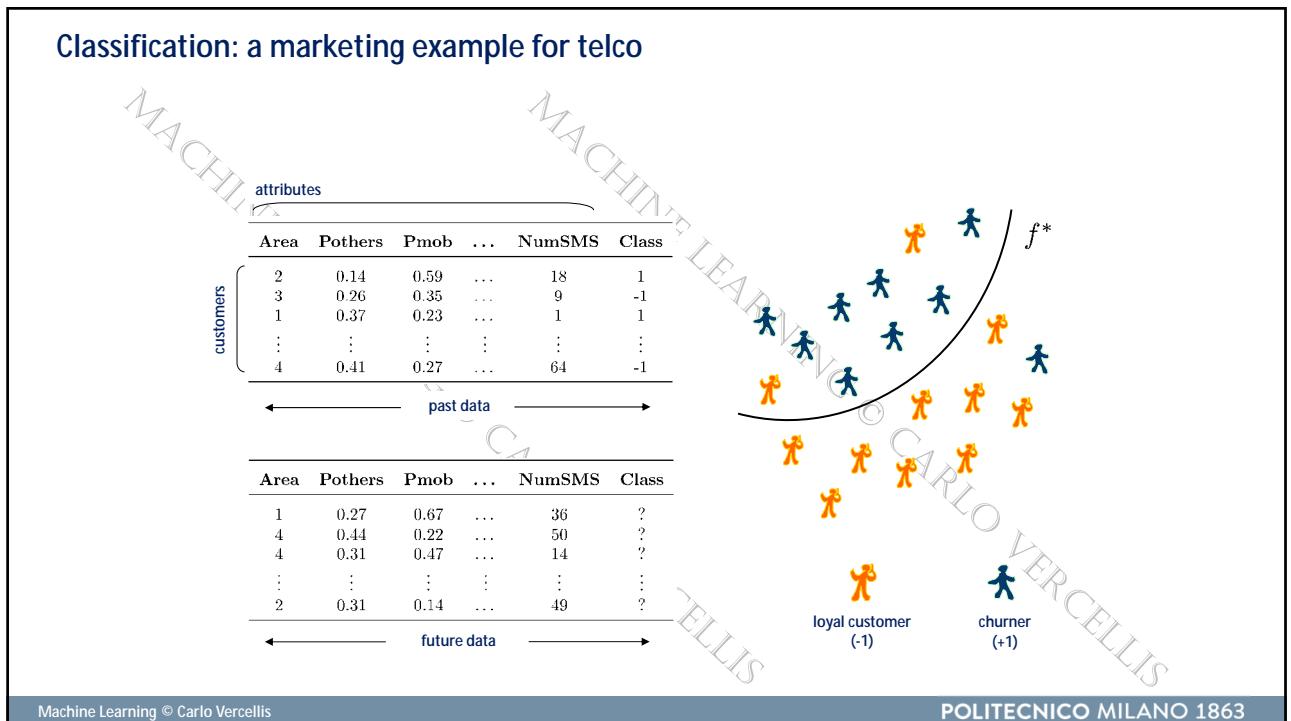




1 finding some options that optimally separates most of good from bads



2

Classification: prediction of HIV protease-cleavable peptides

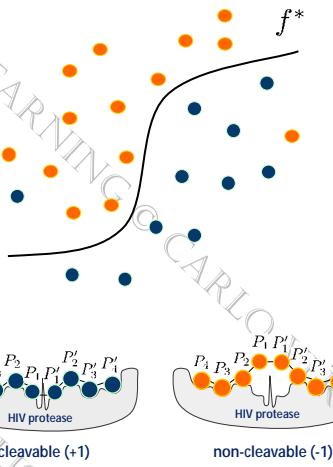
attributes

| | 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



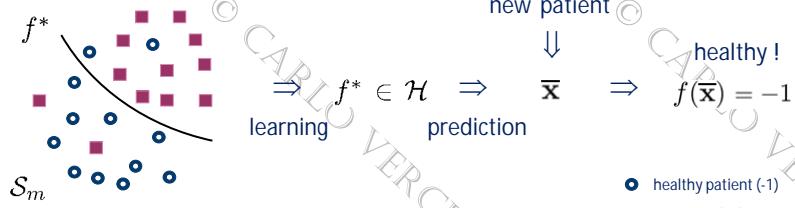
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Classification as a learning task

