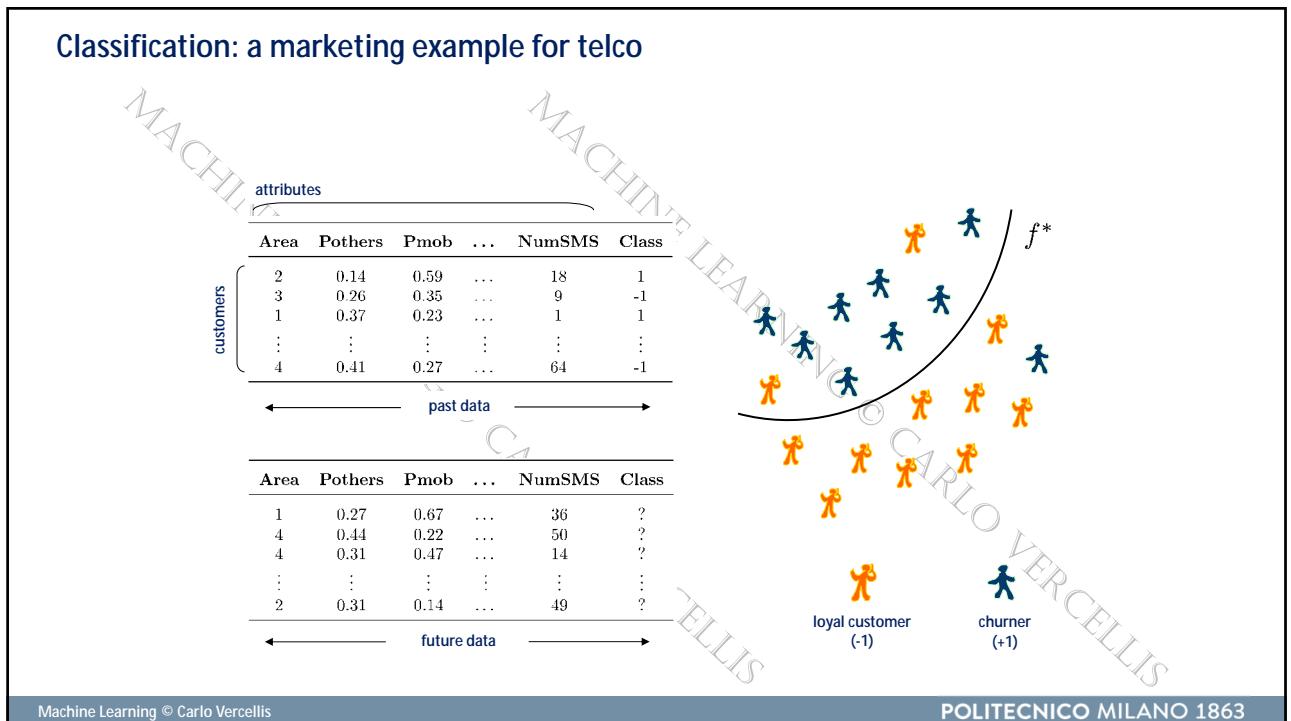




1



2

Classification: prediction of HIV protease-cleavable peptides

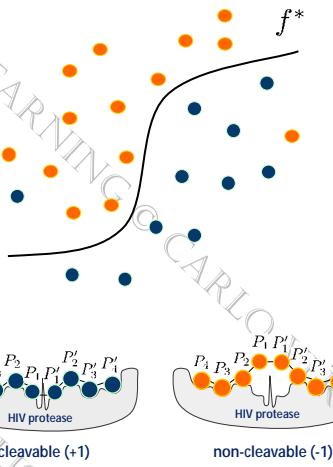
attributes

	P_4	P_3	P_2	P_1	P'_1	P'_2	P'_3	P'_4	Class
T	Q	I	M	F	E	T	F		1
G	Q	V	N	Y	E	E	F		1
Y	T	F	L	F	M	N	S		-1
:	:	:	:	:	:	:	:		:
D	T	V	L	E	E	M	S		1

\longleftrightarrow past data \longleftrightarrow

	P_4	P_3	P_2	P_1	P'_1	P'_2	P'_3	P'_4	Class
S	Q	X	Y	P	I	V	Q		?
T	Q	I	M	F	E	T	F		?
G	L	A	A	P	Q	F	S		?
:	:	:	:	:	:	:	:		:
R	Q	A	G	F	L	G	L		?

\longleftrightarrow future data \longleftrightarrow



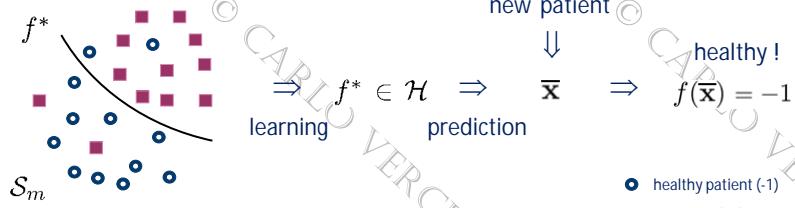
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

3

Classification as a learning task

- $\mathcal{S}_m = \{(\mathbf{x}_i, y_i), i \in \mathcal{M}\}$ training set, where $\mathbf{x}_i \in \mathbb{R}^n$ $y_i \in \mathcal{D}$
- \mathcal{H} denotes a set of functions $f(\mathbf{x}) : \mathbb{R}^n \mapsto \mathcal{D}$
- Classification problem: define a hypotheses space \mathcal{H} and a function $f^* \in \mathcal{H}$ that optimally describes the relationship between \mathbf{x}_i and y_i



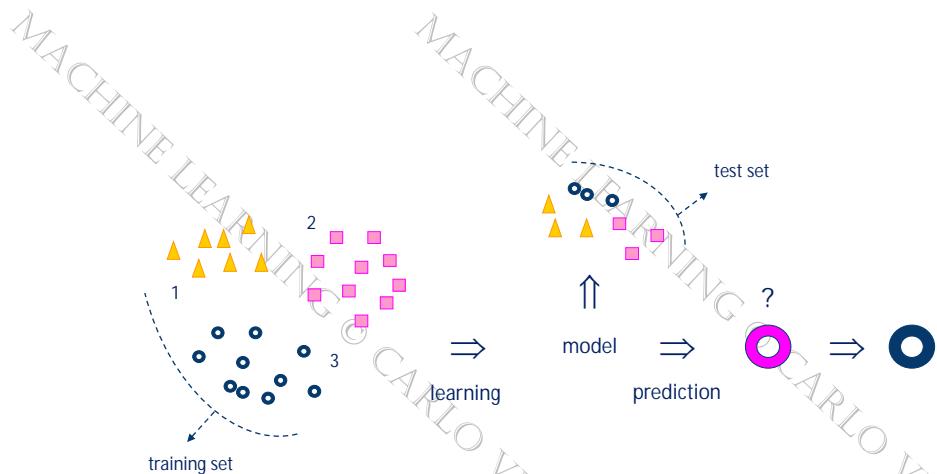
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

4

2

Classification models

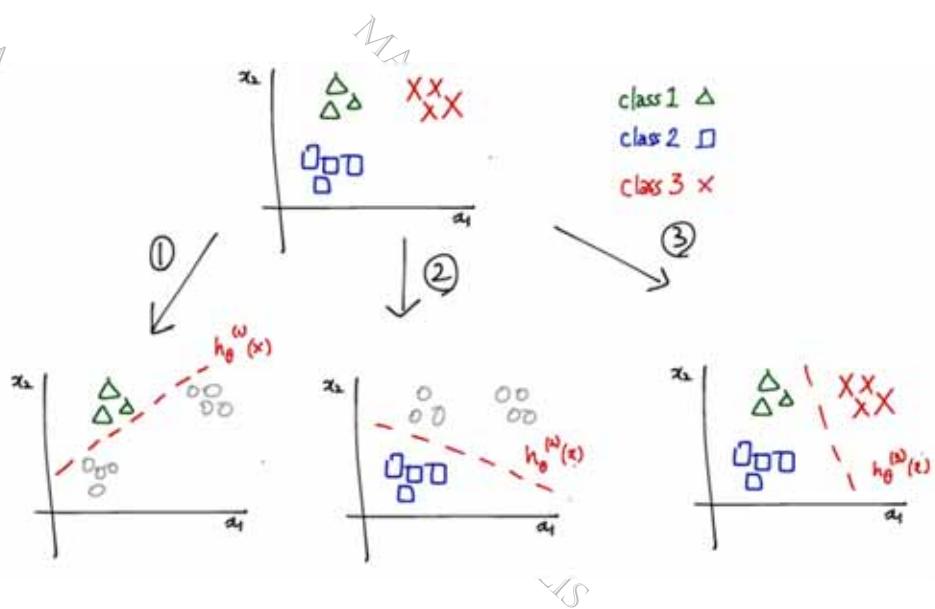


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

5

Multi-class Approaches: 1-against-all



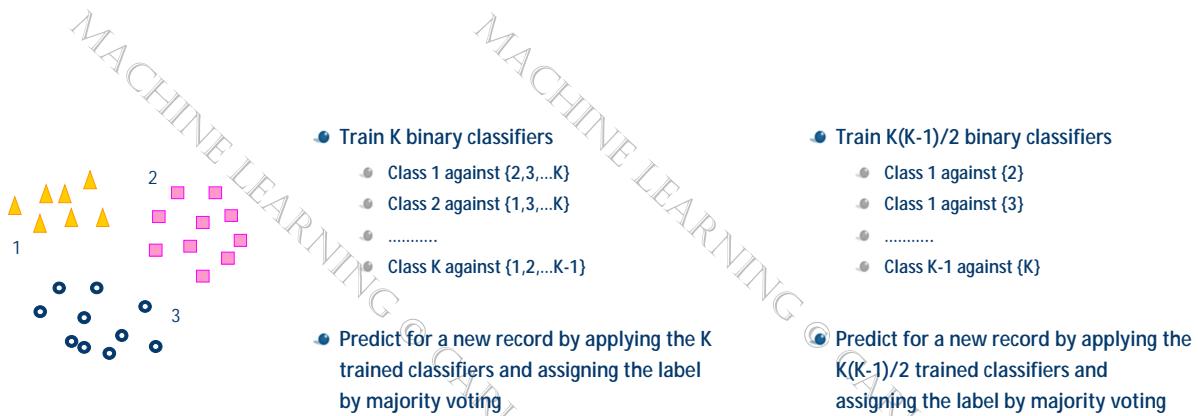
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

6

3

Multi-class Approaches: 1-against-all vs. 1-against-1



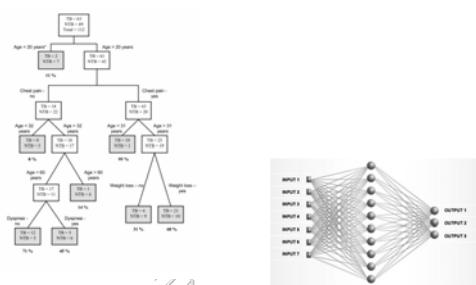
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

7

Taxonomy of classification methods

- Heuristic methods**
 - classification trees
 - nearest neighbor
- Separation methods**
 - perceptron
 - neural networks
 - support vector machines
- Regression methods**
 - logistic regression
- Probabilistic methods**
 - bayesian methods



$$y_{MAP} = \arg \max_{y \in \mathcal{H}} P(y|x) = \arg \max_{y \in \mathcal{H}} \frac{P(x|y)P(y)}{P(x)}$$

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

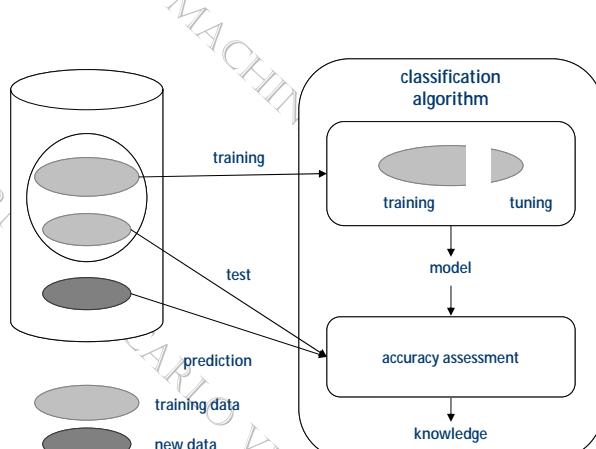
8

4

Assessing classification methods

- Prediction accuracy
- Speed
 - time required to train a model
- Robustness
 - handling noise and missing data
- Scalability
 - effectiveness in handling large datasets
- Interpretability
 - value of the knowledge extracted from the model
- Rules effectiveness
 - number of rules
 - conciseness and significance of the rules

Development of a classification model



Source: C. Vercellis, Business Intelligence. Data Mining and Optimization for Decision Making, Wiley, 2009.

