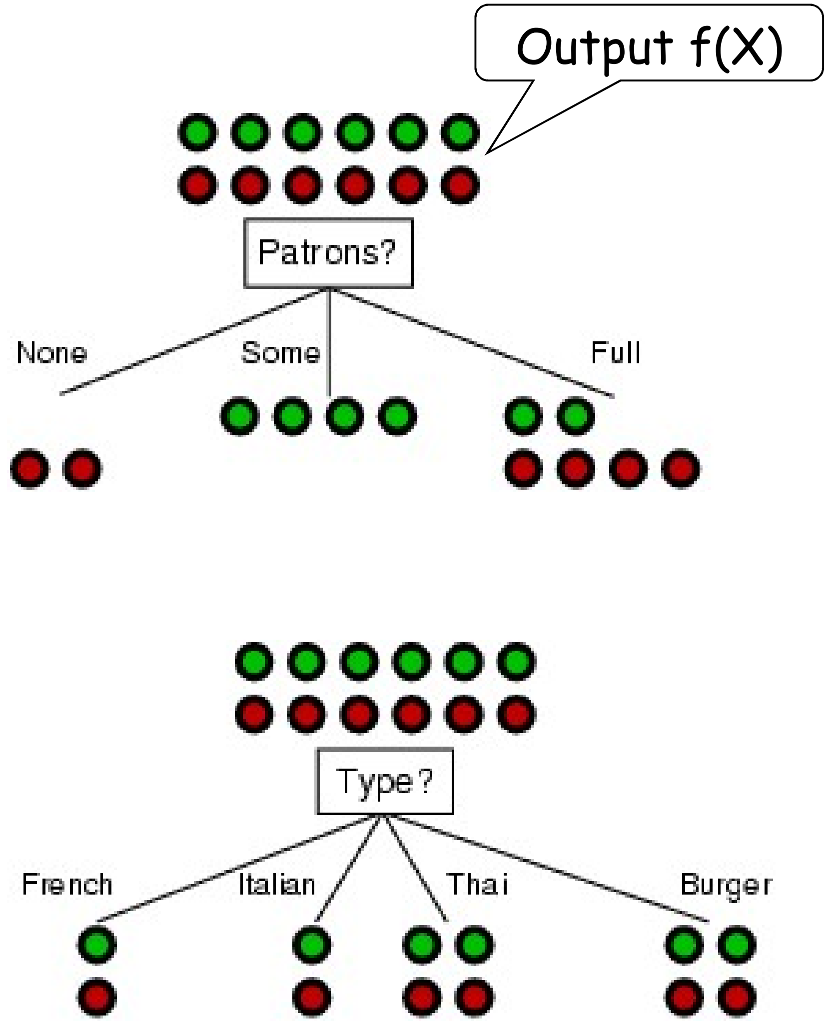
Choosing the Next Attribute

- The key problem is choosing which feature to split a given set of examples

- ID3 uses Maximum Information-Gain:
  - Choose the attribute that has the largest information gain
    - i.e., the attribute that will result in the smallest expected size of the subtrees rooted at its children
    - information theory

Intuitively…

- *Patron*:
  - If value is *Some*… all outputs=*Yes*
  - If value is *None*… all outputs=*No*
  - If value is *Full*… we need more tests
- *Type*:
  - If value is *French*… we need more tests
  - If value is *Italian*… we need more tests
  - If value is *Thai*… we need more tests
  - If value is *Burger*… we need more tests
- …
- So *patron* may lead to shorter tree…



source: Norvig (2003)

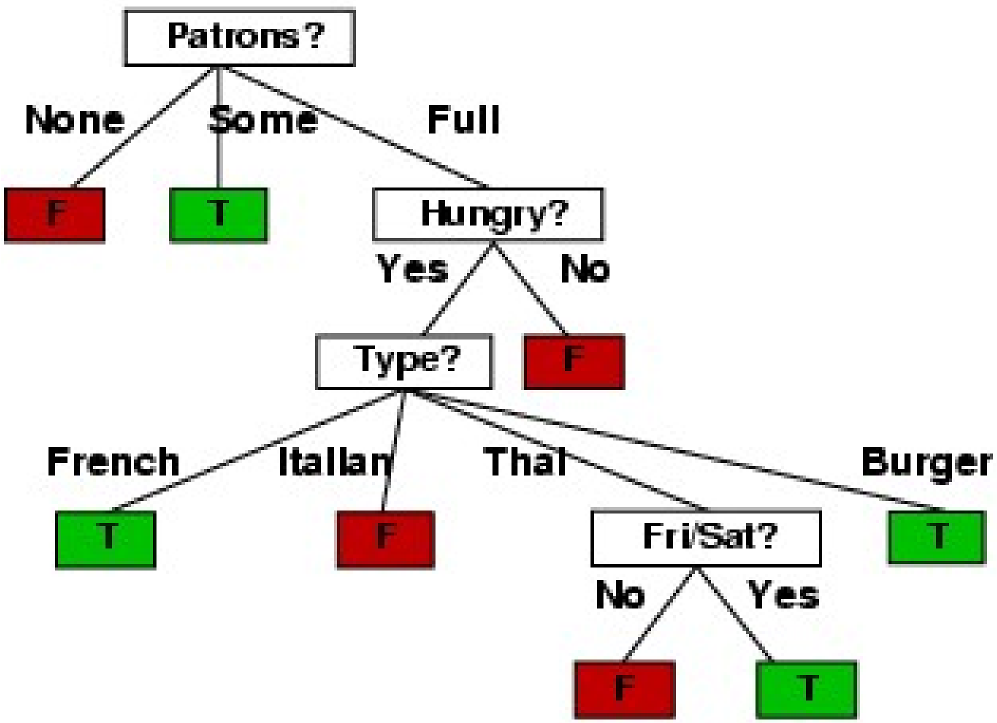
Next Feature…

- For only data where *patron = Full*
- *hungry*
  - If value is *Yes*… we need more tests
  - If value is *No*… all output= *No*
- *type*:
  - If value is *French*… all output= *No*
  - If value is *Italian*… all output= *No*
  - If value is *Thai*… we need more tests
  - If value is *Burger*… we need more tests
- …

- So *hungry* is more discriminating (only 1 new branch)…

A Better Decision Tree

- 4 tests instead of 9
- 11 branches instead of 21



source: Norvig (2003)

Choosing the Next Attribute

- The key problem is choosing which feature to split a given set of examples
- Most used strategy: information theory

$$H(X) = -\sum_{x_i \in X} p(x_i)\log_2 p(x_i)$$ Entropy (or information content)

$$H(\text{fair coin toss}) = -\sum_{x_i \in X} p(x_i)\log_2 p(x_i) = H\left(\frac{1}{2},\frac{1}{2}\right)$$

$$= \left(\frac{1}{2}\log_2\frac{1}{2} + \frac{1}{2}\log_2\frac{1}{2}\right) = 1\text{ bit}$$

entropy of a fair coin toss (the RV) with 2 possible outcomes, each with a probability of 1/2

Essential Information Theory

- Developed by Shannon in the 40s
- Notion of entropy (information content)
- Measure how "predictable" a RV is…
    - If you already have a good idea about the answer (e.g. 90/10 split)
      → low entropy
    - If you have no idea about the answer (e.g. 50/50 split)
      → high entropy

Entropy

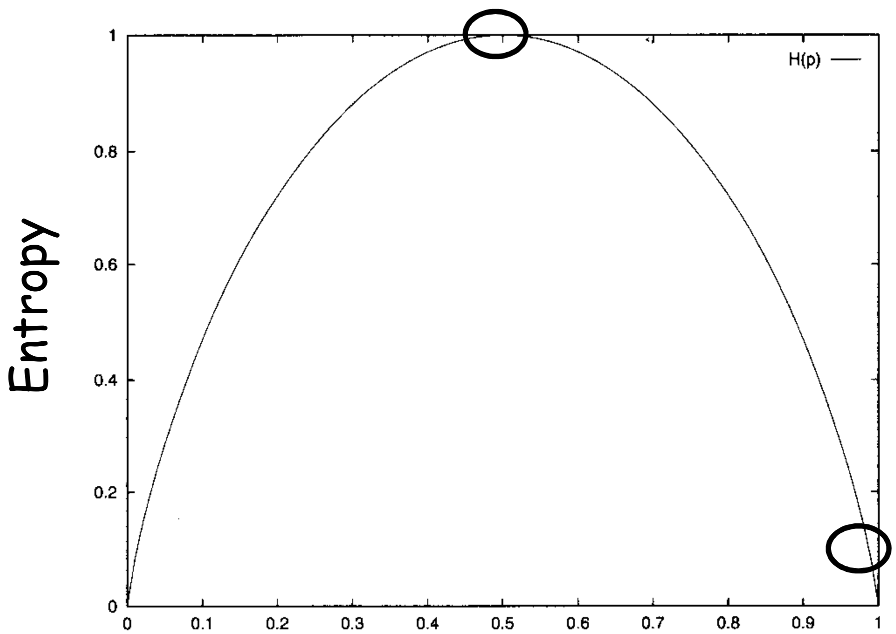
- Let X be a discrete random variable (RV) with *i* possible outcomes x_i
- Entropy (or information content)

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

- measures the *amount of information* in a RV
  - *average uncertainty* of a RV
  - *the average length of the message* needed to transmit an outcome x_i of that variable
- measured in bits
- for only 2 outcomes x_1 and x_2, then $1 \geq H(X) \geq 0$

Example: The Coin Flip

- Fair coin: $H(X) = -\sum_{i=1}^{n} p(x_i)\log_2 p(x_i) = -\left(\frac{1}{2}\log_2\frac{1}{2} + \frac{1}{2}\log_2\frac{1}{2}\right) = 1 \text{ bit}$
- Rigged coin: $H(X) = -\sum_{i=1}^{n} p(x_i)\log_2 p(x_i) = -\left(\frac{99}{100}\log_2\frac{99}{100} + \frac{1}{100}\log_2\frac{1}{100}\right) = 0.08 \text{ bits}$



fair coin -> high entropy

rigged coin -> low entropy

P(head)

Choosing the Best Feature (con't)

- The "discriminating power" of an attribute A given a data set S
- Let Values(A) = the set of values that attribute A can take
- Let S_v = the set of examples in the data set which have value v for attribute A (for each value v from Values(A))

information gain (or entropy reduction)

$$
\begin{aligned}
gain(S, A) &= H(S) - H(S \mid A) \\
&= H(S) - \sum_{v \in values(A)} \frac{|S_v|}{|S|} \times H(S_v)
\end{aligned}
$$