- $\mathcal{S}_m = \{(\mathbf{x}_i, y_i), i \in \mathcal{M}\}$ 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



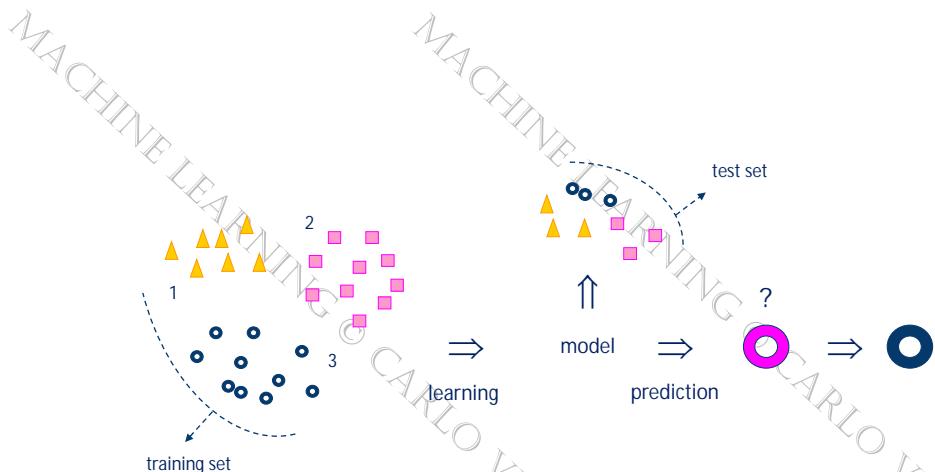
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4

2

Classification models



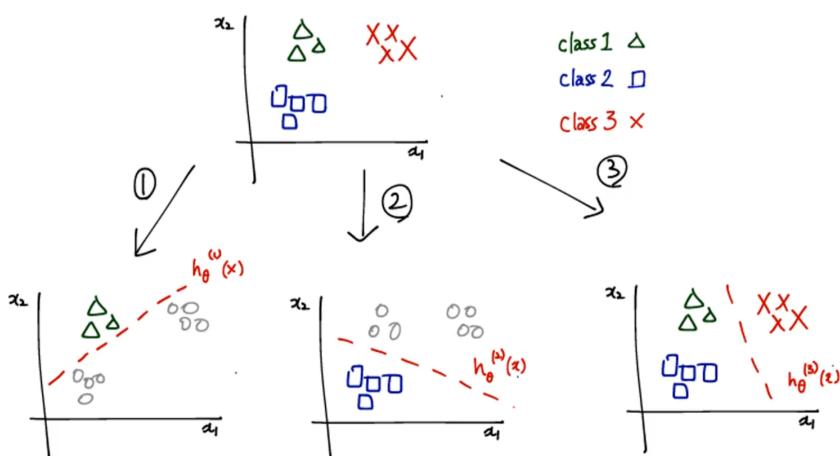
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5

Multi-class Approaches: 1-against-all

multi category ==> binary problems



generate K category, three binary problems, we solve it and come back by majority voting to the main problem which was multi ...

