#### INTELLIGENZA ARTIFICIALE

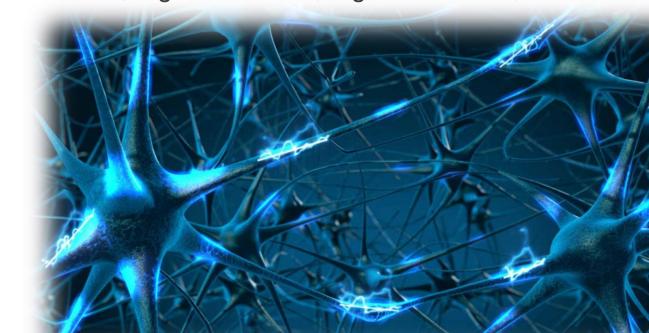
#### APPRENDIMENTO AUTOMATICO DA ESEMPI

Corsi di Laurea in Informatica, Ing. Gestionale, Ing. Informatica,

Ing. di Internet (a.a. 2023-2024)

Roberto Basili

(\*) dalle *slides* di S. Russel



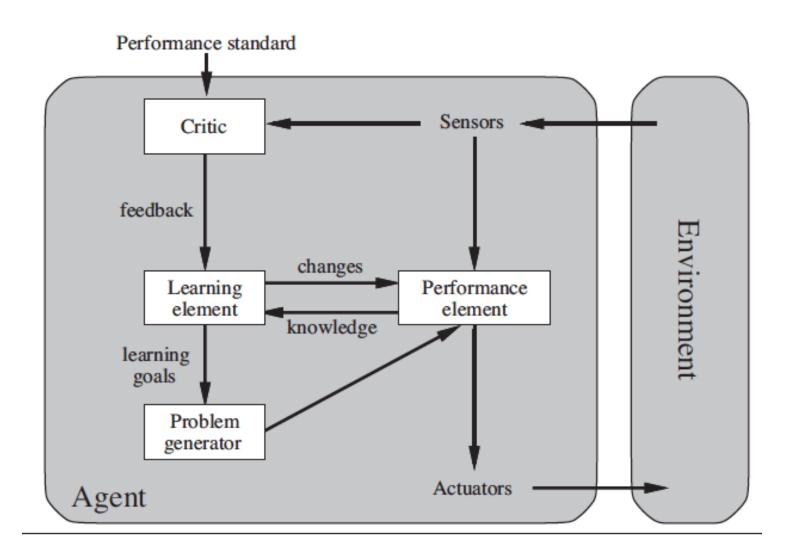
#### Overview (AIMA chpt. 18.1-18.4)

- Agents & machine learning
- Learning from examples:
  - Complexity and Expressiveness
  - The definition of model selection
- Performance Evaluation
- Learning methodology: design, experiment/ evaluation and model selection
  - Cross validation
- An example: Decision Tree learning
  - Recursive search among Boolean formulas
  - Attribute Selection in DT: Information Gain

## Introduction to machine learning

- Introduction to machine learning
  - When appropriate and when not appropriate
  - Task definition
  - Learning methodology: design, experiment, evaluation
  - Learning issues: representing hypothesis
  - Learning paradigms
    - Supervised learning
    - Unsupervised learning
    - Reinforcement learning

# AIMA learning architecture



## Machine learning: definition

- A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E [Mitchell]
- Problem definition for a learning agent
  - Task T
  - Performance measure P
  - Experience E

# Designing a learning system

- 1. Choosing the training experience
  - Examples of best moves, games outcome ...
- 2. Choosing the target function
  - board-move, board-value, ...
- 3. Choosing a representation for the target function
  - linear function with weights (hypothesis space)
- 4. Choosing a learning algorithm for approximating the target function
  - A method for parameter estimation

# Inductive learning

Simplest form: learn a function from examples

f is the target function

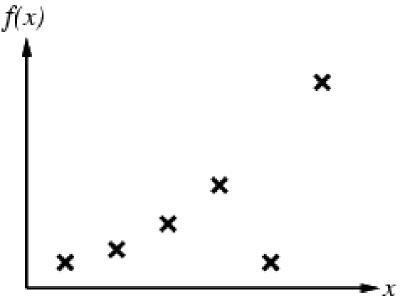
An example is a pair (x, f(x))

Problem: find a hypothesis h such that  $h \approx f$  given a training set of examples

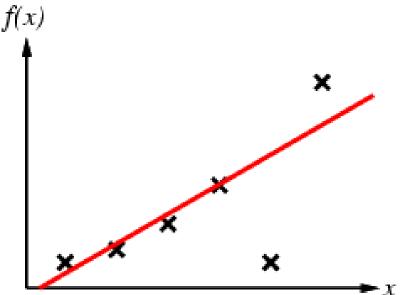
(This is a highly simplified model of real learning:

- Ignores prior knowledge
- Assumes examples are given)

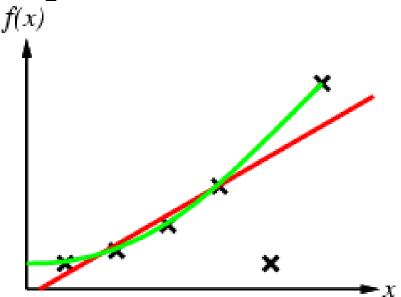
Construct/adjust h to agree with f on training set
 (h is consistent if it agrees with f on all examples)