Some Intuition

Size	Color	Shape	Output
Big	Red	Circle	+
Small	Red	Circle	+
Small	Red	Square	-
Big	Blue	Circle	-

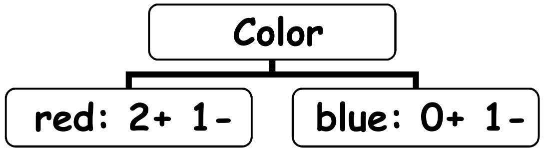
- *Size* is the least discriminating attribute (i.e. smallest information gain)

- *Shape* and *color* are the most discriminating attributes (i.e. highest information gain)

A Small Example (1)

Size	Color	Shape	Output
Big	Red	Circle	+
Small	Red	Circle	+
Small	Red	Square	-
Big	Blue	Circle	-

Values(Color) = {red,blue}



$$gain(S, Color) = H(S) - \sum_{v \in values(Color)} \frac{|S_v|}{|S|} x\, H(S_v)$$

$$H(S) = -\left(\frac{2}{4}\log_2\frac{2}{4} + \frac{2}{4}\log_2\frac{2}{4}\right) = 1$$

for each v of Values(Color)

$$H(S \mid Color = red) = H\left(\frac{2}{3}, \frac{1}{3}\right) = -\left(\frac{2}{3}\log_2\frac{2}{3} + \frac{1}{3}\log_2\frac{1}{3}\right) = 0.918$$

$$H(S \mid Color = blue) = H(1,0) = -\left(\frac{1}{1}\log_2\frac{1}{1}\right) = 0$$

$$H(S \mid Color) = \frac{3}{4}(0.918) + \frac{1}{4}(0) = 0.6885$$

$$gain(Color) = H(S) - H(S \mid Color) = 1 - 0.6885 = 0.3115$$

A Small Example (2)

Size	Color	Shape	Output
Big	Red	Circle	+
Small	Red	Circle	+
Small	Red	Square	-
Big	Blue	Circle	-

Shape

circle: 2+ 1-

square: 0+ 1-

Note: by definition,

- Log 0 = -∞
- 0log0 is 0

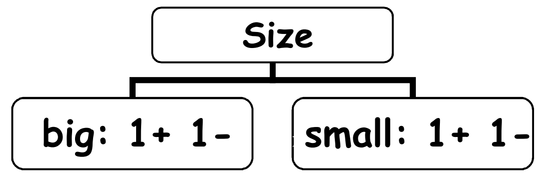
$$H(S) = -\left(\frac{2}{4}\log_2\frac{2}{4} + \frac{2}{4}\log_2\frac{2}{4}\right) = 1$$

$$H(S \mid Shape) = \frac{3}{4}(0.918) + \frac{1}{4}(0) = 0.6885$$

$$gain(Shape) = H(S) - H(S \mid Shape) = 1 - 0.6885 = 0.3115$$

A Small Example (3)

Size	Color	Shape	Output
Big	Red	Circle	+
Small	Red	Circle	+
Small	Red	Square	-
Big	Blue	Circle	-



$$H(S) = -\left(\frac{2}{4}\log_2\frac{2}{4} + \frac{2}{4}\log_2\frac{2}{4}\right) = 1$$

$$H(S\,|\,Size) = \frac{1}{2}(1) + \frac{1}{2}(1) = 1$$

$$gain(Size) = H(S) - H(S\,|\,Size) = 1 - 1 = 0$$

A Small Example (4)

Size	Color	Shape	Output
Big	Red	Circle	+
Small	Red	Circle	+
Small	Red	Square	-
Big	Blue	Circle	-

$$\mathrm{gain}(Shape) = 0.3115$$
$$\mathrm{gain}(Color) = 0.3115$$
$$\mathrm{gain}(Size) = 0$$

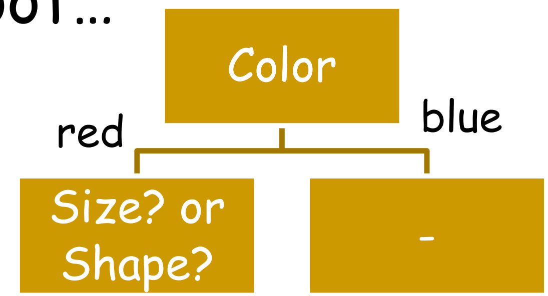
- So first separate according to either *color* or *shape* (root of the tree)

A Small Example (4)

- Let's assume we pick *Color* for the root…

Size	Color	Shape	Output
Big	Red	Circle	+
Small	Red	Circle	+
Small	Red	Square	-
Big	Blue	Circle	-

S_2



$$H(S_2) = -\left(\frac{2}{3}\log_2\frac{2}{3} + \frac{1}{3}\log_2\frac{1}{3}\right)$$

for each v of Values(Size)

$$H(S_2 \mid Size = big) = H\left(\frac{1}{1}, \frac{0}{1}\right) = 0$$

$$H(S_2 \mid Size = small) = H\left(\frac{1}{2}, \frac{1}{2}\right) = 1$$

$$H(S_2 \mid Size) = \frac{1}{3}(0) + \frac{2}{3}(1)$$

$$gain(Size) = H(S_2) - H(S_2 \mid Size)$$

for each v of Values(Shape)

$$H(S_2 \mid Shape = circle) = H\left(\frac{2}{2}, \frac{0}{2}\right) = 0$$

$$H(S_2 \mid Shape = square) = H\left(\frac{0}{1}, \frac{1}{1}\right) = 0$$

$$H(S_2 \mid Shape)$$

$$gain(Shape) = H(S_2) - H(S_2 \mid Shape)$$

Back to the Restaurant

- Training data:

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	\$\$\$	F	T	French	0–10	T
X_2	T	F	F	T	Full	\$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	\$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	\$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	\$\$\$	F	T	French	>60	F
X_6	F	T	F	T	Some	\$\$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	\$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	\$\$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	\$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	\$\$\$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	\$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	\$	F	F	Burger	30–60	T

source: Norvig (2003)

The Restaurant Example

$\text{gain}(alt) = \ldots$ $\text{gain}(bar) = \ldots$ $\text{gain}(fri) = \ldots$ $\text{gain}(hun) = \ldots$

$$\text{gain}(pat) = 1 - \left(\frac{2}{12} \times H\left(\frac{0}{2}, \frac{2}{2}\right) + \frac{4}{12} \times H\left(\frac{0}{4}, \frac{4}{4}\right) + \frac{6}{12} \times H\left(\frac{2}{6}, \frac{4}{6}\right) \right)$$

$$= 1 - \left(\frac{2}{12} \times - \left(\frac{0}{2} \log_2 \frac{0}{2} + \frac{2}{2} \log_2 \frac{2}{2} \right) + \frac{4}{12} \times - \left(\frac{0}{4} \log_2 \frac{0}{4} + \frac{4}{4} \log_2 \frac{4}{4} \right) + \ldots \right) \approx 0.541 \text{bits}$$

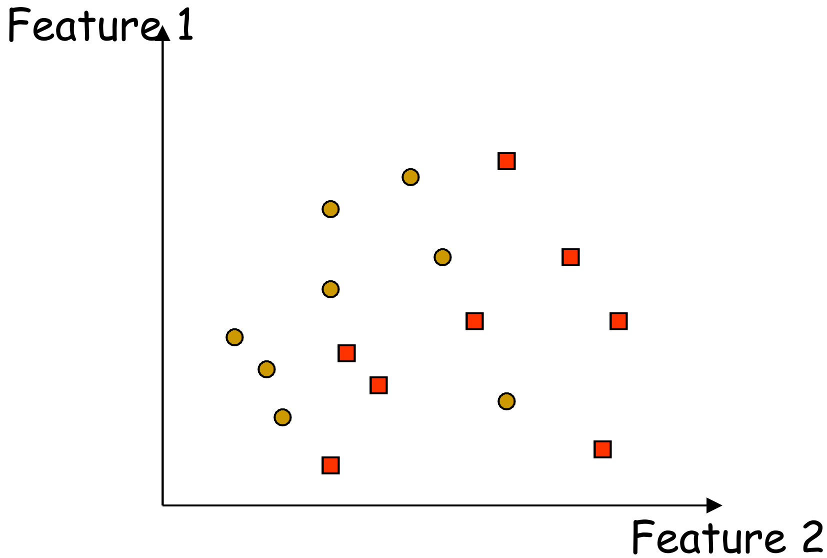
$\text{gain}(price) = \ldots$ $\text{gain}(rain) = \ldots$ $\text{gain}(res) = \ldots$

$$\text{gain}(type) = 1 - \left(\frac{2}{12} \times H\left(\frac{1}{2}, \frac{1}{2}\right) + \frac{2}{12} \times H\left(\frac{1}{2}, \frac{1}{2}\right) + \frac{4}{12} \times H\left(\frac{2}{4}, \frac{2}{4}\right) + \frac{4}{12} \times H\left(\frac{2}{4}, \frac{2}{4}\right) \right) = 0 \text{ bits}$$