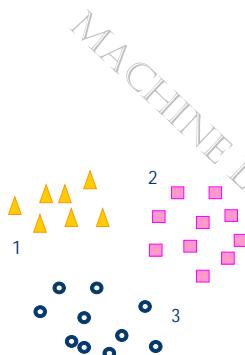
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3

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



- Train K binary classifiers
 - Class 1 against {2,3,...K}
 - Class 2 against {1,3,...K}
 -
 - Class K against {1,2,...K-1}
- Predict for a new record by applying the K trained classifiers and assigning the label by majority voting

around robin (k number of category, take pairs of classification then based on majority)

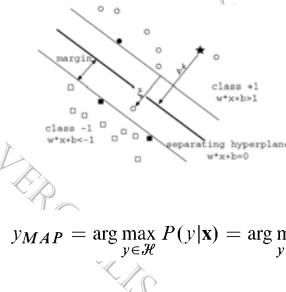
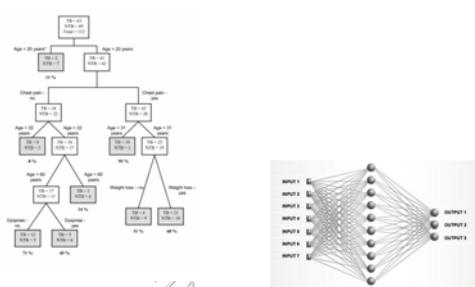
time consuming!

- Train K(K-1)/2 binary classifiers
 - Class 1 against {2}
 - Class 1 against {3}
 -
 - Class K-1 against {K}

- Predict for a new record by applying the K(K-1)/2 trained classifiers and assigning the label by majority voting

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



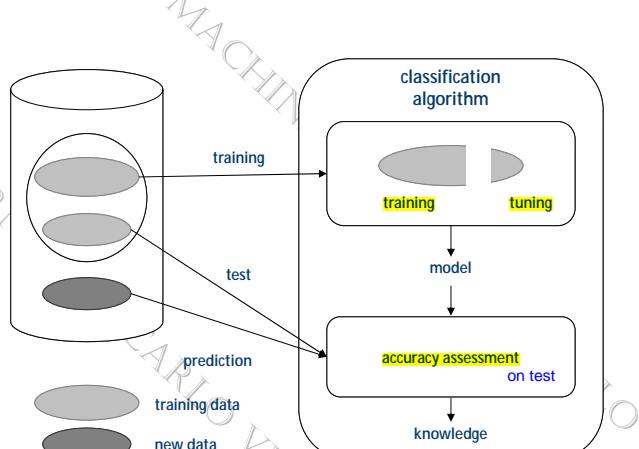
$$y_{MAP} = \arg \max_{y \in \mathcal{H}} P(y|x) = \arg \max_{y \in \mathcal{H}} \frac{P(x|y)P(y)}{P(x)}$$

criteria for evaluating / how to compare

Assessing classification methods

- **Prediction accuracy** several metrics in next slide
- **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

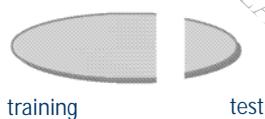
$$R_{\text{emp}} = \frac{1}{m} \sum_{i=1}^m L(f(\mathbf{x}_i))$$

average number of miscalssifications

Prediction accuracy

- Prediction accuracy can be estimated through four main approaches:

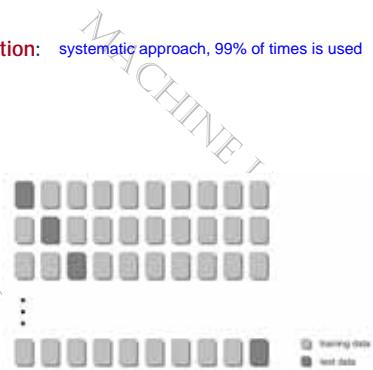
- holdout method:



- repeated random sampling method: repeated applications of holdout method

Prediction accuracy

- **k-fold cross-validation:** systematic approach, 99% of times is used
- **leave-one-out method:** k-fold with $k=m$
best approximation of accuracy