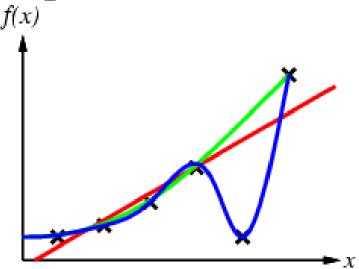
Construct/adjust h to agree with f on training set
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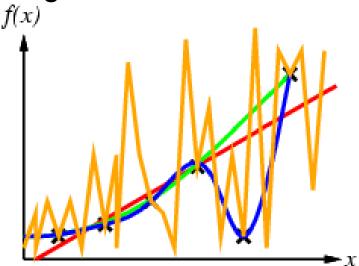
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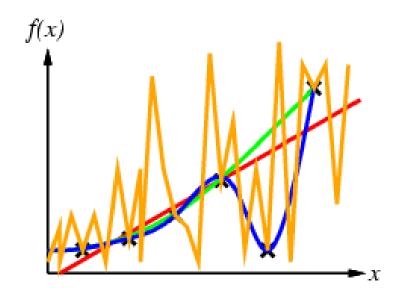
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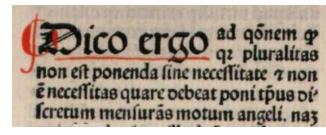




Construct/adjust h to agree with f on training set
 (h is consistent if it agrees with f on all examples)

#### E.g., curve fitting:

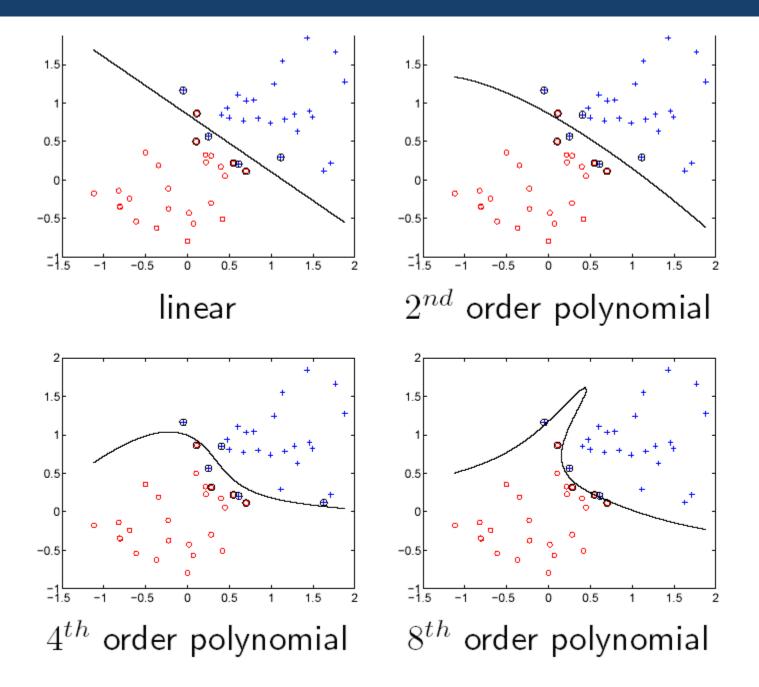




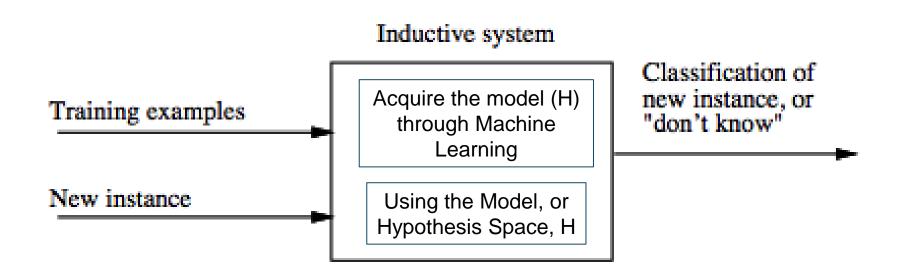
novacula Occami

Ockham's razor:

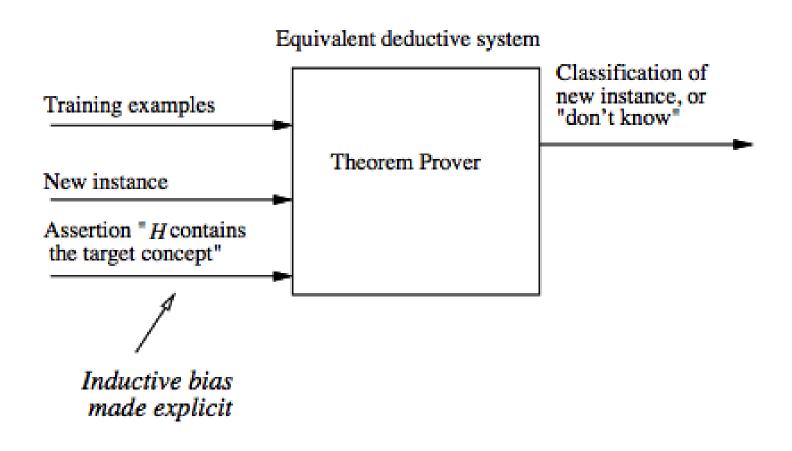
prefer the simplest hypothesis consistent with data