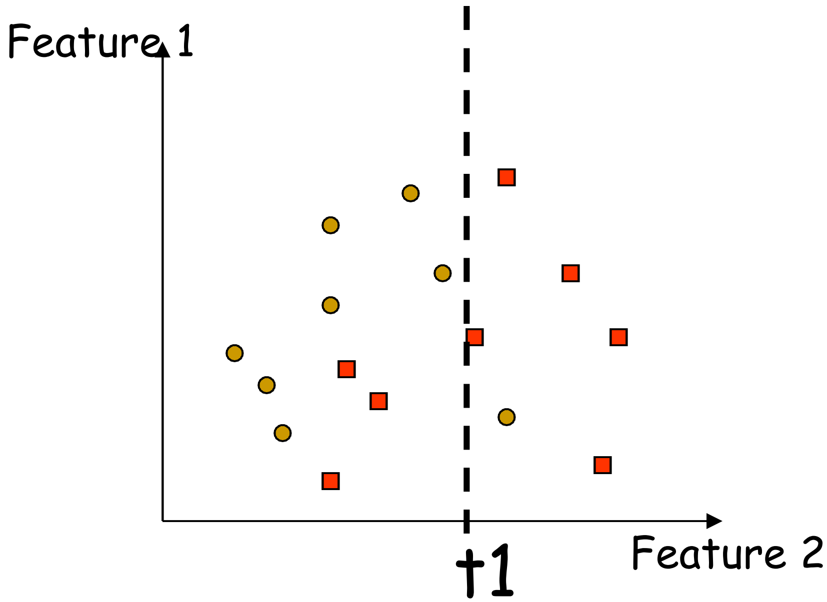
$\text{gain}(est) = \ldots$

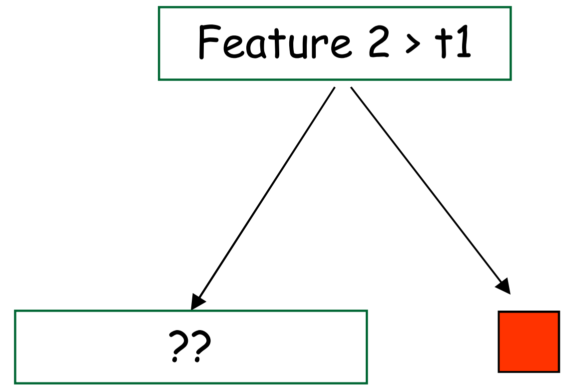
- Attribute pat (Patron) has the highest gain, so root of the tree should be attribute *Patrons*
- do recursively for subtrees

Decision Boundaries of Decision Trees

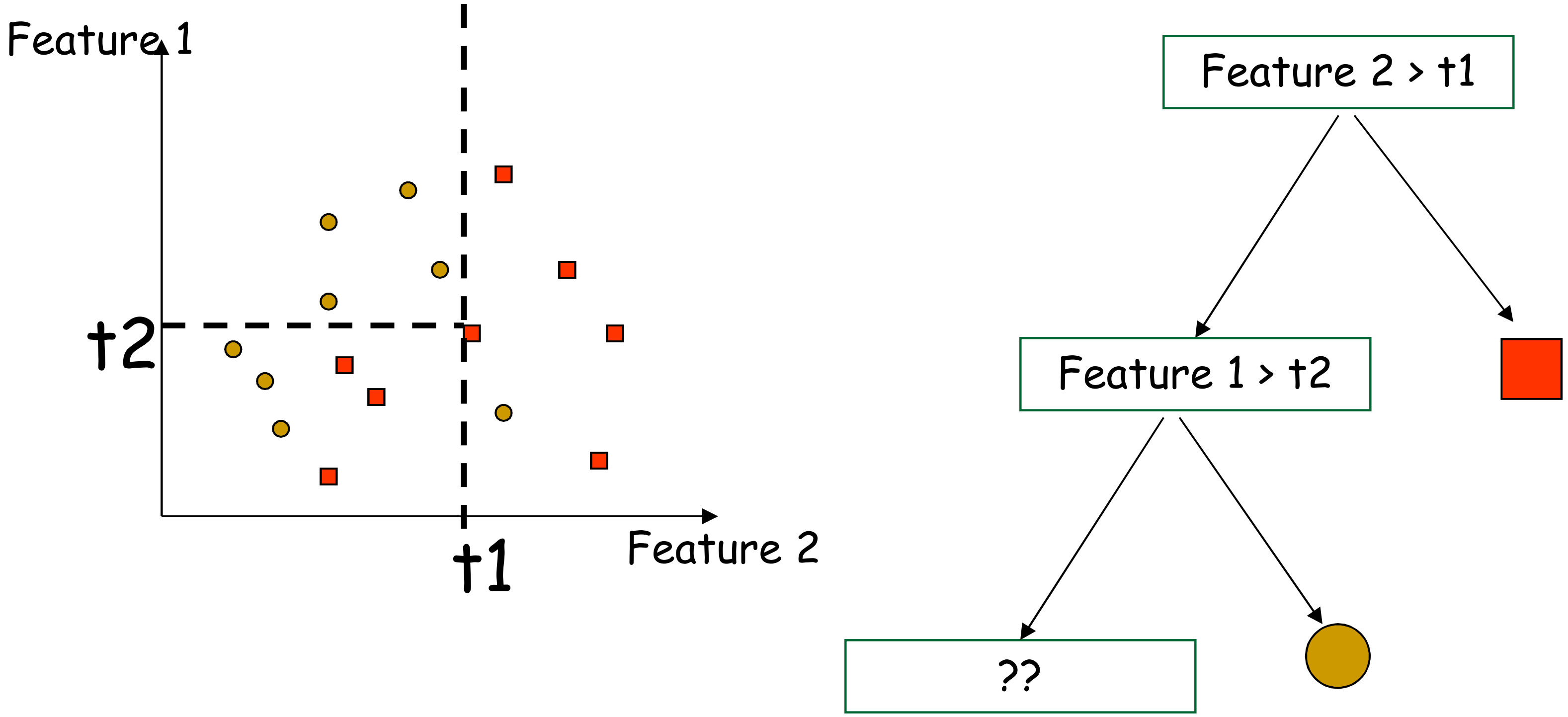


Decision Boundaries of Decision Trees

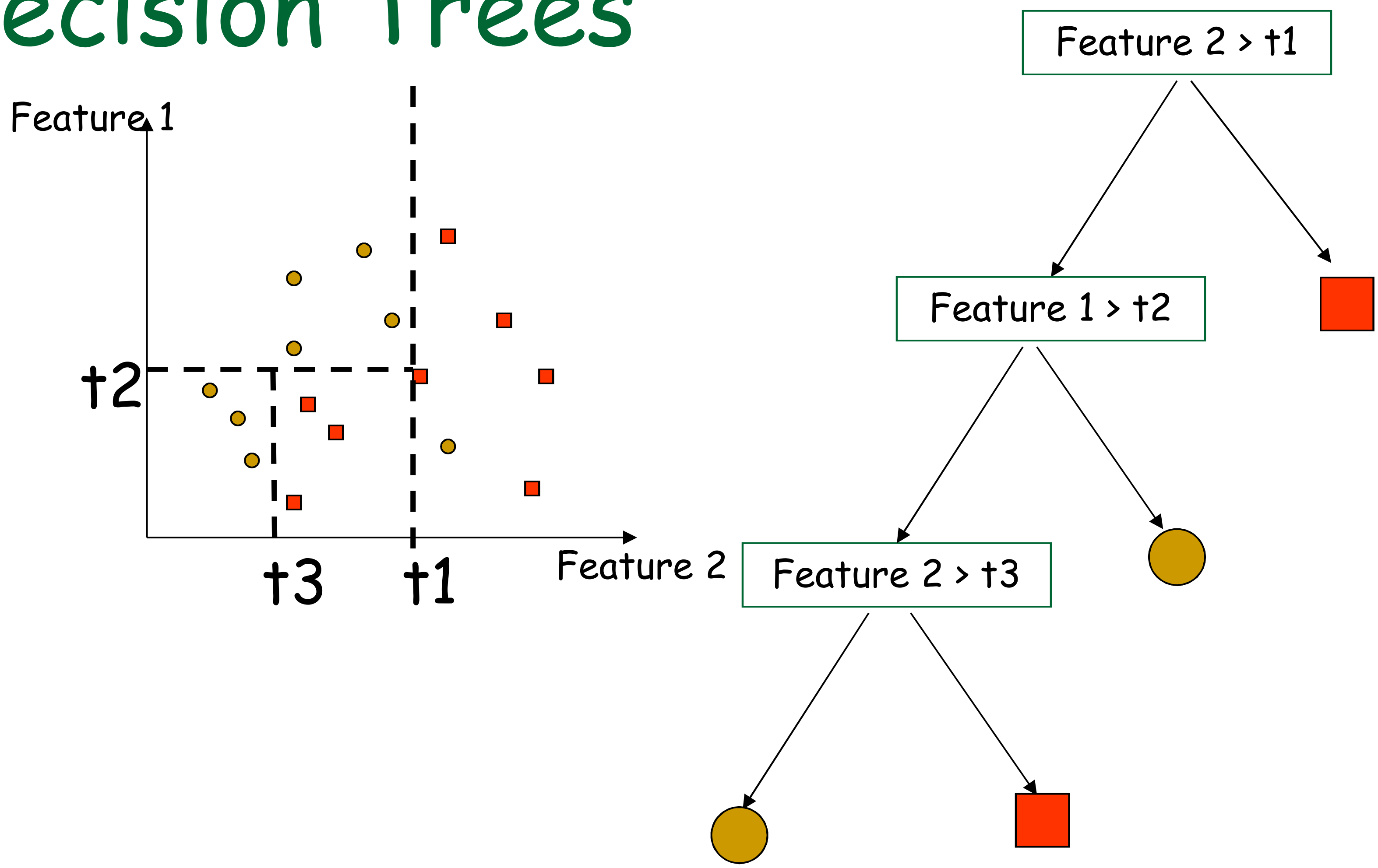




Decision Boundaries of Decision Trees



Decision Boundaries of Decision Trees



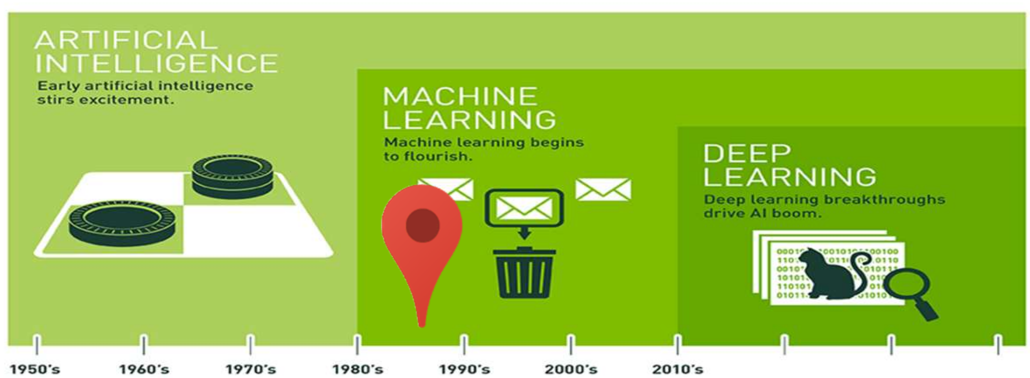
Applications of Decision Trees

- One of the most widely used learning methods in practice
  - Fast, simple, and traceable

- Can out-perform human experts in many problems

Today

1. Introduction to ML
2. Naïve Bayes Classifier
3. Decision Trees
4. (Evaluation
5. Unsupervised Learning)
6. Neural Networks



https://medium.com/machine-learning-for-humans/neural-networks-deep-learning-cdad8aeae49b

Evaluation of Learning Model

- How do you know if what you learned is correct?
- You run your classifier on a data set of unseen examples (that you did not use for training) for which you know the correct classification
- Split data set into 3 sub-sets
  1. Actual **training** set (~80%)
  2. **Validation** set (~20%)
  3. **Test** set

~80%

~20%

Standard Methodology

1. Collect a large set of examples (all with correct classifications)
2. Divide collection into training, validation and test set

Loop:

   3. Apply learning algorithm to training set to learn the parameters
   4. Measure performance with the validation set, and adjust hyper-parameters* to improve performance

5. Measure performance with the test set

- DO NOT LOOK AT THE TEST SET until step 5.