Prediction accuracy

- Loss function counting the number of misclassifications

$$L(y, f(\mathbf{x})) = \begin{cases} 0 & \text{if } y = f(\mathbf{x}) \\ 1 & \text{if } y \neq f(\mathbf{x}) \end{cases}$$

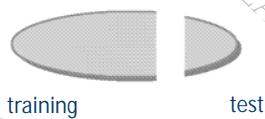
- Empirical error

$$R_{\text{emp}} = \frac{1}{m} \sum_{i=1}^m L(f(\mathbf{x}_i))$$

Prediction accuracy

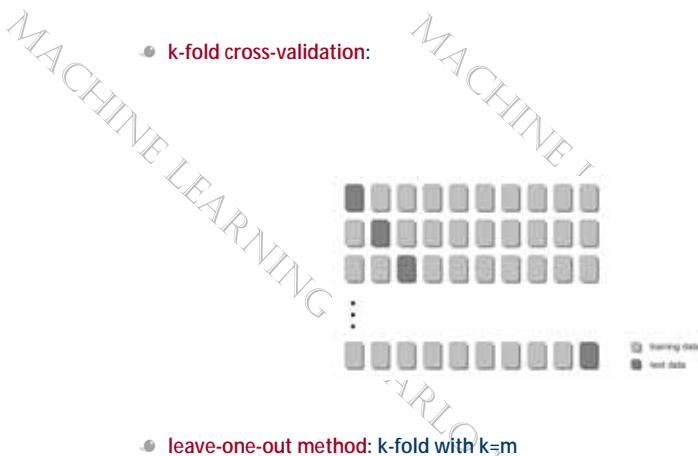
- Prediction accuracy can be estimated through four main approaches:

- **holdout method:**



- **repeated random sampling method:** repeated applications of holdout method

Prediction accuracy

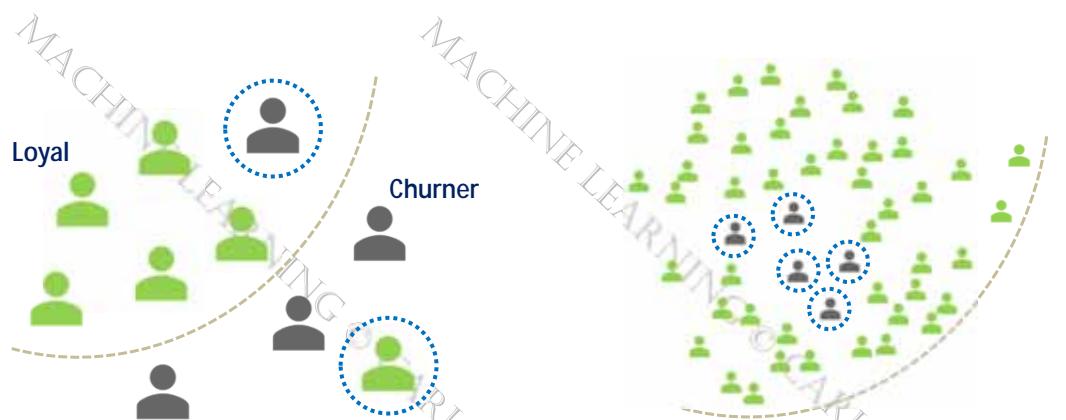


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

13

Model evaluation



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

14

Confusion matrix

- p : true negative
- q : false positive
- u : false negative
- v : true positive

		predictions		total
		-1 (negative)		
examples	-1 (negative)	p	q	$p + q$
	+1 (positive)	u	v	$u + v$
	total	$p + u$	$q + v$	m

Accuracy = % records correctly classified = $(p + v)/m$

Recall (true positive rate tp) = % true positives correctly classified = $v/(u + v)$

Precision (prc) = % true positives among those predicted positives = $v/(q + v)$

False positive rate = $q/(p+q)$

True negative rate = $p/(p+q)$

False negative rate = $u/(u+v)$

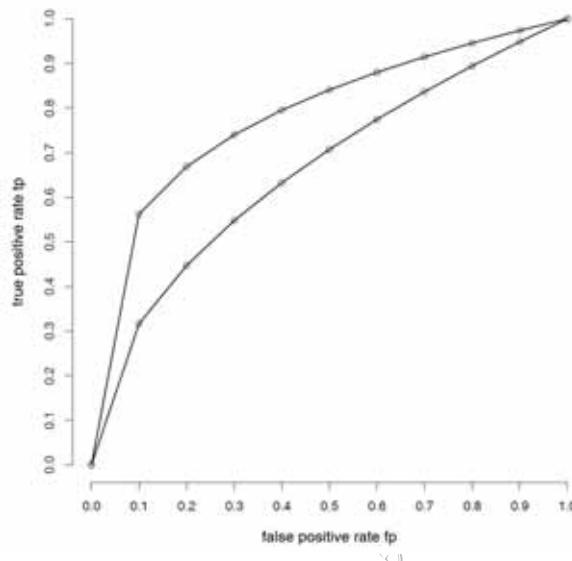
F-measure

$$F = \frac{(\beta^2 + 1) tp \times prc}{\beta^2 prc + tp},$$

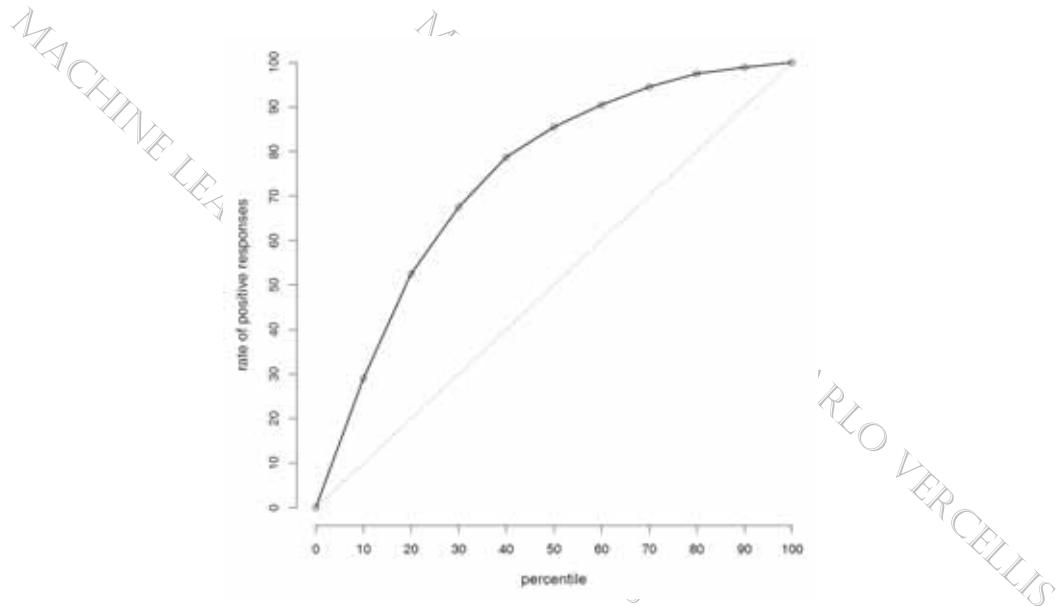
Geometric mean

$$gm = \sqrt{tp \times prc},$$

ROC curves



Cumulative gain

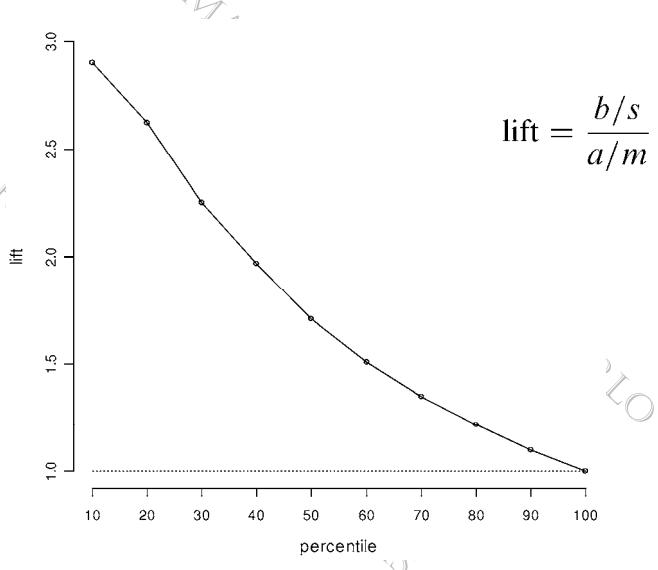


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

17

Lift

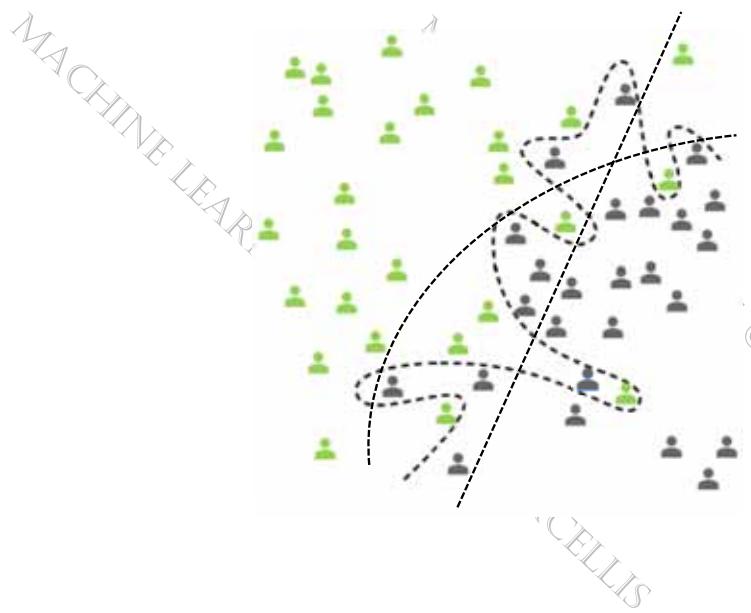


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

18

Overfitting

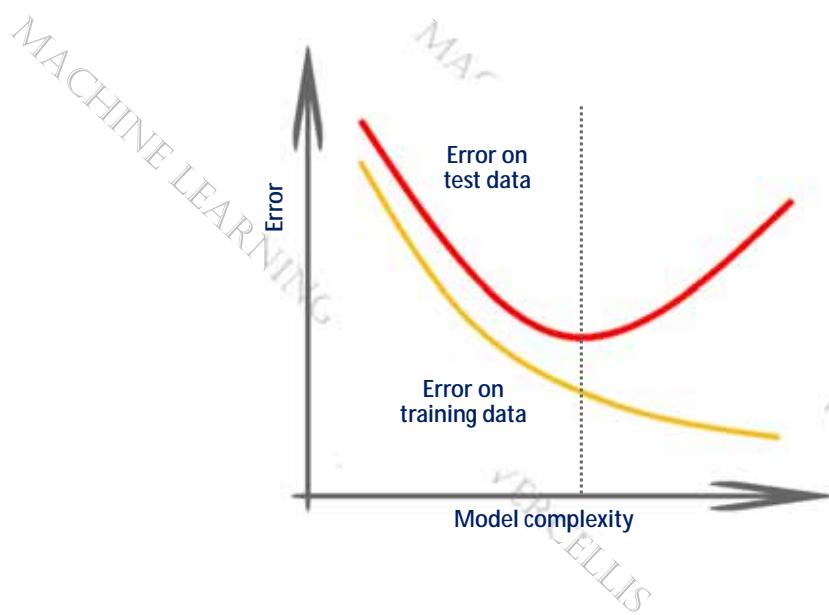


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

19

Bias-variance trade-off



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

20

Numerical representation of categorical variables

- For example, to represent the month associated to an observation

Other Columns	Month	D_Jan	D_Feb	D_Mar	D_Apr	D_May	D_Jun	D_Jul	D_Aug	D_Sep	D_Oct	D_Nov	D_Dec
...	Jan	1	0	0	0	0	0	0	0	0	0	0	0
...	Mar	0	0	1	0	0	0	0	0	0	0	0	0
...	Jun	0	0	0	0	0	1	0	0	0	0	0	0
...	Dec	0	0	0	0	0	0	0	0	0	0	0	1
...	Nov	0	0	0	0	0	0	0	0	0	0	1	0
...	Jan	1	0	0	0	0	0	0	0	0	0	0	0
...
...
...
...
...
...	Feb	0	1	0	0	0	0	0	0	0	0	0	0

Numerical representation of categorical variables

- variable X_j assumes values in the set $V = \{v_1, v_2, \dots, v_H\}$

- $H-1$ dummy variables

$$D_{j1}, D_{j2}, \dots, D_{j,H-1}$$

Predicting survival in patients after myocardial infarction: introduction

All the patients in the dataset suffered heart attacks at some point in the past. Some are still alive and some are not. The problem addressed by past researchers was to predict from the other variables whether or not the patient will survive at least one year.