## Inductive system



## Equivalent deductive system



# Learning decision trees

Problem: decide whether to wait for a table at a restaurant, based on the following attributes:

- 1. Alternate: is there an alternative restaurant nearby?
- 2. Bar: is there a comfortable bar area to wait in?
- 3. Fri/Sat: is today Friday or Saturday?
- 4. Hungry: are we hungry?
- 5. Patrons: number of people in the restaurant (None, Some, Full)
- 6. Price: price range (\$, \$\$, \$\$\$)
- 7. Raining: is it raining outside?
- 8. Reservation: have we made a reservation?
- 9. Type: kind of restaurant (French, Italian, Thai, Burger)
- 10. WaitEstimate: estimated waiting time (0-10, 10-30, 30-60, >60)

### Attribute-based representations

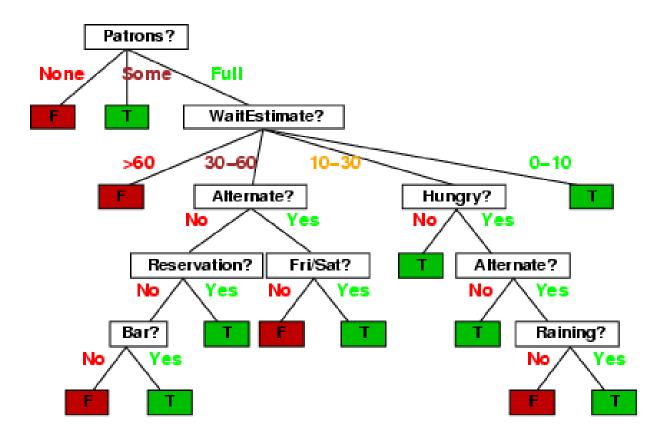
- Examples described by attribute values (Boolean, discrete, continuous)
- E.g., situations where I will/won't wait for a table:

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

Classification of examples is positive (T) or negative (F)

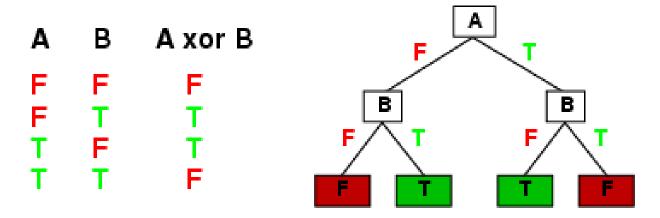
#### **Decision trees**

- One possible representation for hypotheses
- E.g., here is the "true" tree for deciding whether to wait:



## Expressiveness

- Decision trees can express any function of the input attributes.
- E.g., for Boolean functions, truth table row → path to leaf:



- Trivially, there is a consistent decision tree for any training set with one path to leaf for each example (unless f nondeterministic in x) but it probably won't generalize to new examples
- Prefer to find more compact decision trees

## Hypothesis spaces

How many distinct decision trees with *n* Boolean attributes?

- = number of Boolean functions
- = number of distinct truth tables with  $2^n$  rows =  $2^{2^n}$
- E.g., with 6 Boolean attributes, there are 18,446,744,073,709,551,616 trees

# Hypothesis spaces

#### How many distinct decision trees with *n* Boolean attributes?

- = number of Boolean functions
- = number of distinct truth tables with  $2^n$  rows =  $2^{2^n}$
- E.g., with 6 Boolean attributes, there are 18,446,744,073,709,551,616 trees

#### How many purely conjunctive hypotheses (e.g., *Hungry* ∧ ¬*Rain*)?

- Each attribute can be in (positive), in (negative), or out
  - ⇒ 3<sup>n</sup> distinct conjunctive hypotheses
- More expressive hypothesis space
  - increases chance that target function can be expressed
  - increases number of hypotheses consistent with training set
    - ⇒ may get worse predictions

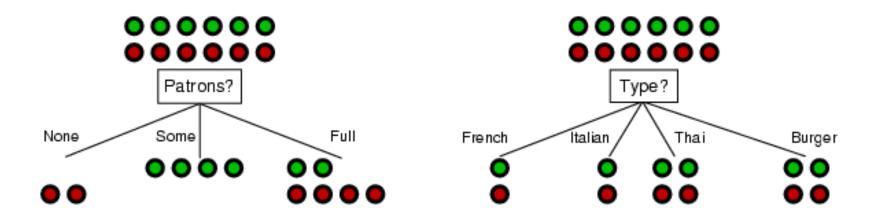
# Decision tree learning

- Aim: find a small tree consistent with the training examples
- Idea: (recursively) choose "most significant" attribute as root of (sub)tree

```
function DTL(examples, attributes, default) returns a decision tree
   if examples is empty then return default
   else if all examples have the same classification then return the classification
   else if attributes is empty then return Mode (examples)
   else
        best \leftarrow \text{Choose-Attributes}, examples)
        tree \leftarrow a new decision tree with root test best
       for each value v_i of best do
            examples_i \leftarrow \{elements of examples with best = v_i\}
            subtree \leftarrow DTL(examples_i, attributes - best, Mode(examples))
            add a branch to tree with label v_i and subtree subtree
       return tree
```