Parameters: basic values learned by the ML model. eg.

- for NB: prior & conditional probabilities
- for DTs: features to split
- for ANNs: weights

Hyper-parameters: parameters used to set up the ML model. eg.

- for NB: value of delta for smoothing,
- for DTs: pruning level
- for ANNs: nb of hidden layers, nb of nodes per layer…

Metrics

- accuracy
  - % of instances of the test set the algorithm correctly classifies
  - when all classes are equally important and represented
- Recall, Precision & F-measure
  - when one class is more important and the others

Accuracy

- % of instances of the test set the algorithm correctly classifies
- when all classes are equally important and represented
- problem:
  - when one class (eg. sick) is more important and the others
  - eg. when data set is unbalanced

	Target	*system 1*
	X1 sick	X1 ok
	X2 sick	X2 ok
	X3 sick	X3 ok
	X4 sick	X4 ok
	X5 sick	X5 ok
	X6 ok	X6 ok
	X7 ok	X7 ok
	…	…
	…	…
	X500 ok	X500 ok
Accuracy		495/500 = 99% !

Recall, Precision

- Recall: What proportion of the instances in the class of interest (eg. sick) are labelled correctly?
- Precision: What proportion of instances labeled with the class of interest (eg. sick) are actually correct?

Model says...	In reality, the instance is... in class C	Is not in class C
instance is in class C	True Positive (TP)	False Positive (FP)
instance is NOT in class C	False Negative (FN)	True Negative (TN)

$$\text{Precision} = \frac{TP}{TP+FP}$$

nb of instances that are in class C and that the model identified as class C

nb of instances that the model labelled as class C

$$\text{Recall} = \frac{TP}{TP+FN}$$

nb of instances that are in class C and that the model identified as class C

All instances that are in class C

Example

	Target	system 1	system 2	system 3
	X1 sick	X1 ok	X1 sick	X1 sick
	X2 sick	X2 ok	X2 ok	X2 sick
	X3 sick	X3 ok	X3 ok	X3 sick
	X4 sick	X4 ok	X4 sick	X4 sick
	X5 sick	X5 ok	X5 ok	X5 sick
	X6 ok	X6 ok	X6 ok	X6 sick
	X7 ok	X7 ok	X7 ok	X7 sick
	… ok	…	… ok	… ok
	… ok	…	… ok	… ok
	X500 ok	X500 ok	X500 ok	X500 ok
Accuracy		495/500 = 99% !	498/500 = 99.6%	498/500 = 99.6%
Precision		0/0	3/3 = 100%	5/7 = 71%
Recall		0/5 = 0%	3/5 = 60%	5/5 = 100%

Which system is better?

Evaluation: A Single Value Measure

- cannot take mean of P&R
  - if R = 50% P = 50% M = 50%
  - if R = 100% P = 10% M = 55% (not fair)
- take harmonic mean

$$HM = \frac{2}{\frac{1}{R} + \frac{1}{P}}$$

HM is high only when both P&R are high

if R = 50% and P = 50% HM = 50%

if R = 100% and P = 10% HM = 18.2%

- take weighted harmonic mean

w_r: weight of R w_p: weight of P $a = 1/w_r$ $b = 1/w_p$

$$WHM = \frac{a+b}{\left(\frac{a}{R} + \frac{b}{P}\right)} = \frac{(a+b)/b}{\left(\frac{a}{Rb} + \frac{b}{Pb}\right)} = \frac{a/b + 1}{\left(\frac{a}{bR} + \frac{1}{P}\right)}$$

  - let $\beta^2 = a/b$

$$WHM = \frac{\beta^2 + 1}{\left(\frac{\beta^2}{R} + \frac{1}{P}\right)} = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

… which is called the F-measure

Evaluation: the F-measure

- A weighted combination of precision and recall

$$F = \frac{(\beta^2 + 1)PR}{(\beta^2 P + R)}$$

- β represents the relative importance of precision and recall
  - when $\beta = 1$, precision & recall have same importance
  - when $\beta > 1$, precision is favored
  - when $\beta < 1$, recall is favored

Example

	Target	system 1	system 2	system 3
	X1 sick	X1 ok	X1 sick	X1 sick
	X2 sick	X2 ok	X2 ok	X2 sick
	X3 sick	X3 ok	X3 ok	X3 sick
	X4 sick	X4 ok	X4 sick	X4 sick
	X5 sick	X5 ok	X5 ok	X5 sick
	X6 ok	X6 ok	X6 ok	X6 sick
	X7 ok	X7 ok	X7 ok	X7 sick
	… ok	…	… ok	… ok
	… ok	…	… ok	… ok
	X500 ok	X500 ok	X500 ok	X500 ok
Accuracy		495/500 = 99% !	498/500 = 99.6%	498/500 = 99.6%
Precision		0/0	3/3 = 100%	5/7 = 71%
Recall		0/5 = 0%	3/5 = 60%	5/5 = 100%
F1 -measure (B=1)		Undef	2PR/P+R = 75%	2PR/P+R = 83%

Error Analysis

- Where did the learner go wrong ?
- Use a confusion matrix / contingency table

correct class (that should have been assigned)	classes assigned by the model							
	C1	**C2**	**C3**	**C4**	**C5**	**C6**	...	**Total**
C1	94	3	0	0	3	0		100%
C2	0	93	3	4	0	0		100%
C3	0	1	94	2	1	2		100%
C4	0	1	3	94	2	0		100%
C5	0	0	3	2	92	3		100%
C6	0	0	5	0	10	85		100%
...								

P, R and F for Multiclass Classification

- previous P, R and F are ok when 1 particular class interests us (eg. sick)
- What if all classes interest us?
- then
  - compute *per-class* P, R, F
  - to have a single measure, combine per-class F-measures via
    - macro F-measure, or
    - weighted-average F-measure

per-class Precision & per-class Recall

		correct		
		Cat	Dog	Fish
predicted	Cat	4	6	3
	Dog	1	2	0
	Fish	1	2	6

nb of samples (not %)

- precision of class Cat: 4/ (4+6+3) = 30.8%
- precision of class Dog: 2 / (1+2+0) = 66.7%
- precision of class Fish: 6/(1+2+6) = 66.7%

- recall of class Cat: 4/(4+1+1) = 66.7%
- recall of class Dog: 2/(2+6+2) = 20%
- recall of class Fish: 6/(3+0+6) = 66.7%

per-class F1-measure

	Precision	Recall	F1
Cat	30.8%	66.7%	42.1%
Dog	66.7%	20.0%	30.8%
Fish	66.7%	66.7%	66.7%

F1 = 2PR/P+R

- F1 of class Cat: (2 x .308 x .667) / (.308 + .667) = 0.421
- F1 of class Dog: (2 x .667 x .200) / (.667 + .200) = 0.308
- F1 of class Fish: (2 x .667 x .667) / (.667 + .667) = 0.667

macro and weighted-average measures

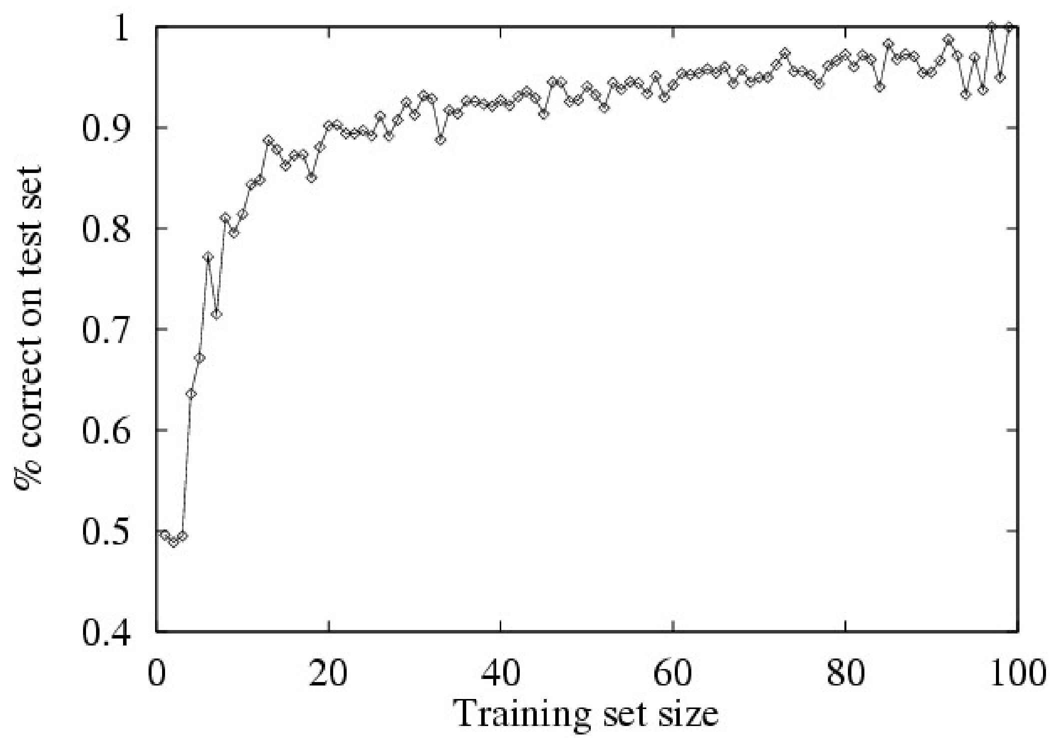
macro precision, macro recall, macro F1

weighted-averaged precision, recall & F1

	Precision	Recall	F1
Cat	30.8%	66.7%	42.1%
Dog	66.7%	20.0%	30.8%
Fish	66.7%	66.7%	66.7%
average	(30.8+66.7+66.7) / 3 = 54.7%	(66.7 + 20.0 + 66.7) / 3 = 51.1%	(42.1+30.8+66.7) = 46.5%
weighted-average	6x30.8 // 6 cat +10x66.7 // 10 dog +9x66.7 // 9 hen / (6+10+9) // 25 samples = 58.1%	(6x66.7 +10x20.0 +6x66.7) / 25 = 48.0%	(6x42.1 +10x30.8 +6x66.7) / 25 = 46.4%