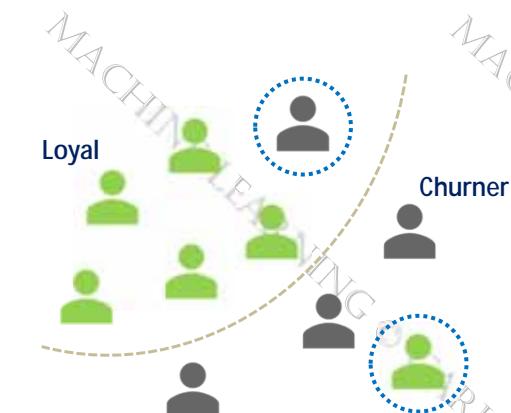


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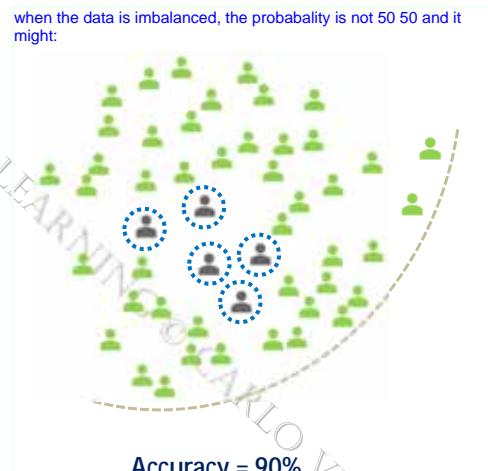
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Model evaluation



Accuracy = % accurate predictions = 80%
Error = 100 - Accuracy = 20%



Accuracy = 90%
Error = 10%

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Confusion matrix contingency tables

- 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

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

بنابراین ما فرض می‌کنیم، فکر کن و قتنی هیچ سلسی نسبت به کاست نداریم میگیریم

۱ تذکر به صورت دلخواه بین کارشناسان پیدا ممکن خواهد بود

Geometric mean

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

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ROC curves recieving operating characteristics

the top one is higher and better

for different models these are obtained

area under the ROC curve => the greater the better

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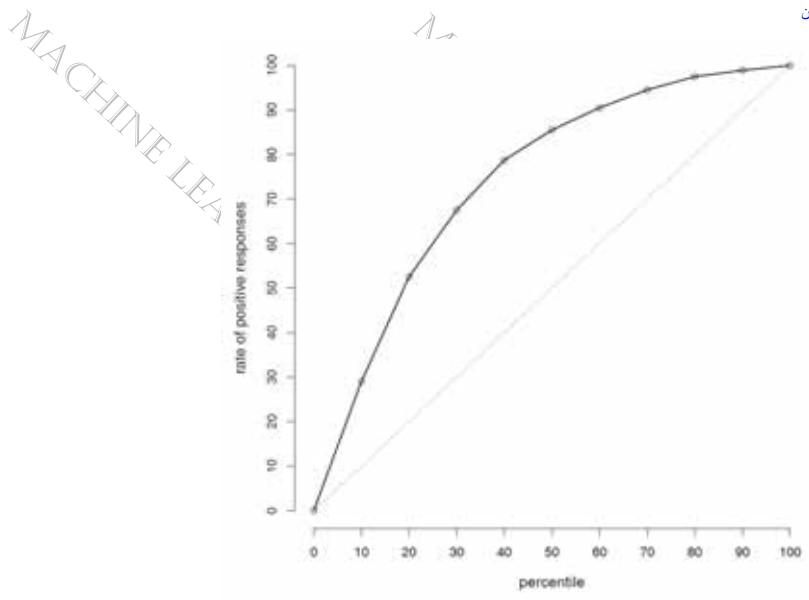
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هیچ مدلی نسبت که توانی همه متريک ها بهتر باشه ... برای همين ما باید انتخاب کنیم

Cumulative gain

رندوم یعنی ۵۰٪ پس خط چین یعنی این ... شبیه به انداختن کوین
... خوبی نفهمیدم دقیقاً چه شکلی تحلیل میشه