## Choosing an attribute

 Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"



Patrons? is a better choice

# Using information theory

To implement Choose-Attribute in the DTL algorithm

Information Content (Entropy):

$$I(P(v_1), ..., P(v_n)) = \sum_{i=1}^{n} -P(v_i) \log_2 P(v_i)$$

 For a training set containing p positive examples and n negative examples:

$$I(\frac{p}{p+n}, \frac{n}{p+n}) = -\frac{p}{p+n} \log_2 \frac{p}{p+n} - \frac{n}{p+n} \log_2 \frac{n}{p+n}$$

# Information gain

 A chosen attribute A divides the training set E into subsets E<sub>1</sub>, ..., E<sub>v</sub> according to their values for A, where A has v distinct values.

remainder(A) = 
$$\sum_{i=1}^{v} \frac{p_i + n_i}{p + n} I(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i})$$

Information Gain (IG) or reduction in entropy from the attribute test:

$$IG(A) = I(\frac{p}{p+n}, \frac{n}{p+n}) - remainder(A)$$

Choose the attribute with the largest IG

# Information gain

For the training set, p = n = 6, I(6/12, 6/12) = 1 bit

Consider the attributes *Patrons* and *Type* (and others too):

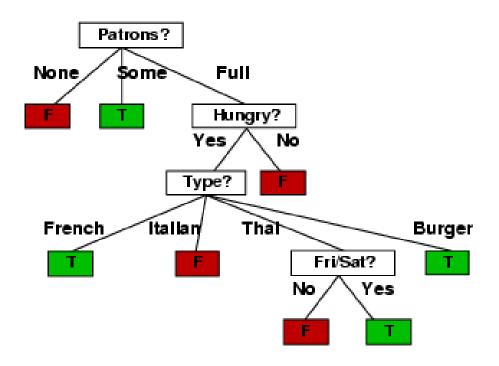
$$IG(Patrons) = 1 - \left[\frac{2}{12}I(0,1) + \frac{4}{12}I(1,0) + \frac{6}{12}I(\frac{2}{6}, \frac{4}{6})\right] = .0541 \text{ bits}$$

$$IG(Type) = 1 - \left[\frac{2}{12}I(\frac{1}{2}, \frac{1}{2}) + \frac{2}{12}I(\frac{1}{2}, \frac{1}{2}) + \frac{4}{12}I(\frac{2}{4}, \frac{2}{4}) + \frac{4}{12}I(\frac{2}{4}, \frac{2}{4})\right] = 0 \text{ bits}$$

Patrons has the highest IG of all attributes and so is chosen by the DTL algorithm as the root

### Example contd.

Decision tree learned from the 12 examples:

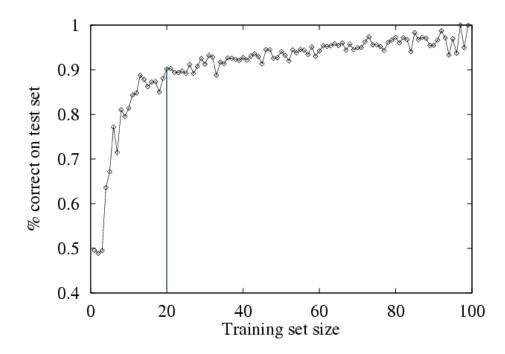


 Substantially simpler than "true" tree---a more complex hypothesis isn't justified by small amount of data

#### Performance measurement

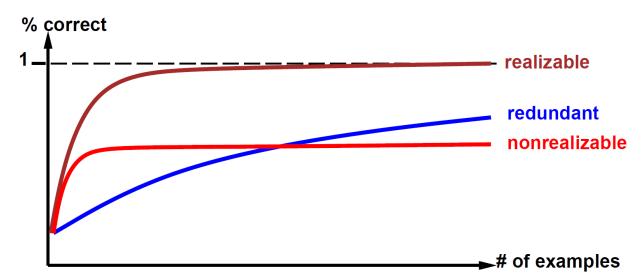
- How do we know that  $h \approx f$ ?
  - Use theorems of computational/statistical learning theory
  - Try h on a new test set of examples
     (use same distribution over example space as training set)