- to combine measures into a single one, we can:
  - take simple average ➔ macro precision, macro recall, macro F1
  - take weighted average ie. weight the average based on the nb of samples from each class ➔ weighted averaged precision, ➔ weighted averaged recall, weighted averaged F1

A Learning Curve



- Size of training set
  - the more, the better
  - but after a while, not much improvement…

source: Mitchell (1997)

Some Words on Training

- In all types of learning… watch out for:
  - Noisy input
  - Overfitting/underfitting the training data

Noisy Input

- In all types of learning… watch out for:
  - Noisy Input:
    - Two examples have the same feature-value pairs, but different outputs

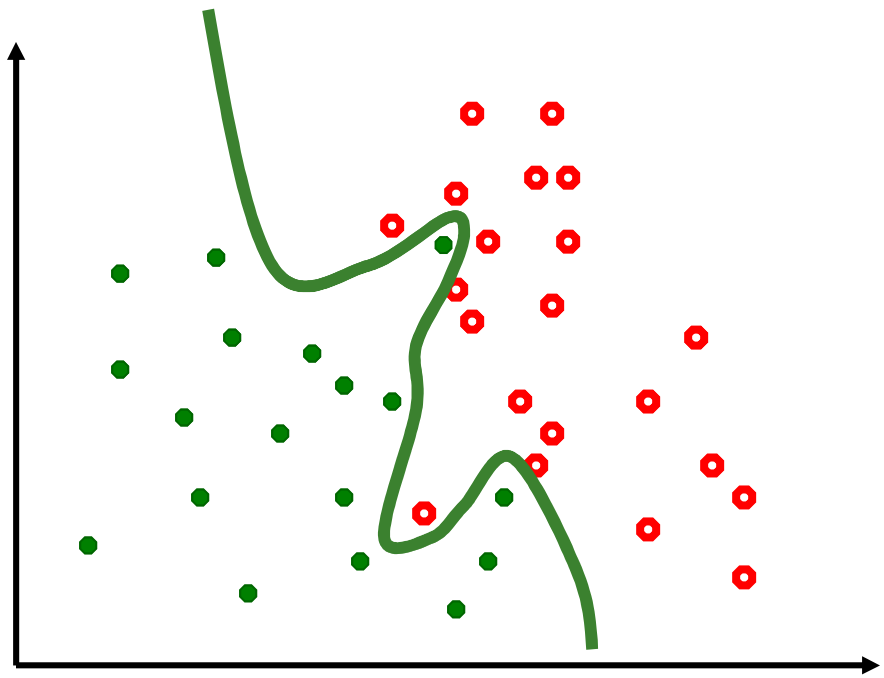
Size	Color	Shape	Output
Big	Red	Circle	+
Big	Red	Circle	-

    - Some values of features are incorrect or missing (ex. errors in the data acquisition)
    - Some relevant attributes are not taken into account in the data set

Overfitting

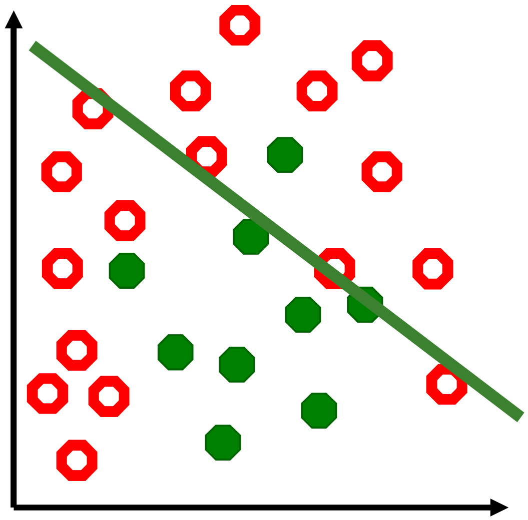
- If a large number of irrelevant features are there, we may find meaningless regularities in the data that are particular to the training data but irrelevant to the problem.
- Complicated boundaries *overfit* the data
- they are too tuned to the particular training data at hand
- They do not *generalize* well to the new data
- Extreme case: "rote learning"

- Training error is low
- Testing error is high



Underfitting

- We can also underfit data, i.e. use too simple decision boundary
- Model is not expressive enough (not enough features)
- There is no way to fit a linear decision boundary so that the training examples are well separated



- Training error is high
- Testing error is high

Cross-validation

- K-fold cross-validation
  - run k experiments, each time you test on 1/k of the data, and train on the rest
  - than you average the results
- ex: 10-fold cross validation
  1. Collect a large set of examples (all with correct classifications)
  2. Divide collection into two disjoint sets: training (90%) and test (10% = 1/k)
  3. Apply learning algorithm to training set
  4. Measure performance with the test set
  5. Repeat steps 2-4, with the 10 different portions
  6. Average the results of the 10 experiments

exp1:	train									test
exp2:	train								test	train
exp3:	train							test	train	
…	…									

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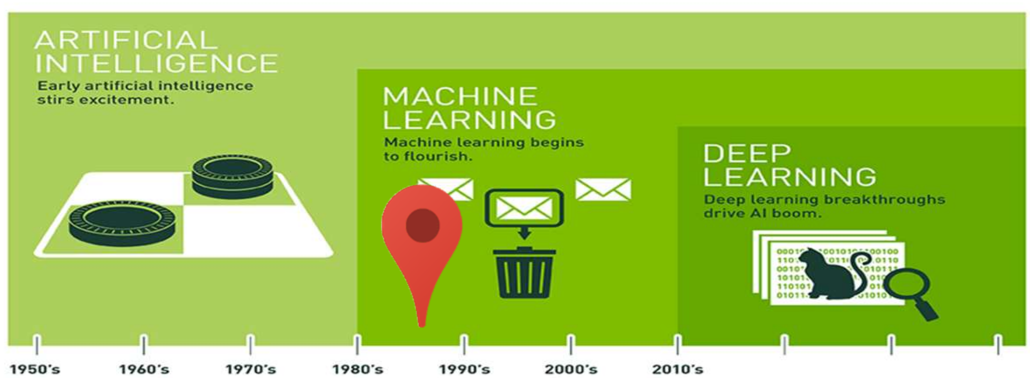
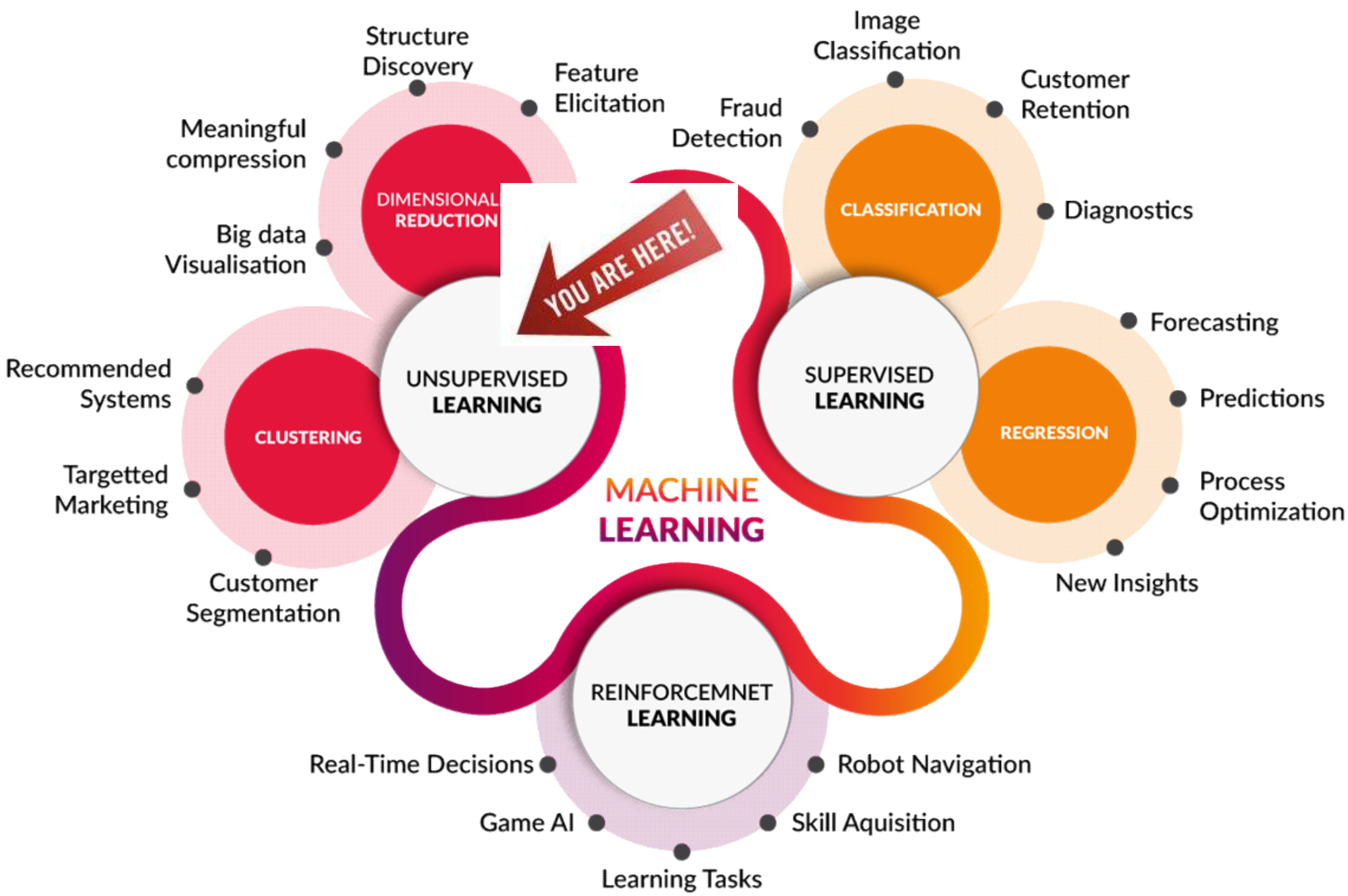