Myocardial infarction (MI) or **acute myocardial infarction (AMI)** occurs when blood flow stops to a part of the heart causing damage to the heart muscle.

Most MIs occur due to coronary artery disease. Risk factors include high blood pressure, smoking, diabetes, lack of exercise, obesity, high blood cholesterol, poor diet, and excessive alcohol intake, among others. Blockages on the **left side** of your heart are usually **more dangerous**.

Binary target Survival is explained by Social Security Number, Nationality, Area, Shortening fraction, Atrial dimension of the LV, Wall motion index, Hematocrit, Pericardial effusion.

Cross-validation for different methods on Heart dataset

Evaluation Results						
Model	AUC	CA	F1	Precision	Recall	
kNN	0.928	0.859	0.855	0.860	0.859	
Tree	0.941	0.936	0.935	0.936	0.936	
SVM	0.892	0.866	0.863	0.866	0.866	
Random Forest	0.992	0.961	0.961	0.961	0.961	
Neural Network	0.922	0.841	0.839	0.839	0.841	
Naive Bayes	0.890	0.796	0.797	0.798	0.796	
Logistic Regression	0.922	0.846	0.845	0.845	0.846	
AdaBoost	0.965	0.971	0.970	0.970	0.971	

Confusion matrix for different methods on Heart dataset

kNN
Tree
SVM
Naive Bayes
Logistic Regression
Random Forest
Neural Network
AdaBoost

		Predicted		<input type="button" value="Show: Number of instances"/>
		0	1	
Actual	0	561	35	596
	1	94	226	320
Σ		655	261	916

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

29

Confusion matrix for different methods on Heart dataset

kNN
Tree
SVM
Naive Bayes
Logistic Regression
Random Forest
Neural Network
AdaBoost

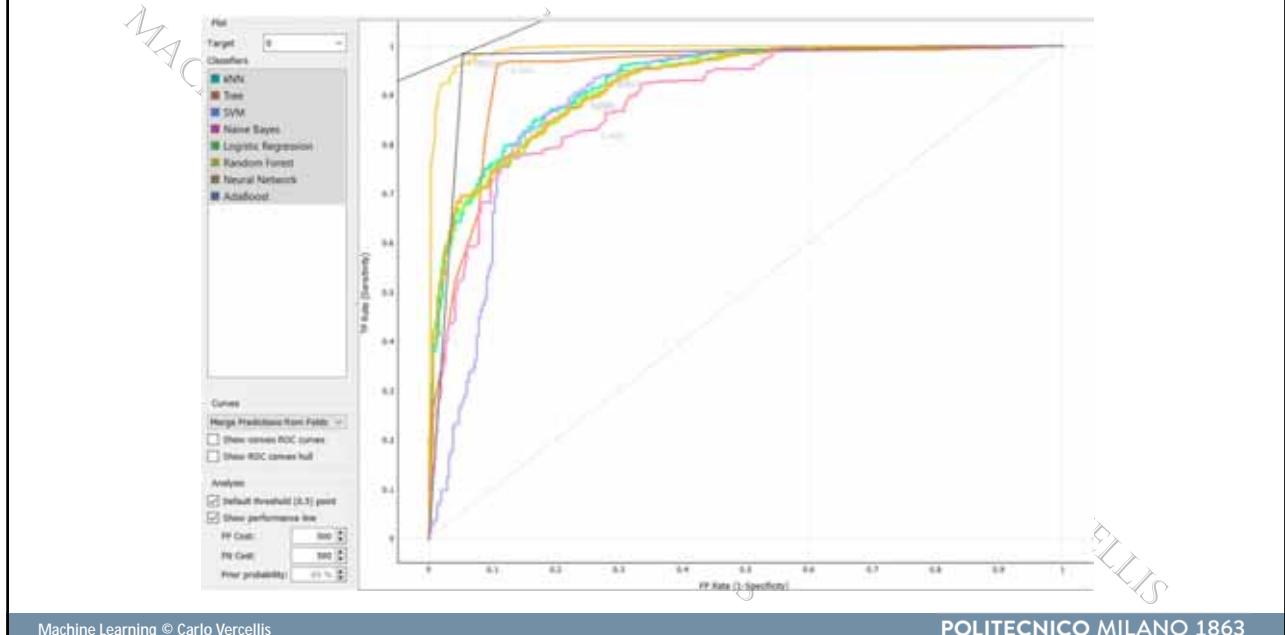
		Predicted		<input type="button" value="Show: Proportion of actual"/>
		0	1	
Actual	0	94.1 %	5.9 %	596
	1	29.4 %	70.6 %	320
Σ		655	261	916

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

30

ROC curve for different methods on Heart dataset



31

K-nearest neighbour (K-NN)

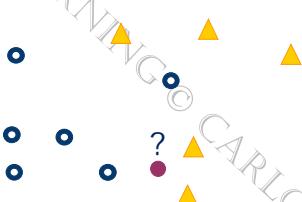
To a new record is attributed the class to which belong the majority of records out of the K closest ones (*majority voting*)

The choice of K affects model robustness and accuracy

By increasing K ...

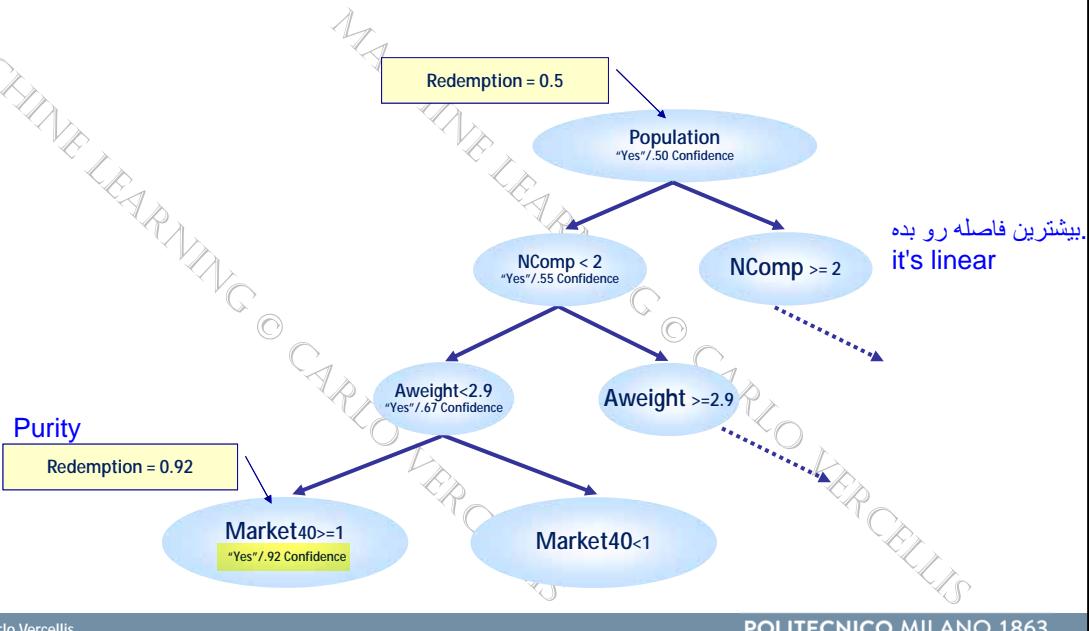
less sensitive to outliers

less distinction among classes



Session Oct 16th

Business case automotive – customer acquisition



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

33

hyper params:

- purity threshhold (90%)
- minumim cardinality - minimum number in a leaf to split
- information gain - difference of heterogeneity reduction.

Classification trees

- Base recursive **greedy** algorithm
 - All records are placed in the root node
 - Records in each node are split according to a heuristic test based on the value of one or more attributes
- **To prevent overfitting**
 - **pre pruning by stopping criteria**
 - purity threshold
 - minimum cardinality
 - minimum information gain
 - **post pruning: identifies and removes ramifications affected by noise**
- **Majority voting is used to classify a leaf**

LaMasa_BL27_BL... An iterative process in which some branches are eliminated from the tree. Again, the idea is if it is better without on the internal test set, the tuning set, then it means the that branching the eliminated branching were LaMasa_BL27_BL... Were producing overfitting. Okay, it's pretty reasonable, pretty rational.

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

34

Classification trees

- Classification trees are distinguished in:

- binary trees

- general trees

and in

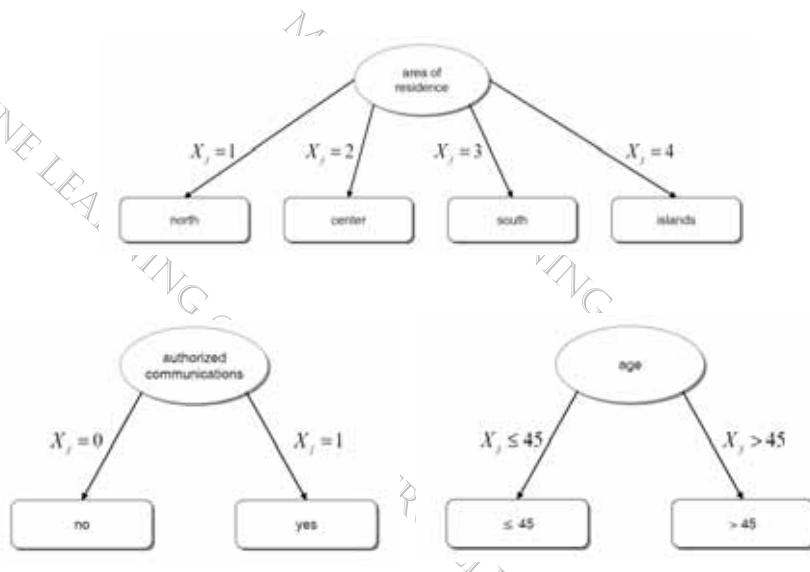
- univariate trees (or axis parallel)

$$\Rightarrow X_j \leq b$$

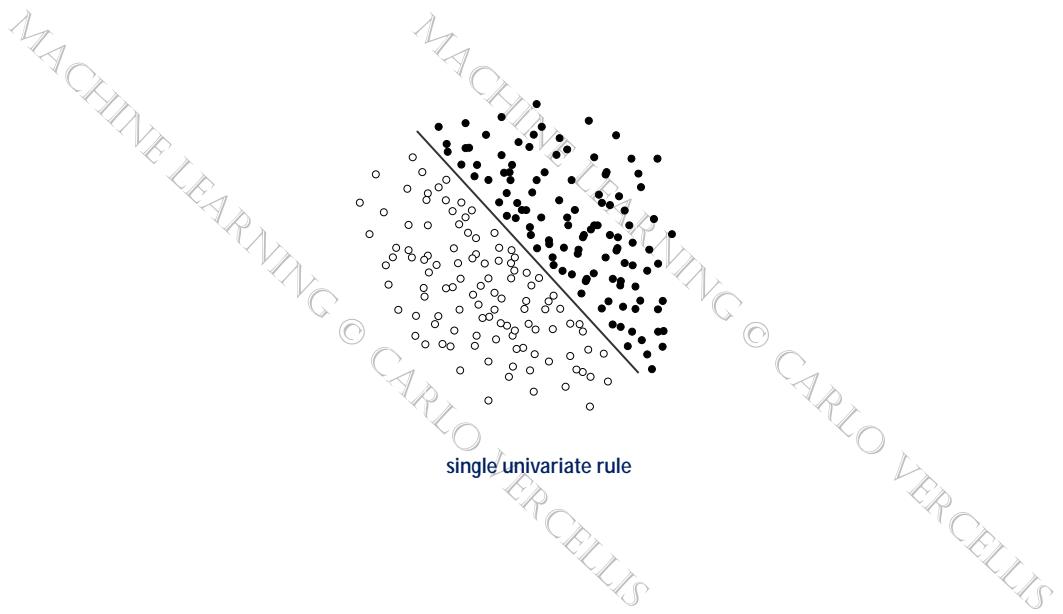
- multivariate trees (or oblique)

$$\Rightarrow \sum_{j=1}^n w_j x_j \leq b$$

Classification trees



Classification trees

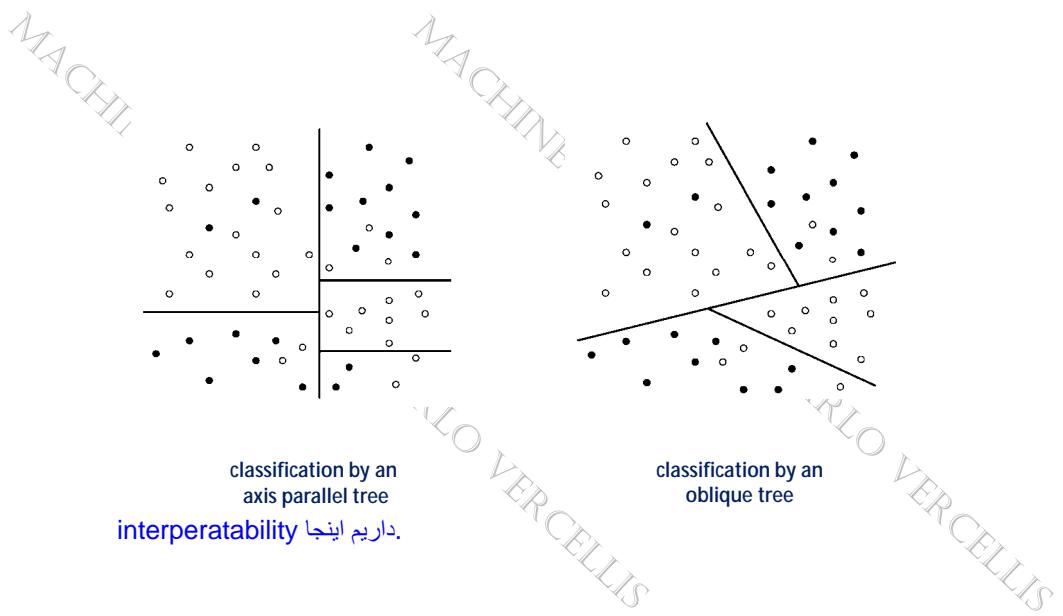


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

37

Classification trees



classification by an
axis parallel tree

interpretability
داریم اینجا

classification by an
oblique tree

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

38

به نظر خوب فیت نمیشن ولی به
خاطر اینترپریتیلیتی باید برایم
سراغشون یا شاید حتی مسائل
حقوقی مارو مجبور کنن.