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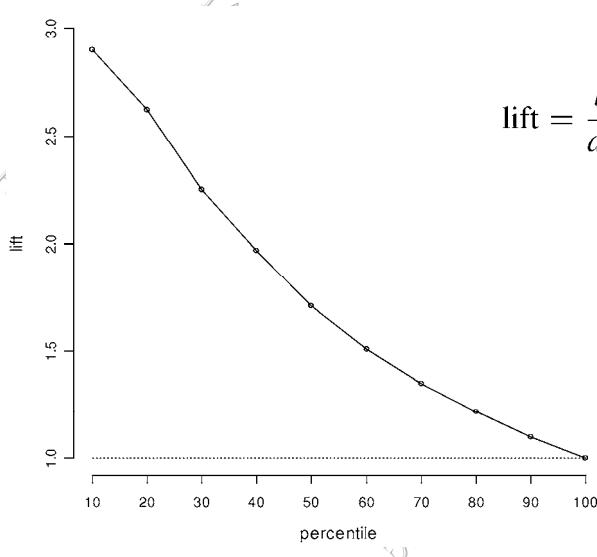
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Lift

$$\text{lift} = \frac{b/s}{a/m}$$

بن نقطه و خیچین ریشو گرفت فک کنم



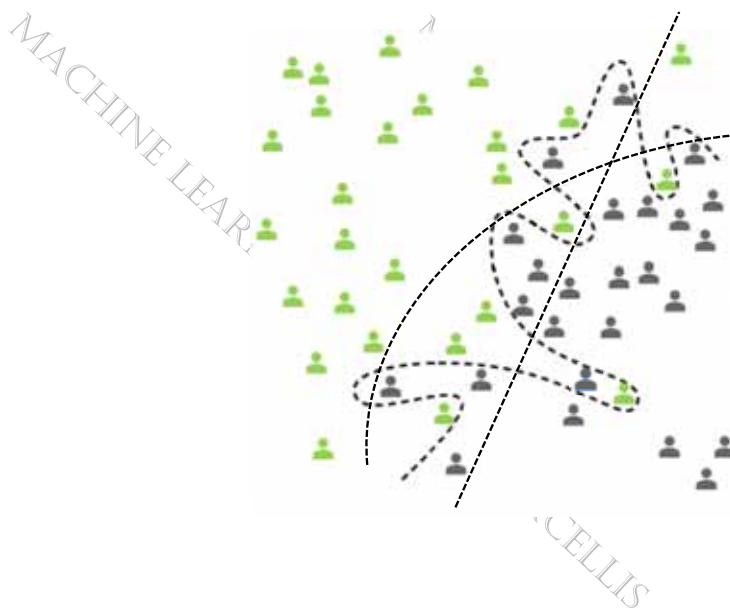
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if accuracy of training set is larger than test set ==>>> overfitting Alert

Overfitting

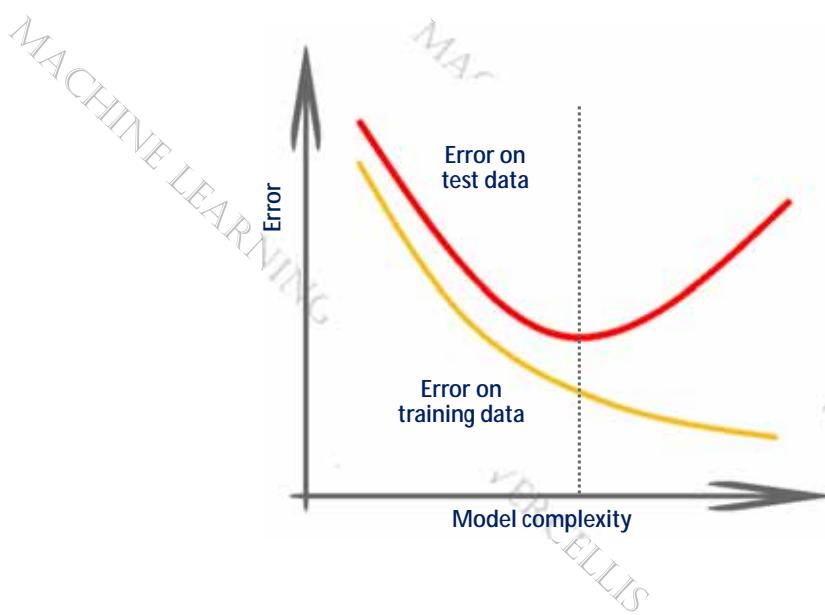


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Bias-variance trade-off



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10

Numerical representation of categorical variables

we need numerical expect for classification trees and bayesian methods

- 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 are under the curve | | | | | | |
|---|-------|-------|-------|-----------|--------|--|
| 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