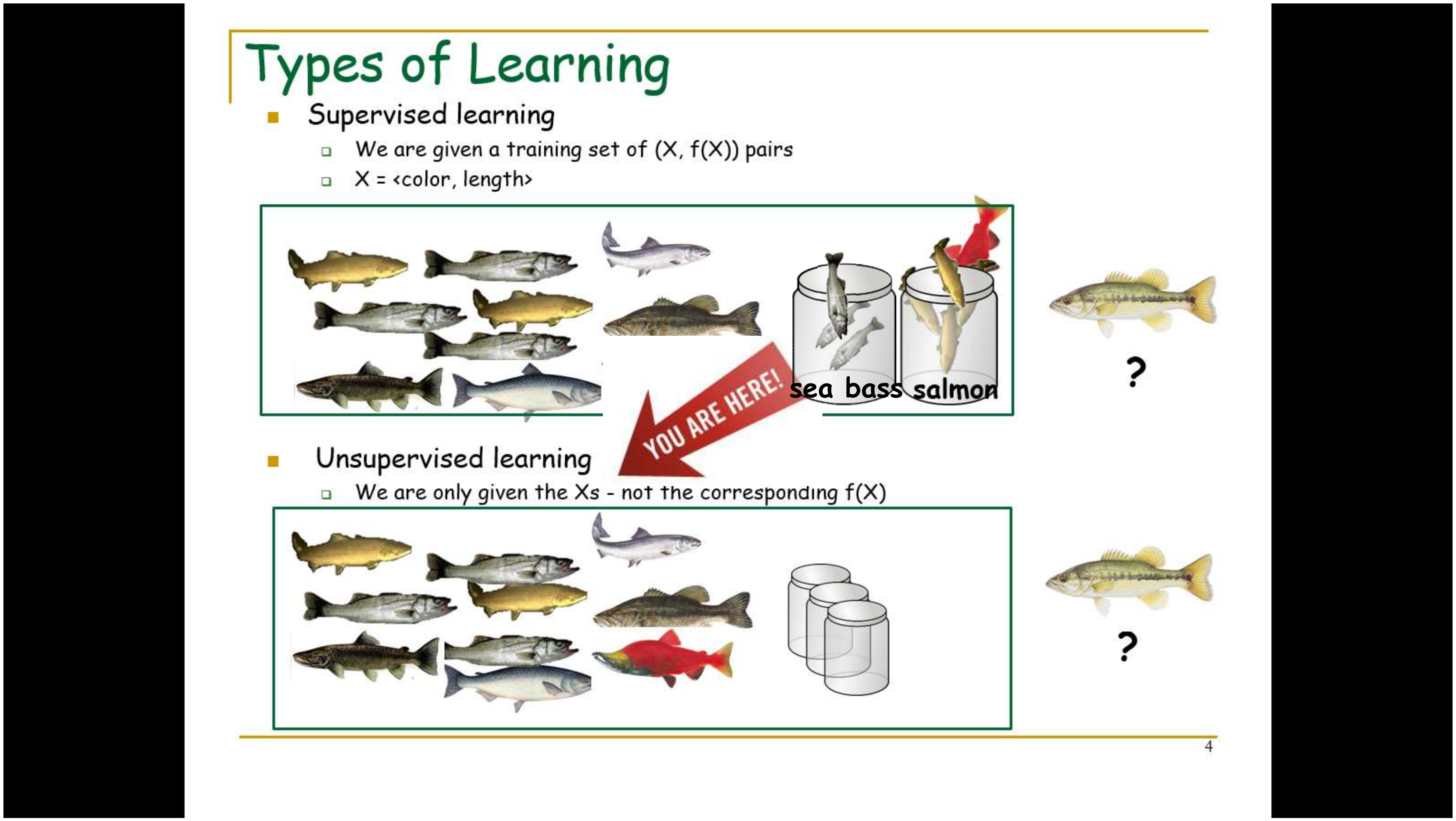
https://medium.com/machine-learning-for-humans/neural-networks-deep-learning-cdad8aeae49b

Types of Machine Learning



http://www.cognub.com/index.php/cognitive-platform/

Remember this slide?



Unsupervised Learning

- Learn without labeled examples
  - i.e. X is given, but not f(X)

small nose	big teeth	small eyes	moustache	f(X) = ?

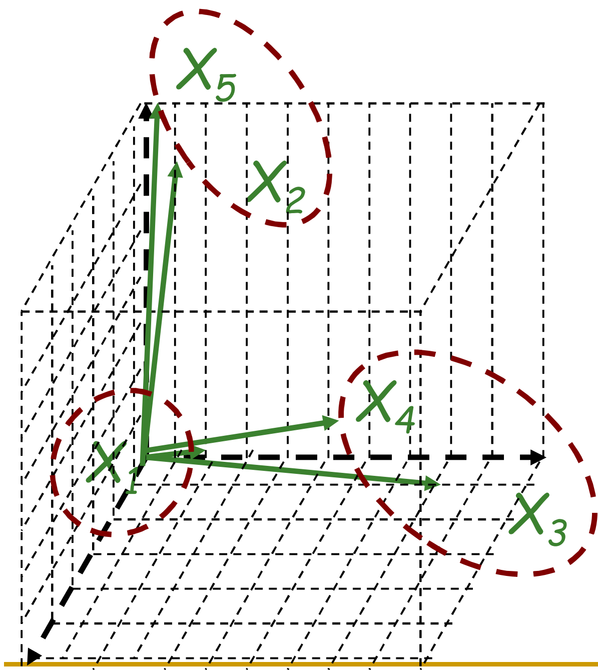
- Without a f(X), you can't really identify/label a test instance

- But you can:
  - Cluster/group the features of the test data into a number of groups
  - Discriminate between these groups without actually labeling them

Clustering

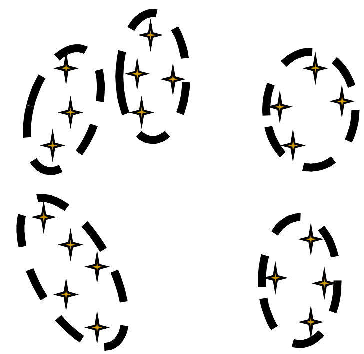
- Represent each instance as a vector <a_1, a_2, a_3,…, a_n>
- Each vector can be visually represented in a n dimensional space

	a_1	a_2	a_3	Output
X_1	1	0	0	?
X_2	1	6	0	?
X_3	8	0	1	?
X_4	6	1	0	?
X_5	1	7	1	?



Clustering

- Clustering algorithm



  - Represent test instances on a n dimensional space
  - Partition them into regions of high density
    - How? … many algorithms (ex. k-means)
  - Compute the centroïd of each region as the average of data points in the cluster

k-means Clustering

- User selects how many clusters they want… (the value of k)

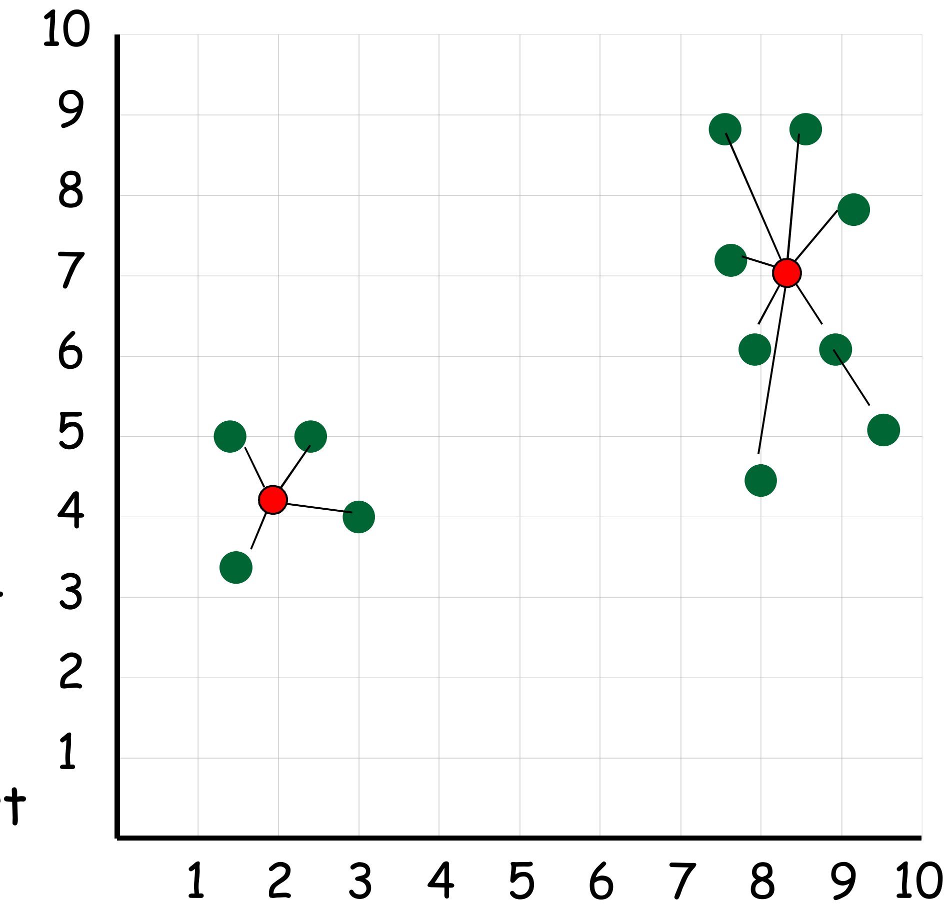
1. Place k points into the space (ex. at random). These points represent initial group centroïds.
2. Assign each data point x_n to the nearest centroïd.
3. When all data points have been assigned, recalculate the positions of the K centroïds as the average of the cluster
4. Repeat Steps 2 and 3 until none of the data instances change group.