17

Classification trees

- In axis parallel trees the best separation rule identifies the most effective attribute and split

- Main criteria for splitting

- misclassification index $\text{Miscl}(q) = 1 - \max_h p_h$

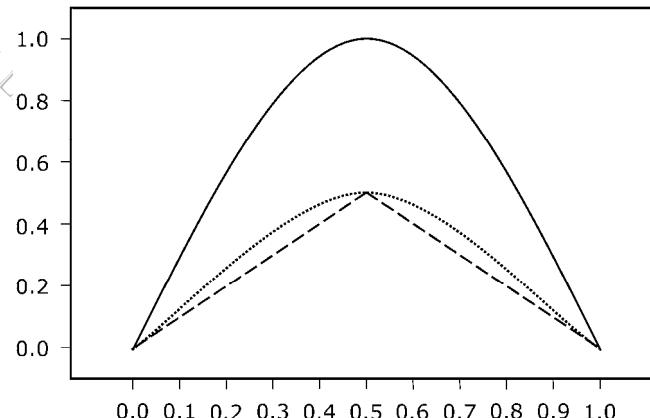
- entropy index $\text{Entropy}(q) = - \sum_{h=1}^H p_h \log_2 p_h$

- Gini index $\text{Gini}(q) = 1 - \sum_{h=1}^H p_h^2$

P_1 negative
 P_2 positive
sum is total number of obs
in this note.

node q

Classification trees



Classification trees

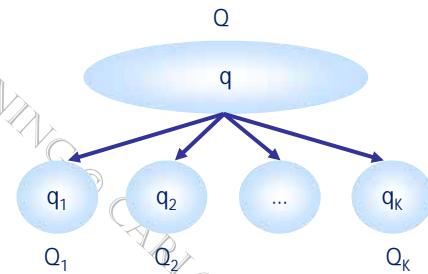
- Impurity of a splitting rule

$$I(q_1, q_2, \dots, q_K) = \sum_{k=1}^K \frac{Q_k}{Q} I(q_k).$$

- At each node select the rule minimizing the impurity or, equivalently, maximizing the information gain

$$\Delta(q, q_1, q_2, \dots, q_K) = I(q) - I(q_1, q_2, \dots, q_K)$$

$$= I(q) - \sum_{k=1}^K \frac{Q_k}{Q} I(q_k).$$



Classification trees

area	numin	timein	numout	Pothers	Pmob	Pland	numsms	numserv	numcall	dropt	churner
3	32	3093	45	0.14	0.75	0.12	18	1	0	0	0
3	277	157842	450	0.26	0.35	0.38	9	3	0	1	0
1	17	15023	20	0.37	0.23	0.40	1	1	0	0	0
1	46	23459	69	0.10	0.39	0.51	33	1	0	0	0
1	19	8640	9	0.00	0.00	1.00	0	0	0	0	0
2	17	7652	66	0.16	0.42	0.43	1	3	0	1	0
3	47	17768	11	0.45	0.00	0.55	0	0	0	0	0
3	19	9492	42	0.18	0.34	0.48	3	1	0	0	1
1	1	84	9	0.09	0.54	0.37	0	0	0	0	1
2	119	87605	126	0.84	0.02	0.14	12	1	0	0	0
4	24	6902	47	0.25	0.26	0.48	4	1	0	0	0
1	32	28072	43	0.28	0.66	0.06	0	1	0	0	0
3	103	112120	24	0.61	0.28	0.11	24	2	0	0	0
3	45	21921	94	0.34	0.47	0.19	45	2	0	1	0
1	8	25117	89	0.02	0.39	0.09	189	0			
3	4	945	16	0.00	0.00	1.00	0				
2	83	44263	83	0.00	0.00	0.67	0				
2	22	15979	59	0.05	0.53	0.41	5				
2	0	0	57	0.00	1.00	0.00	15				
4	162	114108	273	0.18	0.15	0.41	2				
4	21	4141	70	0.14	0.58	0.28	0				
4	33	10066	45	0.12	0.21	0.67	0				
4	5	965	40	0.41	0.27	0.32	64				

Table 5.3 Meaning of the attributes in Table 5.2

attribute	meaning
area	residence area
numin	number of calls received in period $t-2$
timein	duration in seconds of calls received in period $t-2$
numout	number of calls placed in the period $t-2$
Pothers	percentage of calls placed to other mobile telephone companies in period $t-2$
Pmob	percentage of calls placed to the same mobile telephone company in period $t-2$
Pland	percentage of calls placed to land numbers in period $t-2$
numsms	number of messages sent in period $t-2$
numserv	number of calls placed to special services in period $t-2$
numcall	number of calls placed to the call center in period $t-2$
dropt	binary variable indicating whether the customer corresponding to the record has subscribed to a special rate plan for calls placed to selected numbers
churner	binary variable indicating whether the customer corresponding to the record has left the service in period t

Classification trees

attribute	class 1	class 2	class 3	class 4
numin	[0, 20)	[20, 40)	[40, ∞)	
timein	[0, 10 000)	[10 000, 20 000)	[20 000, 30 000)	[30 000, ∞)
numout	[0, 30)	[30, 60)	[60, 90)	[90, ∞)
Pothers	[0, 0,1)	[0,1, 0,2)	[0,2, 0,3)	[0,3, ∞)
Pmob	[0, 0,2)	[0,2, 0,4)	[0,4, 0,6)	[0,6, ∞)
Pland	[0, 0,25)	[0,25, 0,5)	[0,5, ∞)	
numsms	[0, 1)	[1, 10)	[10, 20)	[20, ∞)
numserv	[0, 1)	[1, 2)	[2, 3)	[3, ∞)
numcall	[0, 1)	[1, 3)	[3, ∞)	

Classification trees

area	numin	timein	numout	Pothers	Pmob	Pland	numsms	numserv	numcall	dropt	churner
2	1	1	2	1	4	1	3	2	2	0	1
1	1	3	3	2	4	1	4	2	3	0	0
3	2	1	2	2	4	1	3	2	1	0	0
1	2	3	2	3	4	1	1	2	1	0	0
2	3	4	4	4	1	1	3	2	1	0	0
3	3	4	1	4	2	1	4	3	1	0	0
3	3	3	4	4	3	1	4	3	1	1	0
1	1	1	1	1	3	2	1	1	1	0	1
2	2	2	2	1	3	2	2	3	1	1	1
4	2	1	3	2	3	2	1	2	1	1	1
3	1	1	2	2	2	2	2	2	1	0	1
4	3	4	4	2	1	2	2	4	1	1	1
2	1	1	3	2	3	2	2	4	1	1	0
4	2	1	2	3	2	2	2	2	1	0	0
3	3	4	4	3	2	2	2	4	1	1	0
1	1	2	1	4	2	2	2	2	1	0	0
4	1	1	2	4	2	2	4	2	1	0	1
1	1	1	1	1	1	3	1	1	1	0	0
3	1	1	1	1	1	3	1	1	1	0	1
2	3	4	3	1	1	3	1	1	1	0	1
1	3	3	3	1	2	3	4	2	1	0	0
4	2	2	2	2	2	3	1	1	1	0	1
3	3	2	1	4	1	3	1	1	1	0	0

Classification trees

$$I_E(q) = \text{Entropy}(q) = -\frac{13}{23} \log_2 \frac{13}{23} - \frac{10}{23} \log_2 \frac{10}{23} = 0.988$$

$$\begin{aligned} p_0(q_1) &= 5/6, & p_0(q_2) &= 2/5, & p_0(q_3) &= 5/7, & p_0(q_4) &= 1/5, \\ p_1(q_1) &= 1/6, & p_1(q_2) &= 3/5, & p_1(q_3) &= 2/7, & p_1(q_4) &= 4/5. \end{aligned}$$

$$\begin{aligned} I_E(q_1, q_2, q_3, q_4) &= \frac{6}{23} I_E(q_1) + \frac{5}{23} I_E(q_2) + \frac{7}{23} I_E(q_3) + \frac{5}{23} I_E(q_4) \\ &= \frac{6}{23} 0.650 + \frac{5}{23} 0.971 + \frac{7}{23} 0.863 + \frac{5}{23} 0.722 = 0.8. \end{aligned}$$

$$\Delta_E(\text{area}) = \Delta_E(q, q_1, q_2, q_3, q_4) = I_E(q) - I_E(q_1, q_2, q_3, q_4) = 0.988 - 0.8 = 0.188.$$

$$\begin{aligned} \Delta_E(\text{numin}) &= 0.057, & \Delta_E(\text{Pland}) &= 0.125, \\ \Delta_E(\text{timein}) &= 0.181, & \Delta_E(\text{numsms}) &= 0.080, \\ \Delta_E(\text{numout}) &= 0.065, & \Delta_E(\text{numserv}) &= 0.057, \\ \Delta_E(\text{Pothers}) &= 0.256, & \Delta_E(\text{numcall}) &= 0.089, \\ \Delta_E(\text{Pmob}) &= 0.043, & \Delta_E(\text{diropt}) &= 0.005. \end{aligned}$$

Classification trees

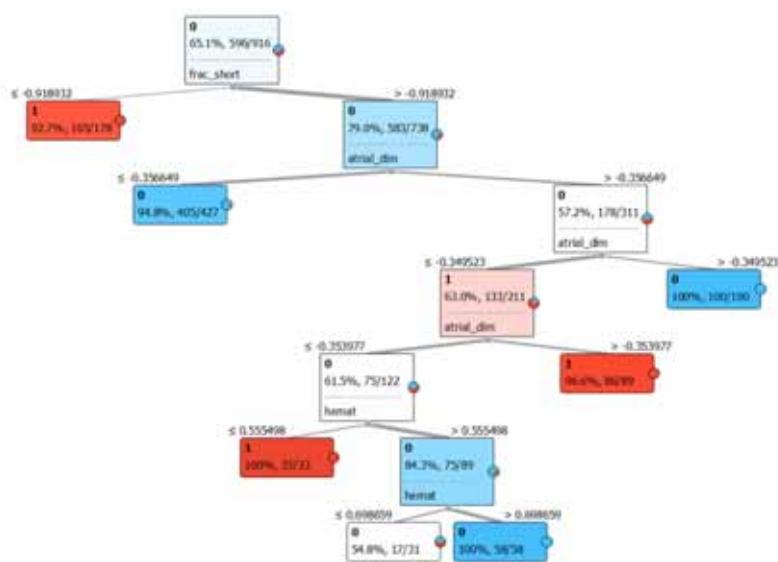
$$I_G(q) = \text{Gini}(q) = 1 - \left(\frac{13}{23}\right)^2 - \left(\frac{10}{23}\right)^2 = 0.491.$$

$$\begin{aligned} I_G(q_1, q_2, q_3, q_4) &= \frac{6}{23} I_G(q_1) + \frac{5}{23} I_G(q_2) + \frac{7}{23} I_G(q_3) + \frac{5}{23} I_G(q_4) \\ &= \frac{6}{23} 0.278 + \frac{5}{23} 0.638 + \frac{7}{23} 0.194 + \frac{5}{23} 0.528 = 0.370. \end{aligned}$$

$$\Delta_G(\text{area}) = \Delta_G(q, q_1, q_2, q_3, q_4) = I_G(q) - I_G(q_1, q_2, q_3, q_4) = 0.491 - 0.370 = 0.121.$$

$$\begin{aligned} \Delta_G(\text{numin}) &= 0.037, & \Delta_G(\text{Pland}) &= 0.078, \\ \Delta_G(\text{timein}) &= 0.091, & \Delta_G(\text{numsms}) &= 0.052, \\ \Delta_G(\text{numout}) &= 0.043, & \Delta_G(\text{numserv}) &= 0.038, \\ \Delta_G(\text{Pothers}) &= 0.146, & \Delta_G(\text{numcall}) &= 0.044, \\ \Delta_G(\text{Pmob}) &= 0.028, & \Delta_G(\text{diropt}) &= 0.003. \end{aligned}$$