Learning curve = % correct on test set as a function of training set size

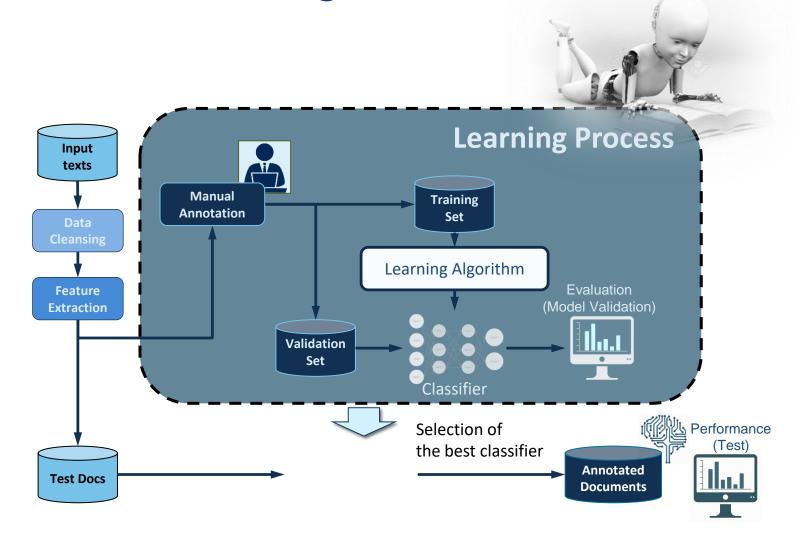


# Performance measurements (2)

- Learnability depends on
  - realizable kind of performances vs.
  - ... non-realizable ones
  - Non-realizability depends on
    - Missing attributes
    - Limitation on the hypothesis space (e.g. non expressive functions)
  - Redundant expressiveness is related to cases where a a largenumber of irrelevant attributes are used



Machine Learning workflow



### Evaluation of a ML system

- Performance Evaluation Metrics
  - Classifier Evaluation Metrics

Tuning and Evaluation Methods

#### Classifier Evaluation: Confusion Matrix

		PREDICTED VALUE			
ш		Class A	Class B	Class C	
VALUI	Class A	38	12	0	
ACTUAL VALUE	Class B	5	43	2	
AC	Class C	6	0	44	

$$accuracy = \frac{\#correct\ classifications}{\#classifications} = \frac{38 + 43 + 44}{150} = 83.33\%$$
 
$$error\ rate = \frac{\#incorrect\ classifications}{\#classifications} = \frac{12 + 5 + 2 + 6}{150} = 16.67\%$$

#### Evaluation with skewed data

 Accuracy is not a suitable metric for task with imbalanced classes (for instance a spam detector)

			PREDICTED VALUE		
			Spam	Non-Spam	
Very bad	TUAL	Spam	Q	10	
performance on the Spam class.		Non-Spam	0	9990	

the Spam class, that is the target of the classifier!! ... nonetheless ...

$$accuracy = \frac{\#correct\ classifications}{\#classifications} = \frac{9990}{10000} = 99.9\%$$

# Single Class Metrics

		PREDICTED VALUE			
		Class C	Not Class C		
ACTUAL VALUE	Class C	<b>TP</b> True Positive	<b>FN</b> False Negative		
	Not Class C	<b>FP</b> False Positive	<b>TN</b> True Negative		

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

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

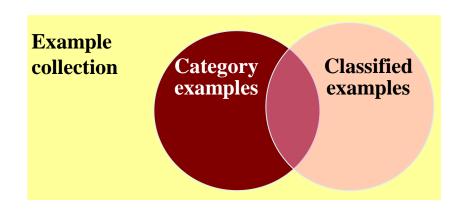
$$F1 = \frac{2 \times precision \times recall}{precision + recall}$$

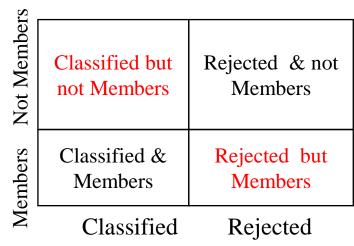
what percentage of instances the classifier labeled as positive are actually positive?

what percentage of positive instances did the classifier label as positive?

F-measure is the harmonic mean of precision and recall

#### Class-based evaluation

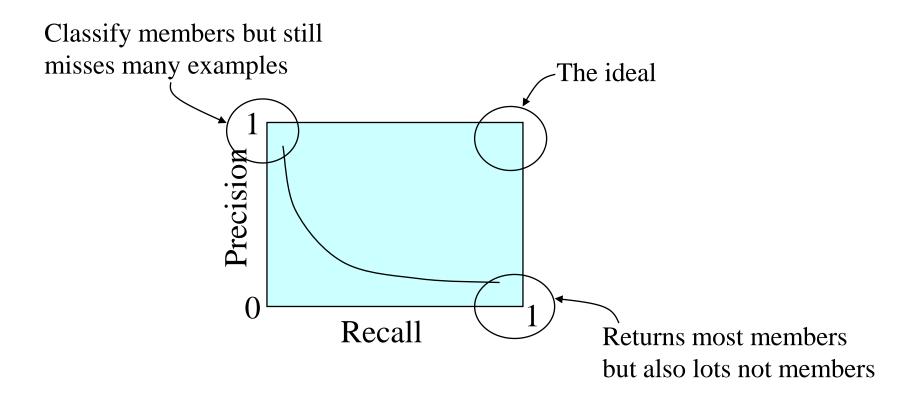




$$precision = \frac{\# \ of \ Members \ Classified}{\# \ of \ Members \ Classified \ + \# \ of \ Classified \ not \ Members}$$
 
$$recall = \frac{\# \ of \ Members \ Classified}{\# \ of \ Members \ Classified \ + \# \ of \ Rejected \ Members}$$

What about accuracy???