Euclidean Distance

- To find the nearest centroïd…
- a possible metric is the Euclidean distance
- distance between 2 pts
  $p = (p_1, p_2, \ldots., p_n)$
  $q = (q_1, q_2, \ldots., q_n)$

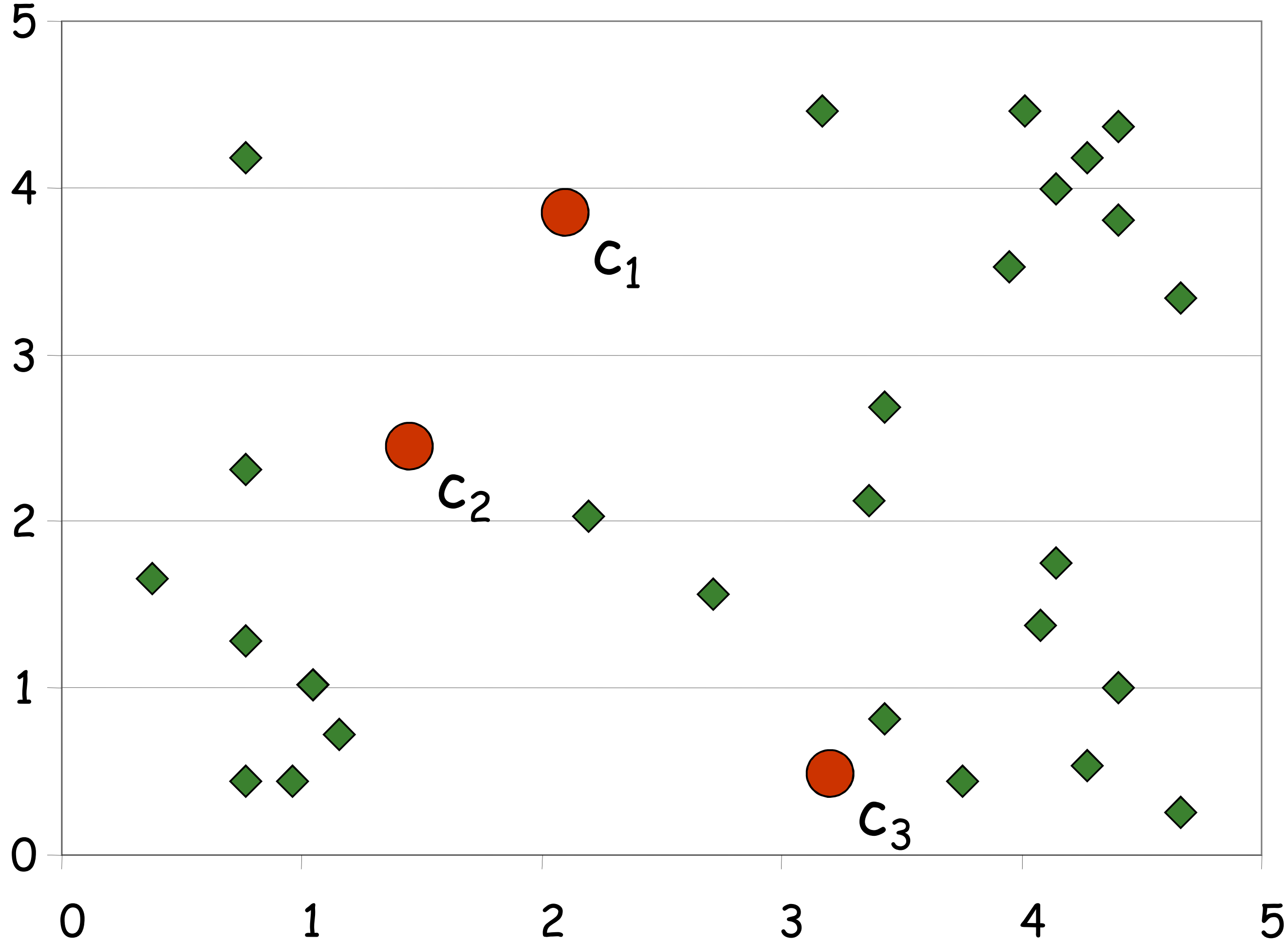
$$d = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

- where to assign a data point x?
- For all k clusters, chose the one where x has the smallest distance



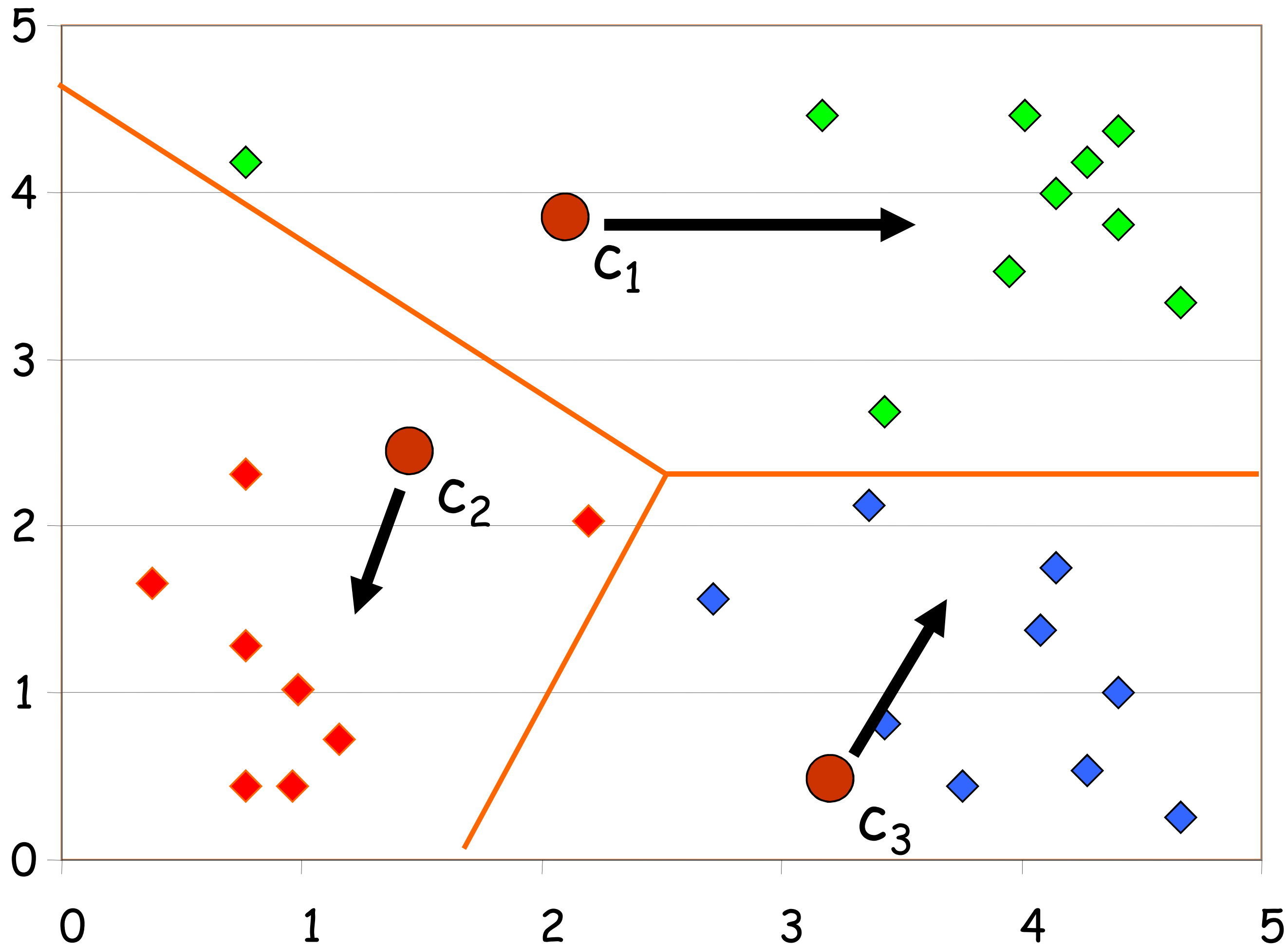
Example (in 2-D… i.e. 2 features)

initial 3 centroïds (ex. at random)