Classification tree for the Heart dataset



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

47

Bayesian methods

- compute posterior probability:

$$P(y|\mathbf{x})$$

- estimate of prior probability

$$P(y) = P(y = v_h) = \frac{m_h}{m}$$

- compute posterior using Bayes theorem

$$P(y|\mathbf{x}) = \frac{P(\mathbf{x}|y)P(y)}{\sum_{l=1}^H P(\mathbf{x}|y_l)P(y_l)} = \frac{P(\mathbf{x}|y)P(y)}{P(\mathbf{x})}$$

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

48

Bayesian methods

- To classify new observations, use *maximum a posteriori hypothesis* (MAP) principle:

$$y_{MAP} = \arg \max_{y \in \mathcal{H}} P(y|\mathbf{x}) = \arg \max_{y \in \mathcal{H}} \frac{P(\mathbf{x}|y)P(y)}{P(\mathbf{x})}$$

- Maximize numerator

$$P(\mathbf{x}|y = v_h)P(y = v_h) \geq P(\mathbf{x}|y = v_l)P(y = v_l), \\ l = 1, 2, \dots, H, l \neq h$$

...but sample estimation of $P(\mathbf{x}|y)$ cannot be hardly done in practice

Naïve Bayesian methods

- assume attributes are independent:

$$P(\mathbf{x}|y) = P(x_1|y) \times P(x_2|y) \times \cdots \times P(x_n|y) = \prod_{j=1}^n P(x_j|y)$$

- two possible cases:

- categorical attributes:

$$P(x_j|y) = P(x_j = r_{jk}|y = v_h) = \frac{s_{j,h}}{m_h}$$

- numerical attributes: postulate a given distribution, such as

$$P(x_j|y = v_h) = \frac{1}{\sqrt{2\pi\sigma_{jh}^2}} e^{-\frac{(x_j - \mu_{jh})^2}{2\sigma_{jh}^2}}$$

Naive Bayesian methods

area

$$P(\text{area} = 1 | \text{churner} = 0) = \frac{5}{13}, \quad P(\text{area} = 1 | \text{churner} = 1) = \frac{1}{10},$$

$$P(\text{area} = 2 | \text{churner} = 0) = \frac{2}{13}, \quad P(\text{area} = 2 | \text{churner} = 1) = \frac{3}{10},$$

$$P(\text{area} = 3 | \text{churner} = 0) = \frac{5}{13}, \quad P(\text{area} = 3 | \text{churner} = 1) = \frac{2}{10},$$

$$P(\text{area} = 4 | \text{churner} = 0) = \frac{1}{13}, \quad P(\text{area} = 4 | \text{churner} = 1) = \frac{4}{10}.$$

Pothers

$$P(\text{Pothers} = 1 | \text{churner} = 0) = \frac{2}{13}, \quad P(\text{Pothers} = 1 | \text{churner} = 1) = \frac{5}{10},$$

$$P(\text{Pothers} = 2 | \text{churner} = 0) = \frac{3}{13}, \quad P(\text{Pothers} = 2 | \text{churner} = 1) = \frac{4}{10},$$

$$P(\text{Pothers} = 3 | \text{churner} = 0) = \frac{3}{13}, \quad P(\text{Pothers} = 3 | \text{churner} = 1) = 0,$$

$$P(\text{Pothers} = 4 | \text{churner} = 0) = \frac{5}{13}, \quad P(\text{Pothers} = 4 | \text{churner} = 1) = \frac{1}{10}.$$

VERCELLIS

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

51

Naive Bayesian methods

...and relative frequencies of the two classes

$$P(\text{churner} = 0) = \frac{13}{23} = 0.56, \quad P(\text{churner} = 1) = \frac{10}{23} = 0.44,$$

Predict the target class for a new observation

$$\mathbf{x} = (1, 1, 1, 2, 1, 4, 2, 1, 2, 1, 0)$$

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

52

Naive Bayesian methods

Compute probabilities

$$P(\mathbf{x}|0) = \frac{5}{13} \cdot \frac{4}{13} \cdot \frac{4}{13} \cdot \frac{3}{13} \cdot \frac{2}{13} \cdot \frac{3}{13} \cdot \frac{4}{13} \cdot \frac{3}{13} \cdot \frac{7}{13} \cdot \frac{12}{13} \cdot \frac{10}{13} = 0.81 \cdot 10^{-5}$$

$$P(\mathbf{x}|1) = \frac{1}{10} \cdot \frac{5}{10} \cdot \frac{6}{10} \cdot \frac{5}{10} \cdot \frac{5}{10} \cdot \frac{1}{10} \cdot \frac{6}{10} \cdot \frac{5}{10} \cdot \frac{4}{10} \cdot \frac{9}{10} \cdot \frac{7}{10} = 5.67 \cdot 10^{-5}$$

obtaining the posterior probability

$$P(\text{churner} = 0|\mathbf{x}) = P(\mathbf{x}|0)P(\text{churner} = 0)$$

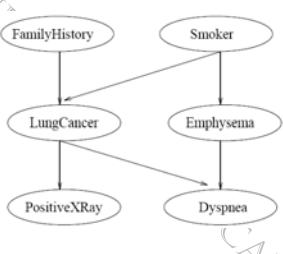
$$= 0.81 \cdot 10^{-5} \cdot 0.56 = 0.46 \cdot 10^{-5},$$

$$P(\text{churner} = 1|\mathbf{x}) = P(\mathbf{x}|1)P(\text{churner} = 1)$$

$$= 5.67 \cdot 10^{-5} \cdot 0.44 = 2.495 \cdot 10^{-5}.$$

Bayesian belief networks

BAYESIAN BELIEF NETWORKS allow to define dependency relationships between (small) subsets of attributes



Acyclic oriented graph

Conditional probability table

	FH,S	FH, \sim S	\sim FH,S	\sim FH, \sim S
LC	0.8	0.5	0.7	0.1
\sim LC	0.2	0.5	0.3	0.9

Logistic regression

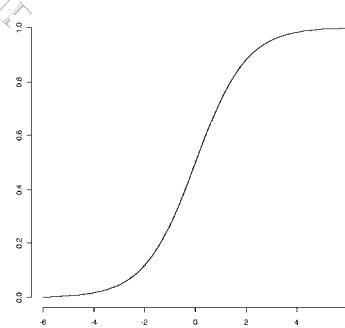
- A logistic function (sigmoid)

$$S(t) = \frac{1}{1 + e^{-t}}$$

Postulate posterior probability

$$P(y = 0|\mathbf{x}) = \frac{1}{1 + e^{\mathbf{w}'\mathbf{x}}}$$

$$P(y = 1|\mathbf{x}) = \frac{e^{\mathbf{w}'\mathbf{x}}}{1 + e^{\mathbf{w}'\mathbf{x}}}$$



Logistic regression

- odds ratio

$$\log \frac{P(y = 1|\mathbf{x})}{P(y = 0|\mathbf{x})} = \mathbf{w}'\mathbf{x}$$

- linear regression model

$$z = \log \frac{P(y = 1|\mathbf{x})}{P(y = 0|\mathbf{x})} \Rightarrow z = \mathbf{w}'\mathbf{x}$$

Logistic regression: an example

January 1986: Explosion of the Space Shuttle Challenger

launch	temp.	failure	launch	temp.	failure	launch	temp.	failure
1	53	Y	9	68	N	17	75	N
2	56	Y	10	69	N	18	75	Y
3	57	Y	11	70	N	19	76	N
4	63	N	12	70	Y	20	76	N
5	66	N	13	70	Y	21	78	N
6	67	N	14	70	Y	22	79	N
7	67	N	15	72	N	23	80	N
8	67	N	16	73	N	24	81	N

$$\text{Odds Ratio} = \ln \frac{p(x)}{1 - p(x)} = \beta_0 + \beta_1 x$$

$p(x)$ is the success probability
(failure = N) when temp. = x

Logistic regression: an example

Parameters estimate:

$$\beta_1 = 0.17$$

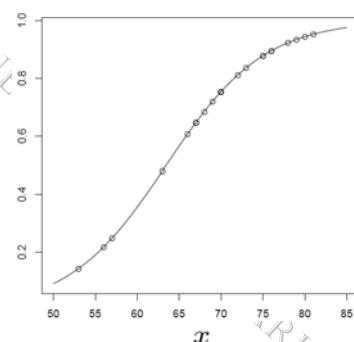
$$\beta_0 = -10.8 \text{ (intercept)}$$

Temperature when Challenger exploded
was 31°F...

... the Odds Ratio was

?

$$x = 31 \quad \text{Odds Ratio} = 0.0038 !!!$$



Classification and statistical learning theory

Choose the function $f^* \in \mathcal{H}$ (hypothesis) to minimize the empirical risk

$$R_{emp}(f) = \frac{1}{m} \sum_{i=1}^m V(y_i, f(\mathbf{x}_i))$$

Two critical issues:

- overfitting
- ill-posed optimization problem

Choose $f^* \in \mathcal{H}$ to minimize the structural risk (SRM principle)

$$\hat{R}(f) = \frac{1}{m} \sum_{i=1}^m V(y_i, f(\mathbf{x}_i)) + \lambda \|f\|_K$$

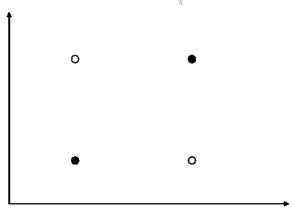
↓ ↓
loss function regularizer

Classification and statistical learning theory

Probabilistic upper bound on the expected risk (structural risk)

$$\begin{aligned} R(f) &\leq \sqrt{\frac{\gamma \log(2t/\gamma) + 1 - \log(\eta/4)}{t}} + R_{emp}(f) \\ &\leq \Psi(t, \gamma, \eta) + R_{emp}(f), \end{aligned}$$

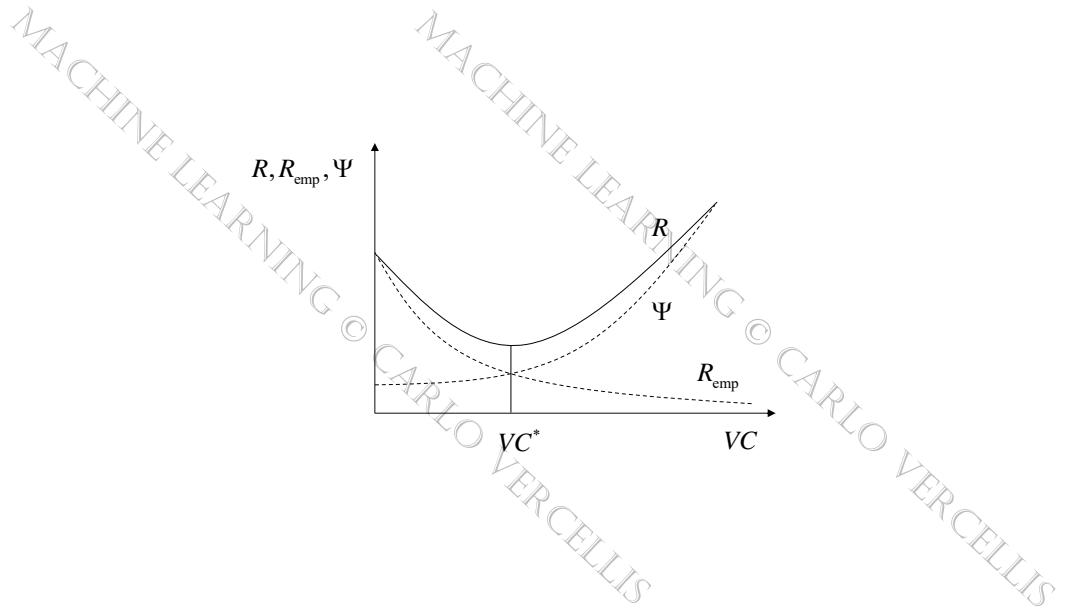
γ is the VC-dimension (Vapnik-Chervonenkis) expressing the complexity of the hypothesis space \mathcal{F}