#### Trade-off between Precision and Recall



### Other class based measures

#### Precision and Recall of $C_i$

- a, corrects (TP<sub>i</sub>)
- b, mistakes (FP<sub>i</sub>)
- c, instances of a Class<sub>i</sub> that are not actually retrieved,
   (FN<sub>i</sub>)

The *Precision* and *Recall* are defined by the above counts:

$$Precision_i = \frac{a_i}{a_i + b_i}$$
 
$$Recall_i = \frac{a_i}{a_i + c_i}$$

		PREDICTED VALUE		
ш		Class A	Class B	Class C
ACTUAL VALUE	Class A	38	12	0
	Class B	5	43	2
	Class C	6	0	44

- Precision<sub>A</sub>= 38/(38+5+6)=38/49
- $Recall_A = 38/(38+12)=38/50$
- Precision<sub>B</sub> = 43/(43+12)=43/55
- Recall<sub>C</sub> = 44/(44+6)=44/50

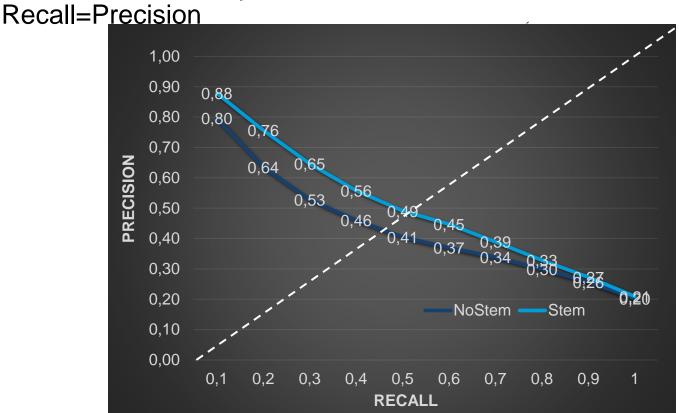
## Performance Measurements (cont'd)

- Breakeven Point
  - Find thresholds for which

- Interpolation
- F-measure  $F_1 = \frac{2 \times Precision \times Recall}{Precision + Recall}$ 
  - Harmonic mean between precision and recall
- Global performance on more than two categories
  - Micro-average
    - The counts refer to classifiers
  - Macro-average (average measures over all categories)

#### Break-even Point

The BEP is the interpolated estimate of the value for which

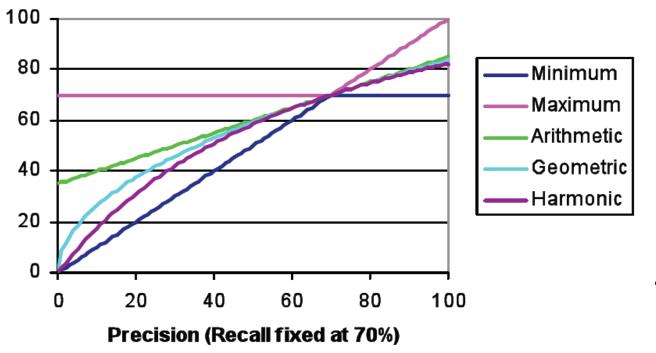


 It shows the superiority of methods whose behavior is closer to the (1,1) ideal performance

# Averaging Precision & Recall: comparison

A

$$F_1 = rac{2}{rac{1}{Precision} + rac{1}{Recall}} = rac{2 \cdot Precision \cdot Recall}{Precision + Recall}$$



min(p,r)max(p,r)

$$arithM(p,r) = \frac{p+r}{2}$$

$$geomM(p,r) = \sqrt{p \cdot r}$$

$$harm M(p,r) = \frac{2}{p^{-1} + 1}$$

# Averaging Precision & Recall: cross-categorical analysis

- Individual scores characterize the performance about each specific class
- Simple macro averaging can be applied to have

$$MPrecision = \sum_{i=1}^{n} Precision_{i}$$
 $MRecall = \sum_{i=1}^{n} Recall_{i}$ 
 $= \frac{MF_{1}}{MPrecision \cdot MRecall}$ 
 $= \frac{2 \cdot MPrecision \cdot MRecall}{MPrecision + MRecall}$ 

#### F-measure e MicroAverages

$$F_{1} = \frac{2 \times Precision \times Recall}{Precision + Recall}$$

$$\mu Precision = \frac{\sum_{i=1}^{n} a_{i}}{\sum_{i=1}^{n} a_{i} + b_{i}}$$

$$\mu Recall = \frac{\sum_{i=1}^{n} a_{i}}{\sum_{i=1}^{n} a_{i} + c_{i}}$$

$$\mu BEP = \frac{\mu Precision + \mu Recall}{2}$$

$$\mu f_{1} = \frac{2 \times \mu Precision \times \mu Recall}{\mu Precision + \mu Recall}$$

		PREDICTED VALUE		
ш		Class A	Class B	Class C
ACTUAL VALUE	Class A	38	12	0
	Class B	5	43	2
	Class C	6	0	44

- Precision<sub>A</sub>= 38/(38+5+6)=38/49
- Precision<sub>B</sub> = 43/(43+12)=43/55
- Segue che:

Mprecision=1/3(38/49 + 43/55 +...)