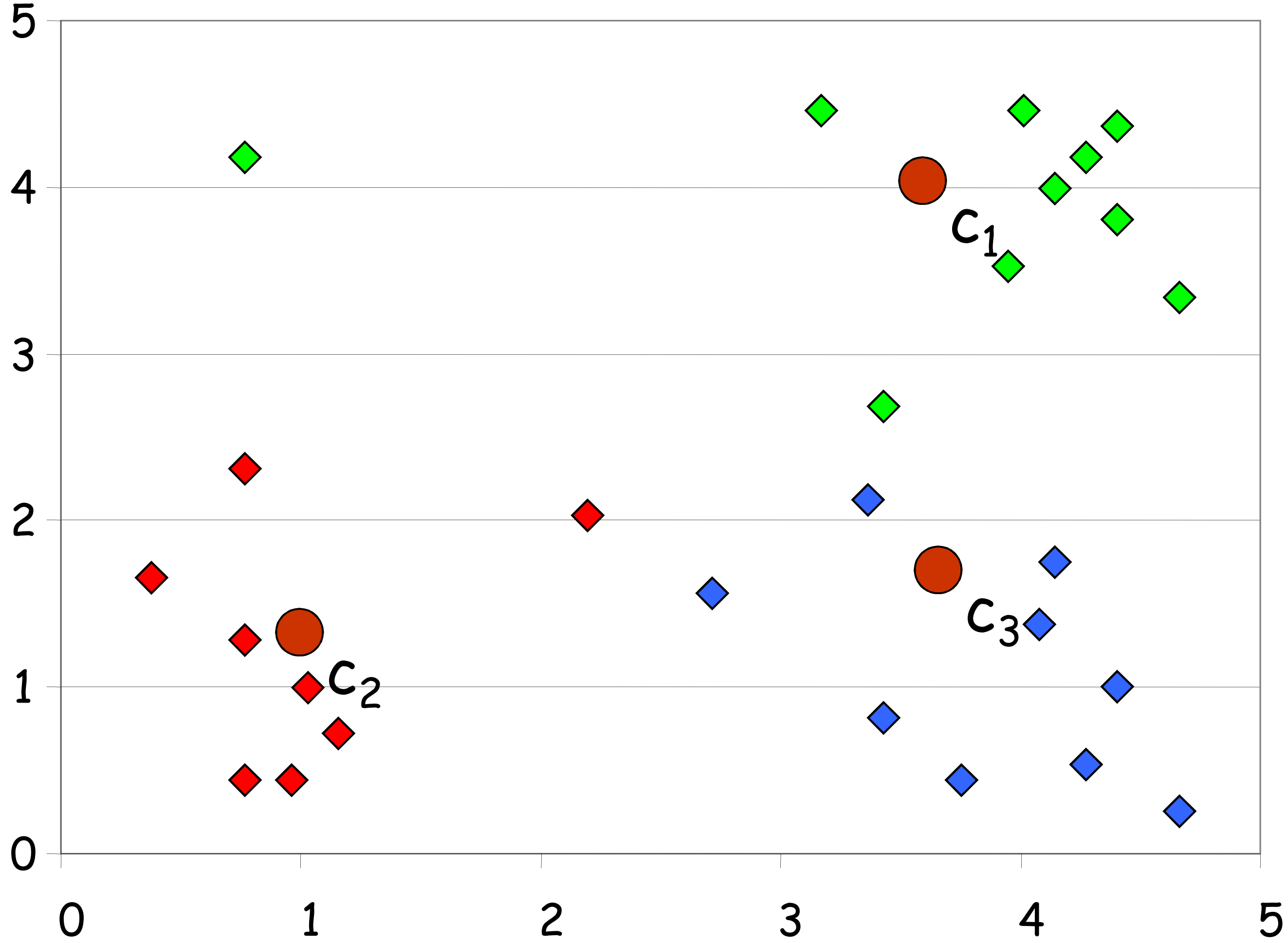
Example

partition data points to closest centroïd



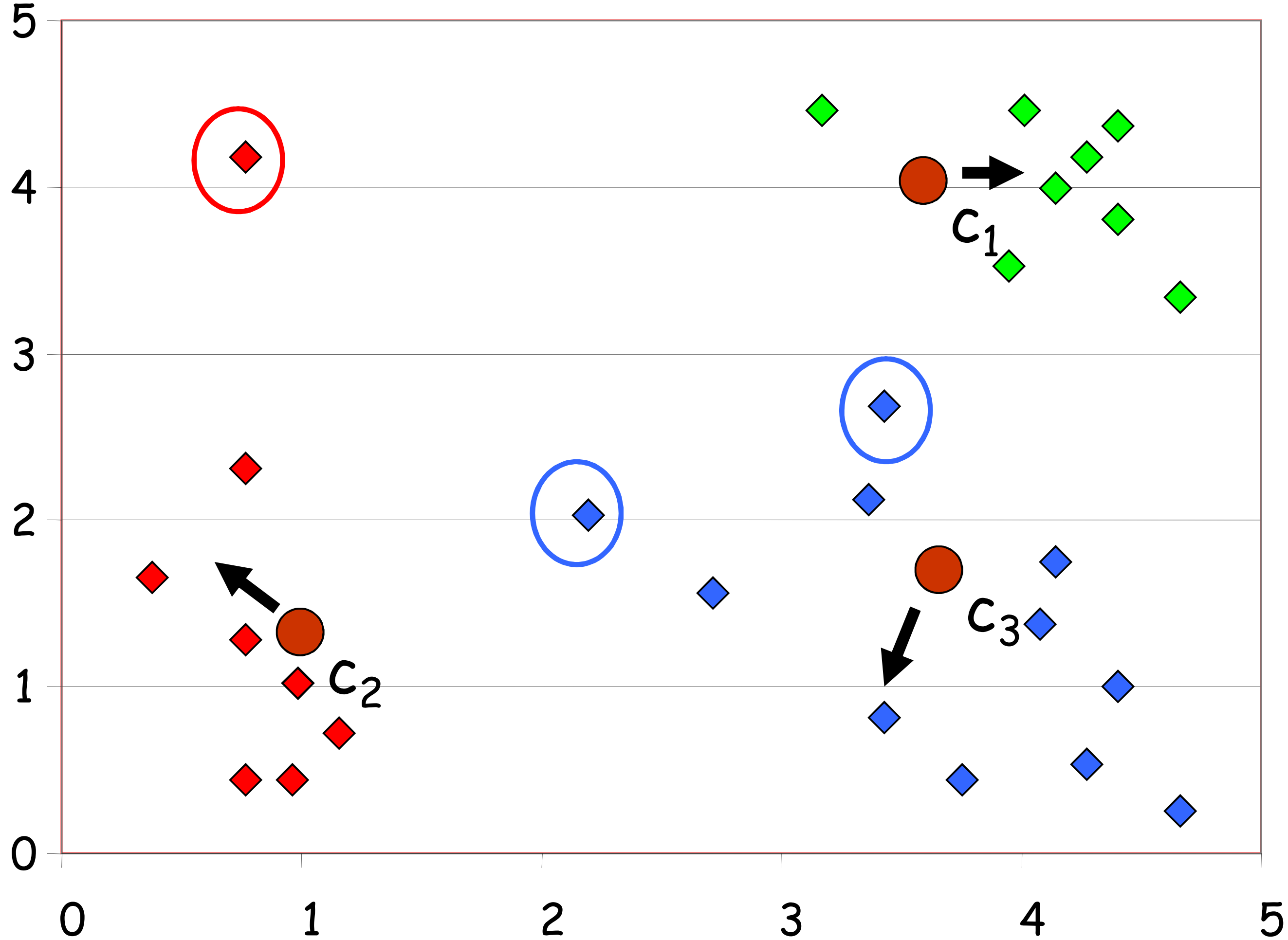
Example

re-compute new centroïds

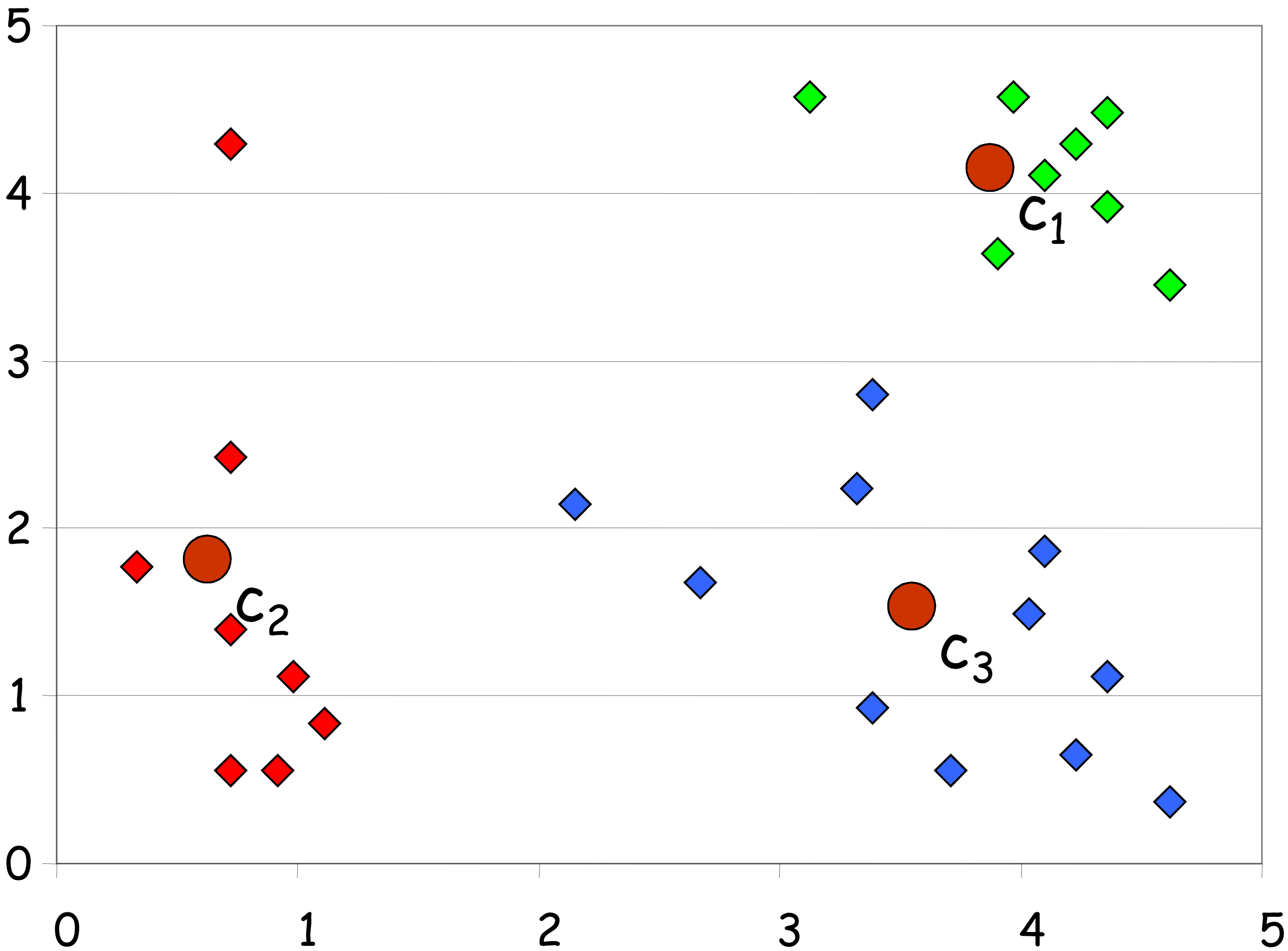


Example

re-assign data points to new closest centroïds



Example



Notes on k-means

- converges very fast!
- BUT:
  - very sensitive to initial choice of centroids
    - many find useless clusters…
  - user must set initial k
    - not easy to do…

- many other clustering algorithms…

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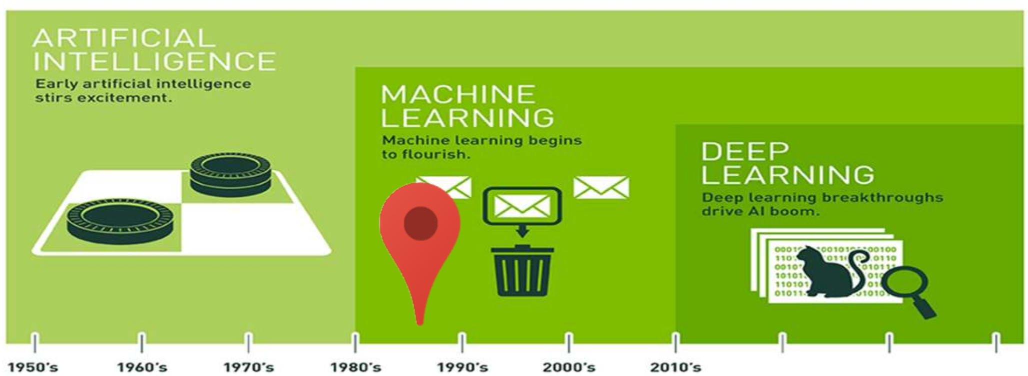

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