- The VC dimension of the lines in the plane is 3

- the VC dimension of the hyperplanes in the n -dimensional space is $n+1$

Classification and statistical learning theory

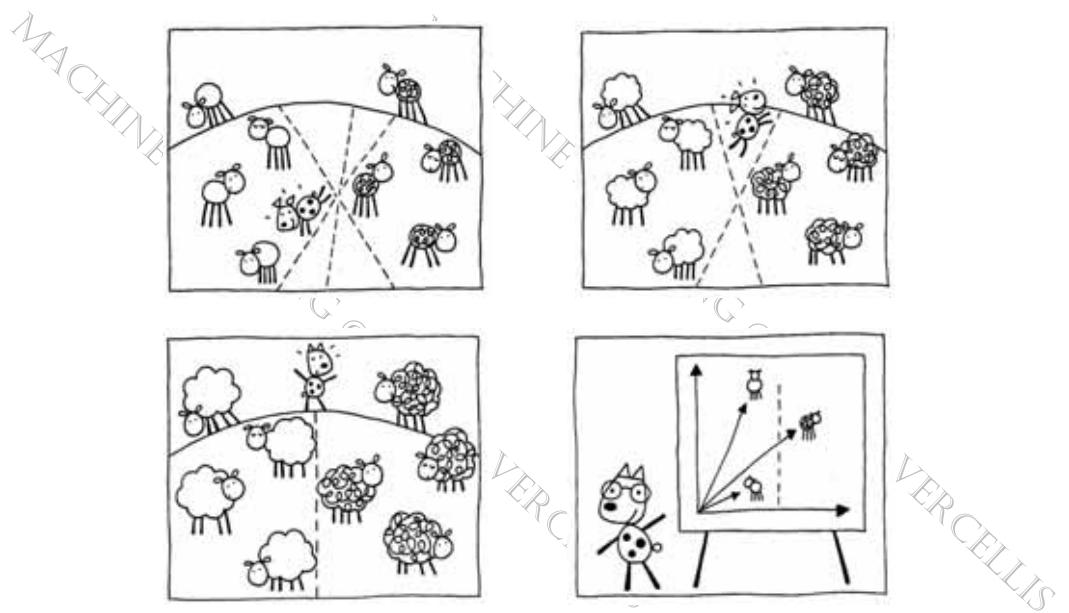


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

63

Accuracy vs. generalization

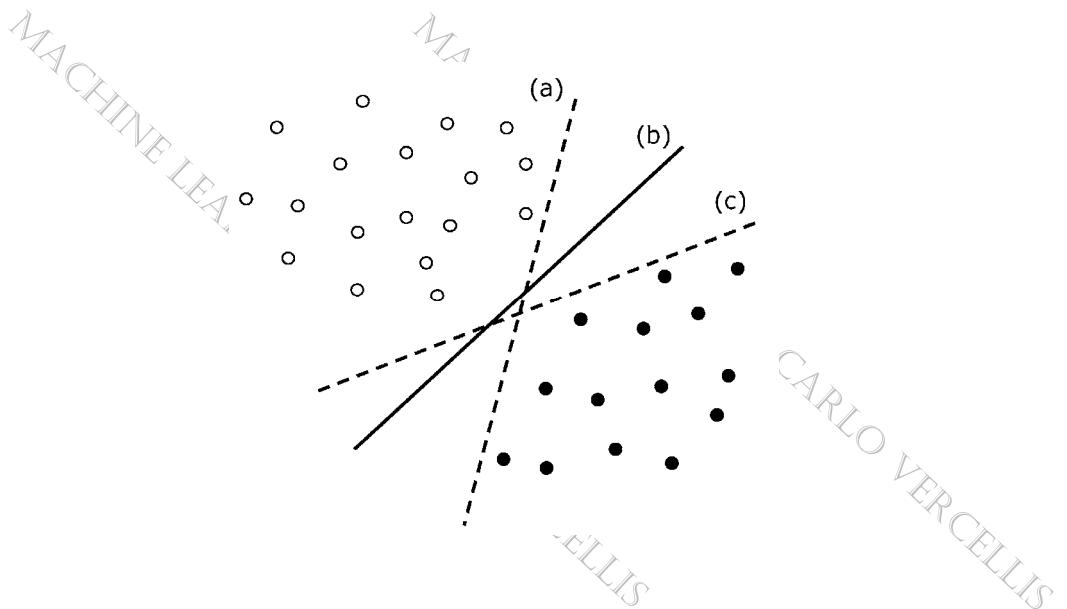


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

64

Support vector machines

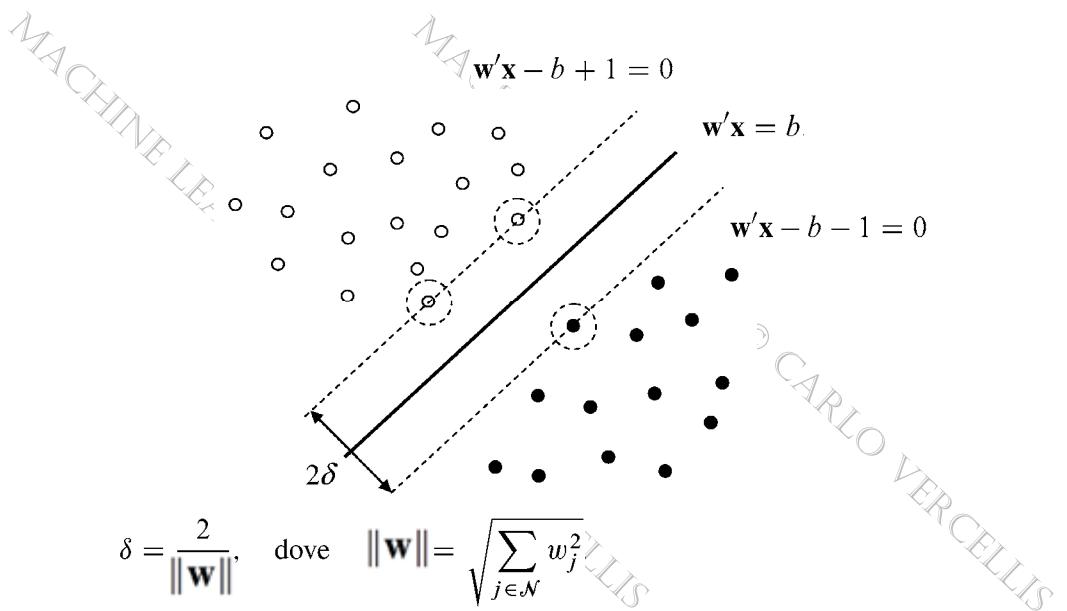


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

65

Support vector machines



Machine Learning © Carlo Vercellis

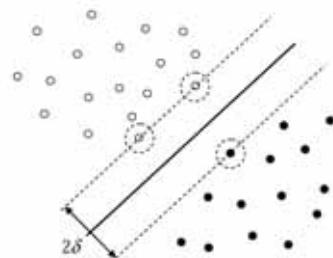
POLITECNICO MILANO 1863

66

Support vector machines: SVM formulation

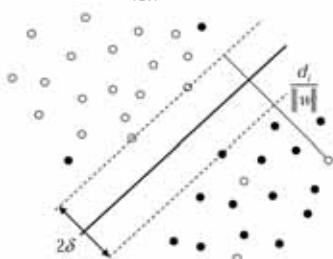
$$\text{MACH}_{\text{SVM}} \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2^2$$

$$\text{s. t. } y_i(\mathbf{w}' \mathbf{x}_i - b) \geq 1 \quad i \in \mathcal{M}^{\text{INEQ}}$$



$$\min_{\mathbf{w}, b, d} \frac{1}{2} \|\mathbf{w}\|_2^2 + \lambda \sum_{i=1}^m d_i$$

$$\text{s. t. } y_i(\mathbf{w}' \mathbf{x}_i - b) \geq 1 - d_i \quad i \in \mathcal{M}^{\text{EQ}} \\ d_i \geq 0 \quad i \in \mathcal{M}^{\text{LL}}$$



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

67

Support vector machines

$$L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \frac{1}{2} \|\mathbf{w}\|^2 + \lambda \sum_{i=1}^m d_i$$

$$- \sum_{i=1}^m \alpha_i [y_i(\mathbf{w}' \mathbf{x}_i - b) - 1 - d_i] - \sum_{i=1}^m \mu_i d_i$$

$$\frac{\partial L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu})}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i = \mathbf{0},$$

$$\frac{\partial L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu})}{\partial b} = \lambda - \alpha_i - \mu_i = 0,$$

$$\frac{\partial L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu})}{\partial \mathbf{d}} = \sum_{i=1}^m \alpha_i y_i = 0,$$

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

68

Support vector machines

$$\mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i,$$

$$\lambda = \alpha_i + \mu_i,$$

$$\sum_{i=1}^m \alpha_i y_i = 0.$$

$$L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{k=1}^m y_i y_k \alpha_i \alpha_k \mathbf{x}_i' \mathbf{x}_k$$

Support vector machines

Lagrangian function

$$L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \frac{1}{2} \|\mathbf{w}\|^2 + \lambda \sum_{i=1}^m d_i - \sum_{i=1}^m \alpha_i [y_i (\mathbf{w}' \mathbf{x}_i - b) - 1 + d_i] - \sum_{i=1}^m \mu_i d_i$$

Representation form

$$\mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i$$

Lagrangian function expressed as

$$L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{h=1}^m y_i y_h \alpha_i \alpha_h \mathbf{x}_i' \mathbf{x}_h$$

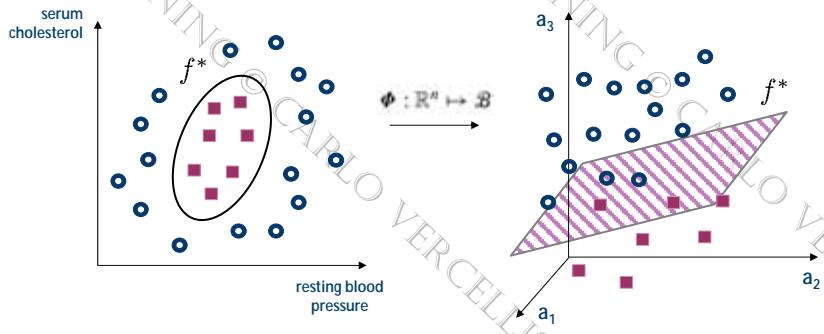
Prediction

$$f(\mathbf{x}) = \text{sgn}(\mathbf{w}' \mathbf{x} - b)$$

Nonlinear separation with SVM

Kernel methods: projection of the original input data into a higher dimensional Hilbert space, in an efficient way due to kernels

- Vapnik, 1998, Statistical learning theory
- Scholkopf & Smola, 2002, Learning with kernels
- Shawe-Taylor & Cristianini, 2006, Kernel methods for pattern analysis



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

71

Nonlinear separation with SVM

Kernel

$$\Phi(\mathbf{x}_i)' \Phi(\mathbf{x}_h) = k(\mathbf{x}_i, \mathbf{x}_h)$$

Lagrangean function

$$L(\mathbf{w}, b, \mathbf{d}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{h=1}^m y_i y_h \alpha_i \alpha_h k(\mathbf{x}_i, \mathbf{x}_h)$$

- Existence of meaningful kernel functions is guaranteed by Mercer Theorem

- polynomial kernels

- radial basis kernels

- neural networks kernels

$$k(\mathbf{x}_i, \mathbf{x}_h) = (\mathbf{x}_i' \mathbf{x}_h + 1)^d$$

$$k(\mathbf{x}_i, \mathbf{x}_h) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_h\|^2}{2\sigma^2}\right)$$

$$k(\mathbf{x}_i, \mathbf{x}_h) = \tanh(\kappa \mathbf{x}_i' \mathbf{x}_h - \delta)$$

Prediction

$$f(\mathbf{x}) = \text{sgn} \left(\sum_{i=1}^m \alpha_i y_i \Phi(\mathbf{x})' \Phi(\mathbf{x}_i) - b \right)$$

Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

72

Support vector machines

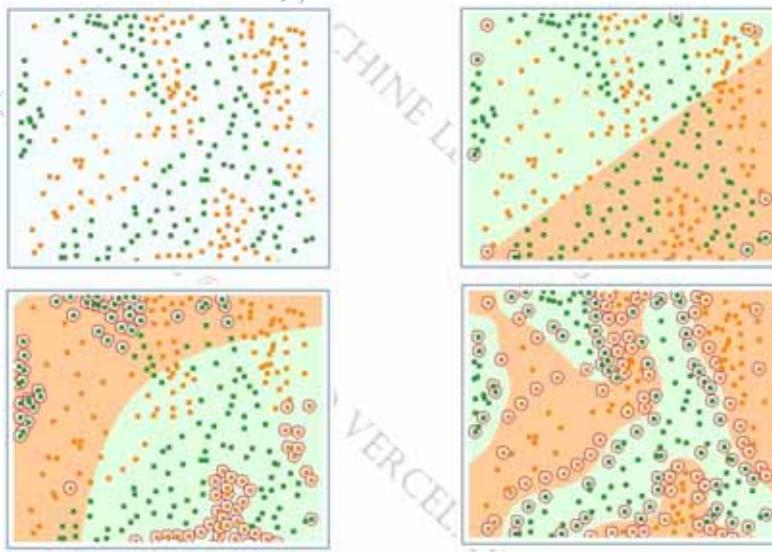
- complementarity conditions (KKT theorem)

$$\alpha_i[y_i(\mathbf{w}'\mathbf{x}_i - b) - 1 + d_i] = 0, \quad i \in \mathcal{M}$$

$$\mu_i(\alpha_i - \lambda) = 0, \quad i \in \mathcal{M}$$

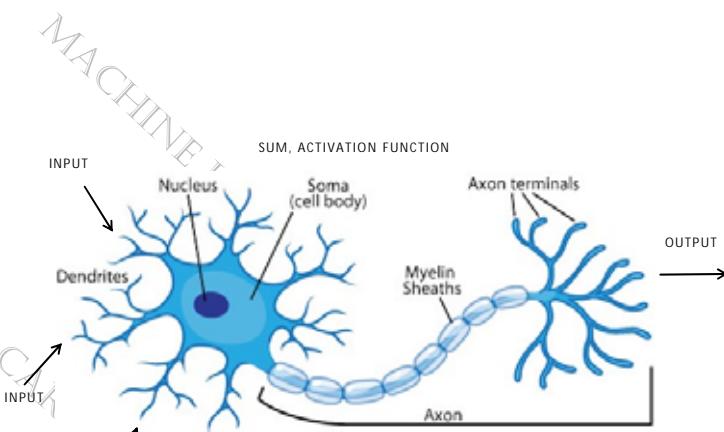
- the observations for which $0 < \alpha < \lambda$ are at distance $\frac{1}{\|\mathbf{w}\|}$ from separating hyperplane and therefore lie on the canonical hyperplanes: **support vectors**

SVM: linear and nonlinear learning with kernels



Neural networks: brain analogy

- It takes inputs (signals) from its dendrites (i.e. other neurons).
- The signals received from the dendrites are joined in the soma (a weighted sum of these inputs is computed).
- The result is passed on to the axon hillock (a specialized part of the soma that controls the firing of the neuron).
- If the weighted sum (i.e. total strength of the signal) is larger than a threshold limit, the neuron fires, otherwise it stays at rest.
- The state of the neuron (on/off) propagates through its axon and is passed on to the other connected neurons via its synapses.

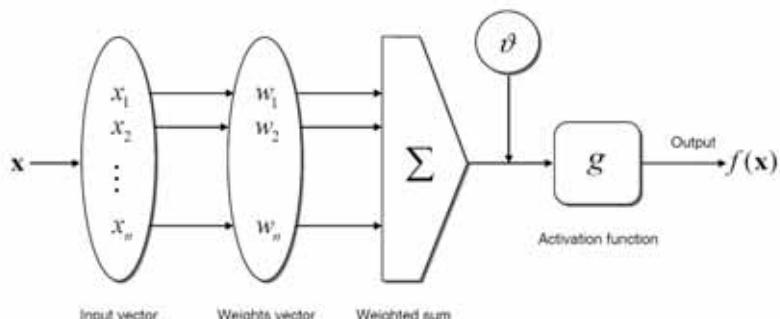


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

75

Neural networks (artificial): perceptron



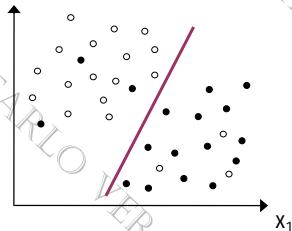
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

76

Neural networks

separation by a hyperplane
 $z = w_1x_1 + w_2x_2 + \dots + w_nx_n - \vartheta = \mathbf{w}'\mathbf{x} - \vartheta$

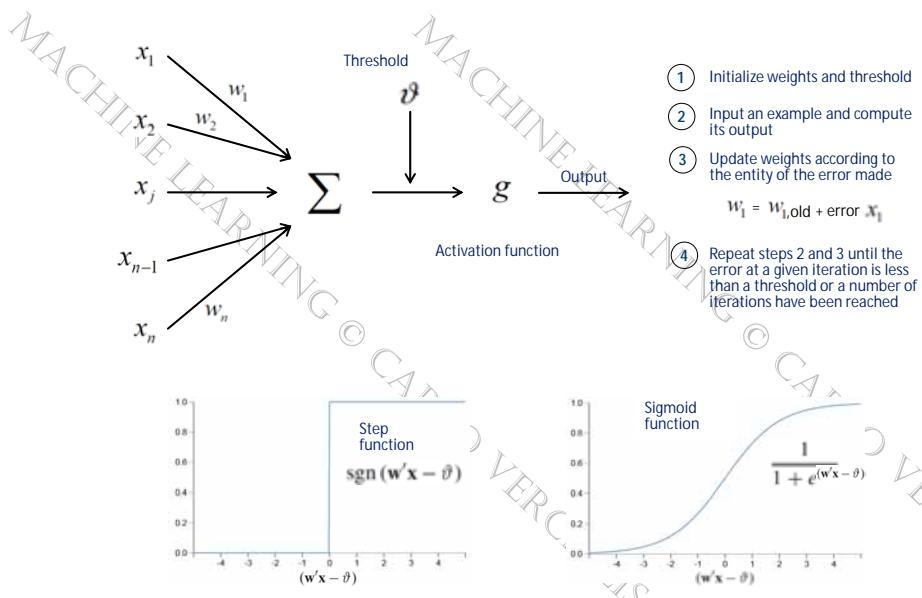


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

77

Rosenblatt's Perceptron



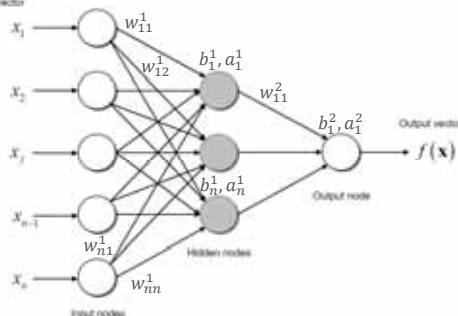
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

78

Multi-layer feed-forward neural networks

Each hidden unit can be considered as a single perceptron.

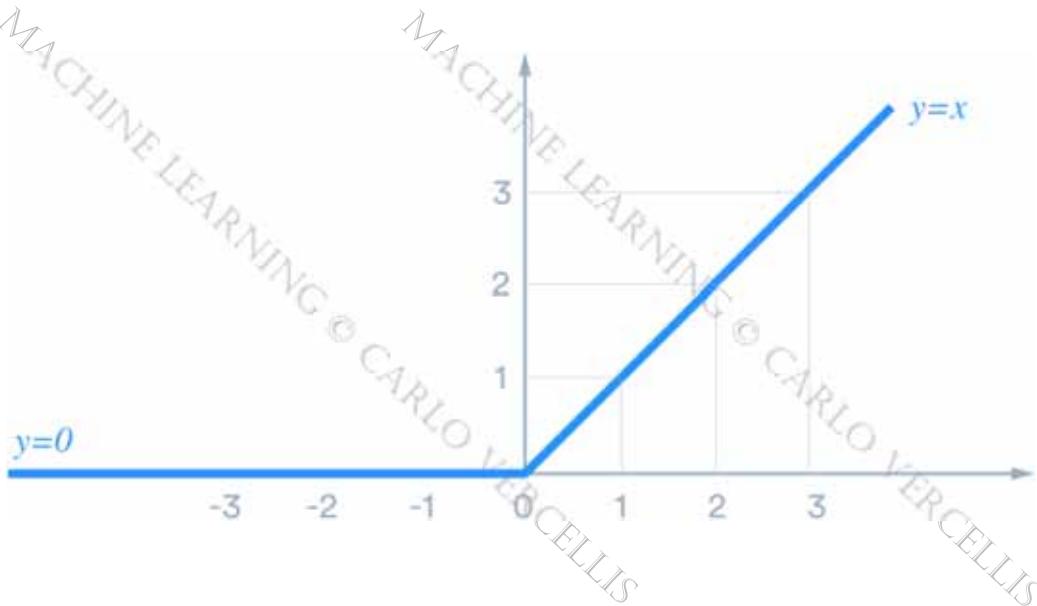


- 1 Initialize weights and threshold.
- 2 Input an example, compute its output and the corresponding error.
- 3 Starting with the output layer propagate the error back to the previous layer and update the weights according to the "strength" of the connection.
- 4 Repeat steps 2 and 3 for all the training examples.

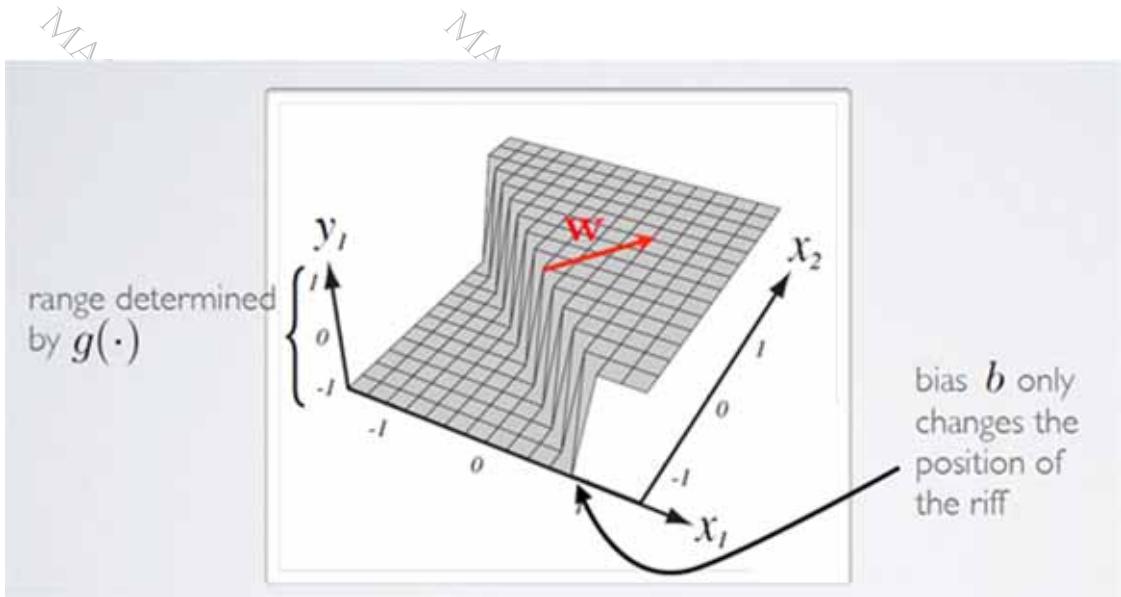
$$w_j^{(k+1)} = w_j^{(k)} + \lambda(y_i - \hat{y}_i^{(k)})x_{ij}$$

$$a_i^l = \phi(\sum_n w_{ni}^l a_n^{l-1} + b_i^l), \text{ where } \phi \text{ is the element-wise activation function}$$