		PREDICTED VALUE		
ш		Class A	Class B	Class C
ACTUAL VALUE	Class A	38	12	0
	Class B	5	43	2
	Class C	6	0	44

- Precision<sub>A</sub>= 38/(38+5+6)=38/49
- Precision<sub>B</sub> = 43/(43+12)=43/55
- Segue che:
   μPrecision=(38+43+44)/(38+43+44+11+12+2)

#### Overview

- Performance Evaluation Metrics
  - Classifier Evaluation Metrics
  - Information Retrieval Systems Evaluation Metrics

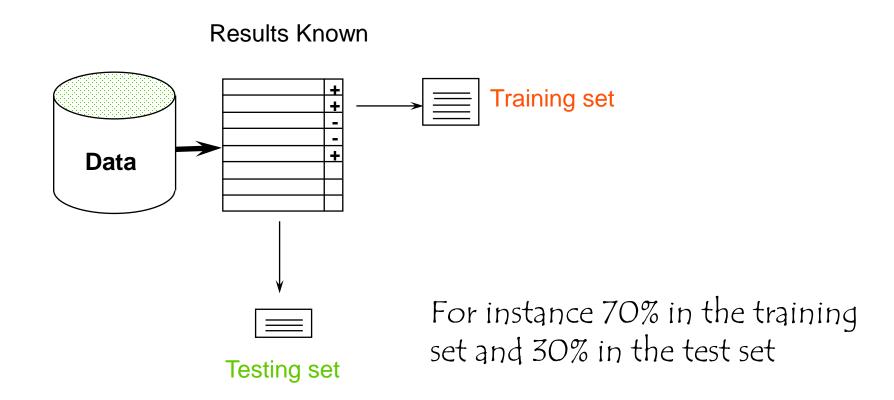
Tuning and Evaluation Methods

Error Diagnostics

# **Testing Data**

- To obtain a reliable estimation, test data must be instances not employed for the training step:
  - Error on the training data is not a good indicator of performance on future data, because new data will probably not be exactly the same as the training data!
  - Overfitting fitting the training data too precisely usually leads to poor results on new data
  - We want to evaluate how much accurate predictions of the model we learned are, and not other computational aspects (e.g. its memorization capability)

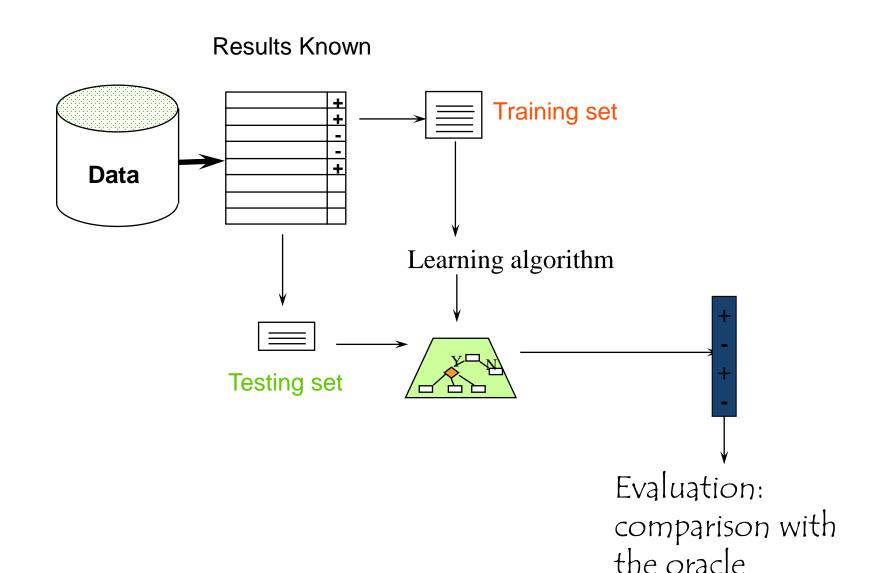
# Step 1: dataset splitting



# Step 2: learning phase

# Results Known Training set **Data** Learning algorithm Testing set

# Step 3: testing the model

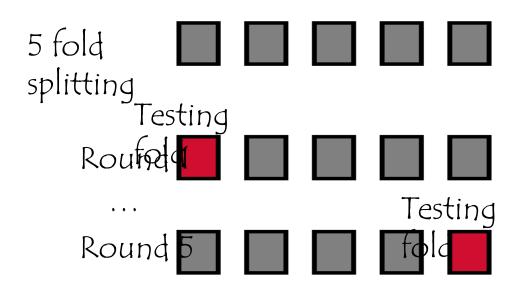


#### **Evaluation on Few Data**

- When data is scarce (totally or for a single class), a single evaluation process could not be enough representative
  - The testing set could contain too few instances to produce a reliable result
- SAMPLING: The evaluation process must be repeated with different splitting

#### N-Fold Cross Validation

- Data is split into n subsets of equal size
- Each subset in turn is used for testing and the remainders n-1 for training
- The metrics estimated in each round are averaged

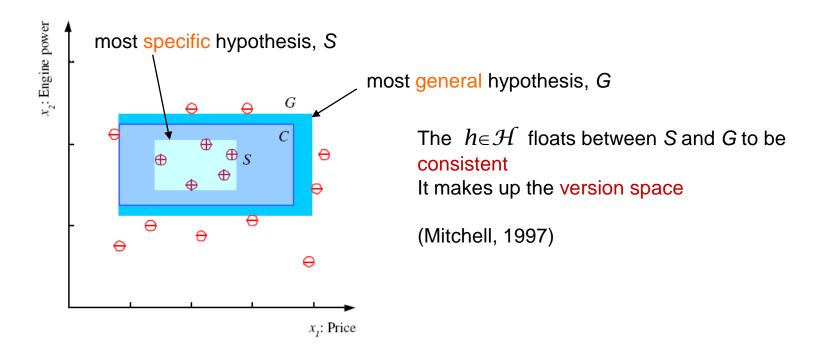


# Tuning a Classifier

- Most of ML algorithms depends on some parameters
  - Examples: k in KNN,  $w_i$  in Rocchio,  $p(w_i | c_i)$  for NB
- The best configuration must be choosen after a proper tuning stage:
  - A set of configurations must be established (for instance, k=1,2,5,10,...,50)
  - Each configuration must be evaluated on a validation (or tuning) set

### ... short look at model selection

## (Vector) Spaces, Functions and Learning



$$h \in \mathcal{H}$$

#### Model selection

- We try to find the model with the best balance of complexity and the fit to the training data
- Ideally, we would select a model from a nested sequence of models of increasing complexity (VC-dimension)

```
Model 1 d_1
```

Model 2  $d_2$ 

Model 3  $d_3$ 

where  $d_1 \leq d_2 \leq d_3 \leq \dots$ 

 The model selection criterion is: find the model class that achieves the lowest upper bound on the expected loss

Expected error  $\leq$  Training error + Complexity penalty

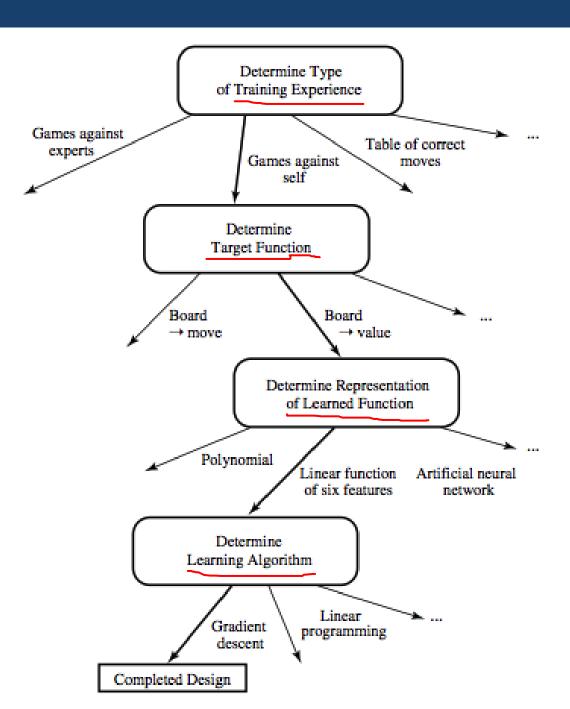
# Alternatives to VC-dim-based model selection

- What could we do instead of the scheme below?
  - Cross-validation

i	$f_i$	TRAINERR	10-FOLD-CV-ERR	Choice
1	$f_1$			
2	$f_2$			
3	$f_3$			?
4	$f_4$			
5	$f_5$			
6	$f_6$			

# Design of a learning system

Mitchell, 1997

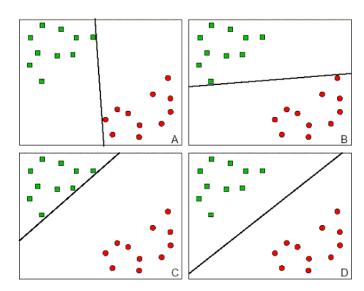


# Machine Learning Tasks

- Supervised learning da esempi
  - Classification
    - Approcci dicriminativi
    - Approcci generative
    - Outlier and deviation detection
  - Regression
  - Dependency modeling
    - Discovery di Associazioni/Relazioni, Sommari, Inferenza/Causalità
  - Sequence Classification
    - Temporal learning
    - Trend analysis and change/anomaly detection
- Unsupervised learning
  - Clustering
  - Embedding ottimo: Enconding/Decoding
    - Representation Learning for Images
    - PreTraining as optimal encoding

#### Metodi di ML: selezione dei modelli

- Approcci discriminativi
  - Lineari
  - $h(x) = sign(W \cdot x + b)$



- Approcci probabilistici
  - Stima delle probabilità  $p(C_k|\mathbf{x})$  attraverso un training set
  - Modello generativo ed uso della inversione Bayesiana

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})}.$$

# Riferimenti Bibliografici

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- READING. Machine Learning, Tom Mitchell, Mc Graw-Hill International Editions, 1997 (Cap 3).
- L'Algoritmo Definitivo, Pedro Domingos, Bollati Boringhieri, 2016