ReLU activation function



Nonlinear learning

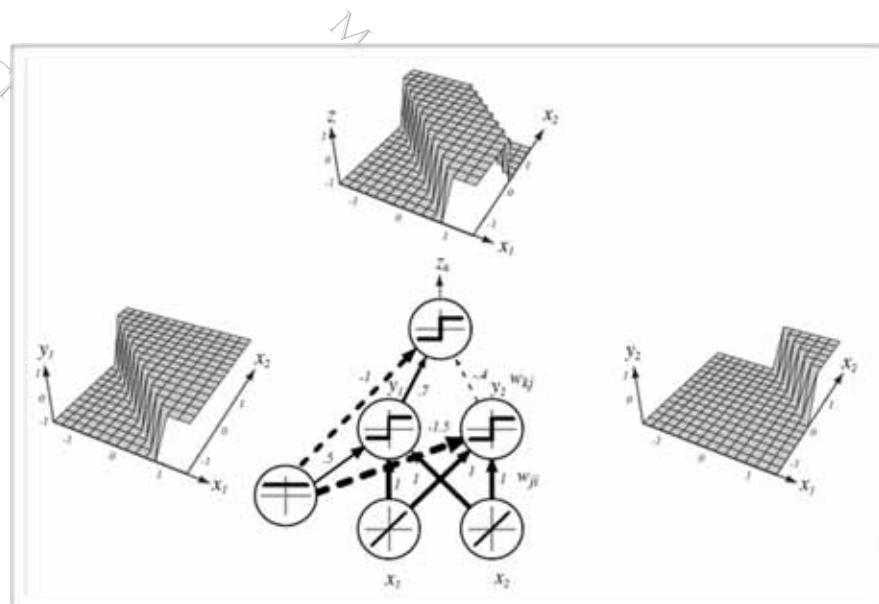


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

81

Nonlinear learning

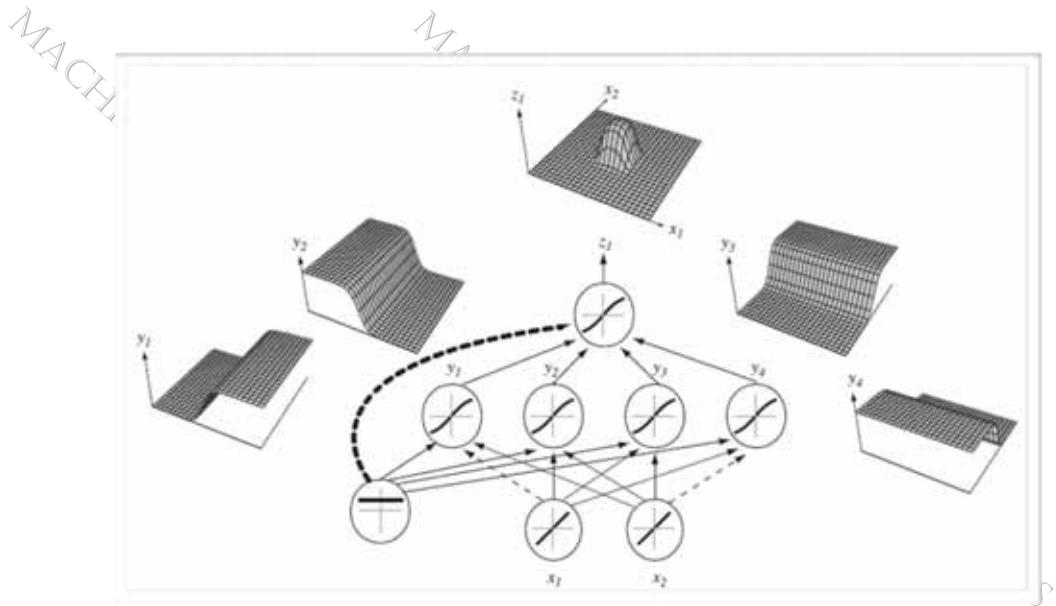


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

82

Nonlinear learning

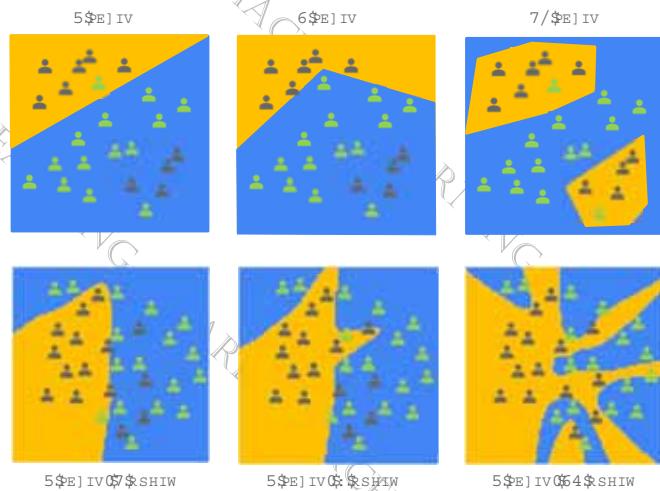


Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

83

Nonlinear learning



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

84

Deep Learning as Hierarchical Feature Learning

Machine
Learning

Deep learning can be summarized as learning both the representation and the classifier out of it

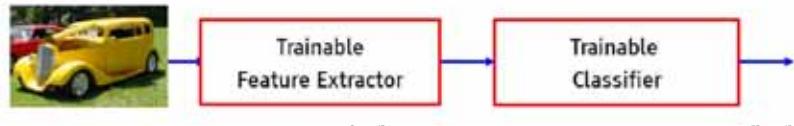
- Fixed engineered features (or kernels) + trainable classifier



VS.

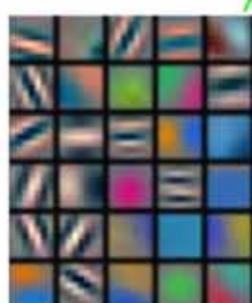
Deep
Learning

- End-to-end learning / feature learning / deep learning



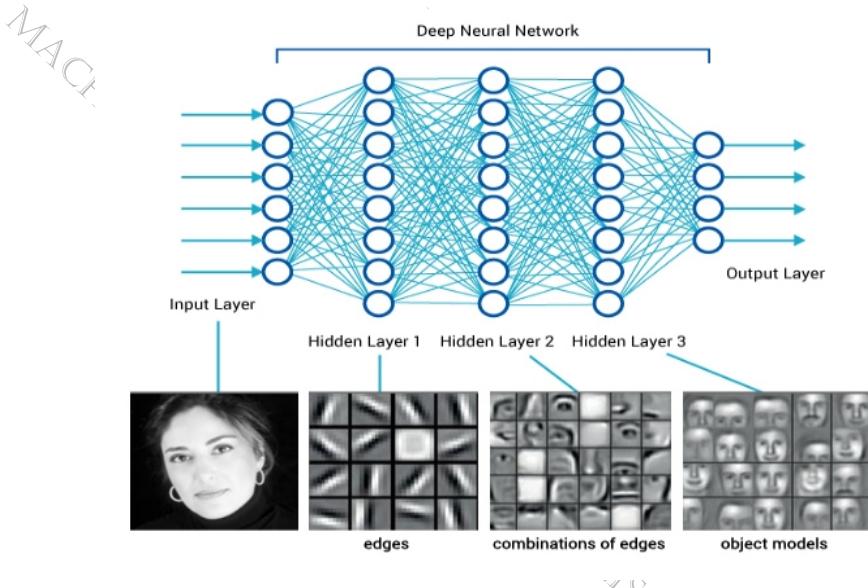
Deep Learning as Hierarchical Feature Learning

In deep learning we have multiple stages of non linear feature transformation



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

Image analysis



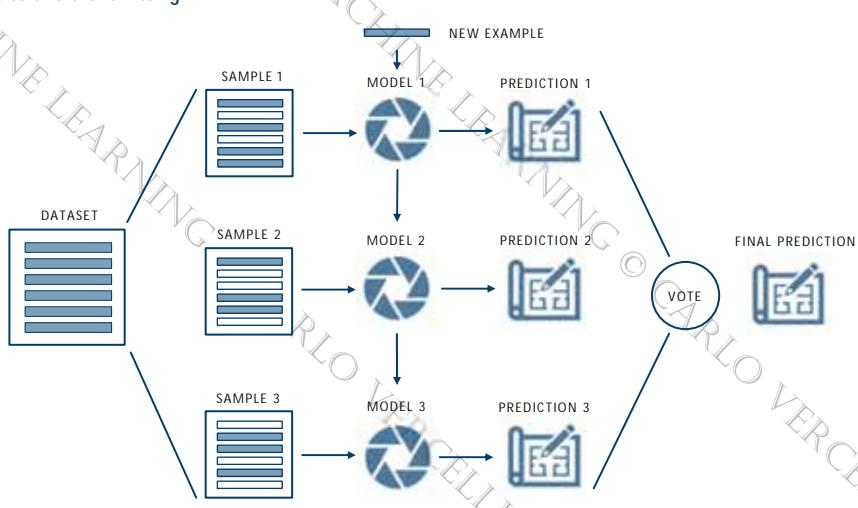
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

87

Ensemble framework: Bagging

Bagging (bootstrap aggregating) is an ensemble framework aimed at improving the stability and accuracy of a classifier. It helps to avoid overfitting.



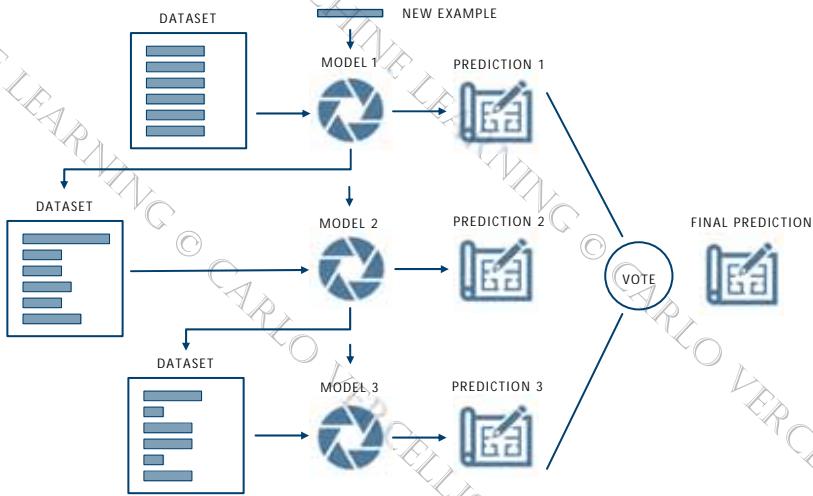
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

88

Ensemble framework : Adaptive Boosting

Adaptive Boosting (AdaBoost) is another ensemble framework. It focuses on "harder-to-classify" examples.



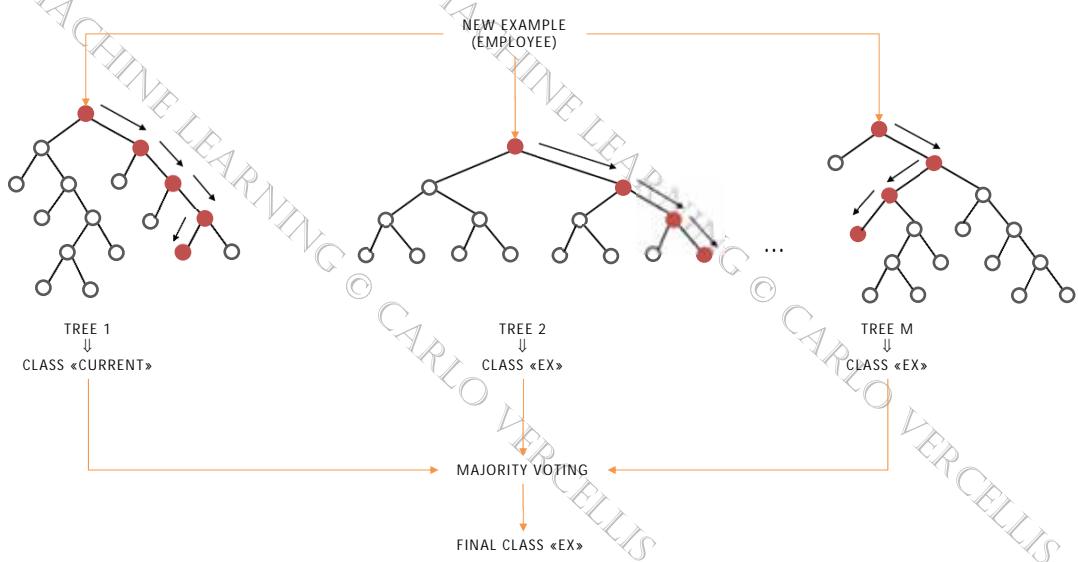
Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

89

Random Forest

Each classifier is a classification tree and is generated using a random selection of attributes at each node to determine the split.



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863

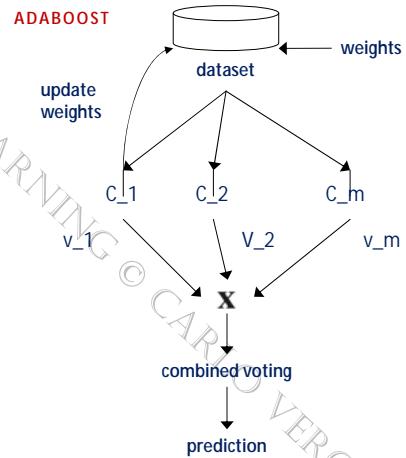
90

Adaboost

- Initially, all the weights of tuples are set the same ($1/d$)
 - Generate k classifiers in k rounds. At round i ,
 - Tuples from D are sampled (with replacement) to form a training set of the same size
 - Each tuple's chance of being selected is based on its weight
 - A classification model M_i is derived from D_i and its error rate is calculated
 - If a tuple is misclassified, its weight is increased, otherwise it is decreased
 - Error rate: $\text{err}(X_j)$ is the misclassification error of tuple X_j . Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$\text{error } (M_i) = \sum_j^d w_j \times \text{err} (\mathbf{X}_j)$$

classifier M_i 's vote is $\log \frac{1 - \text{error}(M_i)}{\text{error}(M_i)}$



Machine Learning © Carlo Vercellis

POLITECNICO MILANO 1863