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

MACHIN
Show: Number of instances

| | | Predicted | | |
|--------|---|-----------|-----|----------|
| | | 0 | 1 | Σ |
| Actual | 0 | 561 | 35 | 596 |
| | 1 | 94 | 226 | 320 |
| | | Σ | 655 | 261 916 |

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Confusion matrix for different methods on Heart dataset

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

MACHIN
Show: Proportion of actual

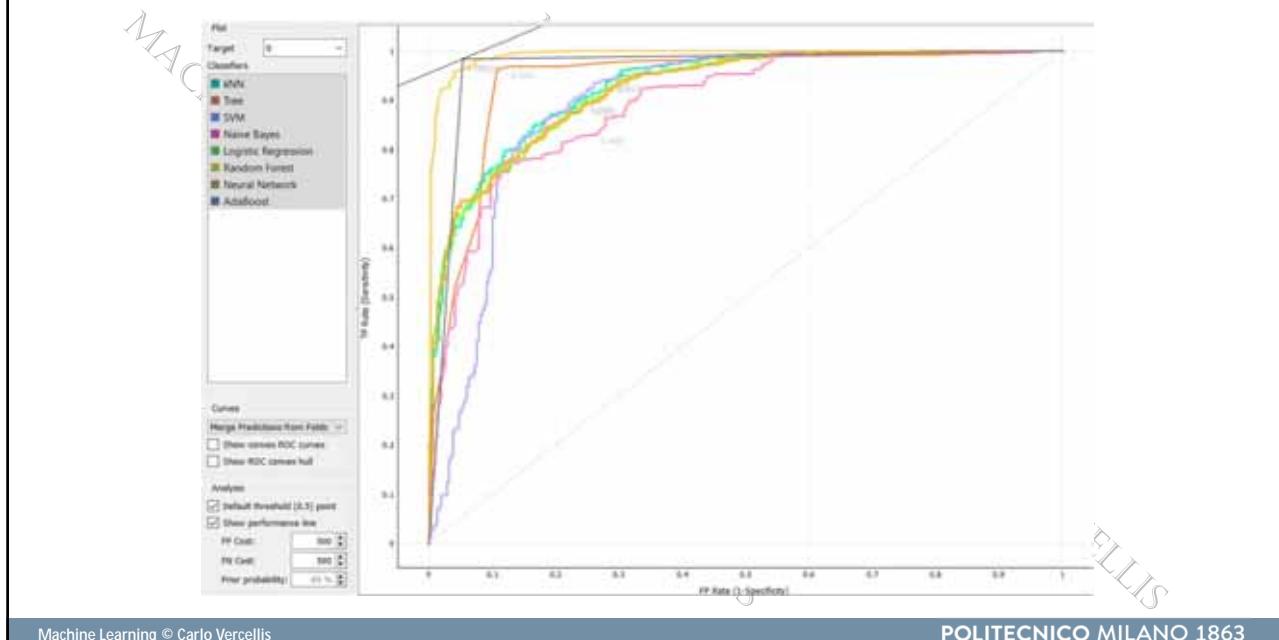
| | | Predicted | | |
|--------|---|-----------|--------|----------|
| | | 0 | 1 | Σ |
| Actual | 0 | 94.1 % | 5.9 % | 596 |
| | 1 | 29.4 % | 70.6 % | 320 |
| | | Σ | 655 | 261 916 |

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ROC curve for different methods on Heart dataset



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1st algo. no training phase, predicting based on distances

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

فاحصه با هر کدوم رو بررسی میکنه و نزدیک ترین رو به عنوان نیل انتخاب میکنه.

هایبر پارامتر رو با اکسپریمنت انتخاب میکنیم

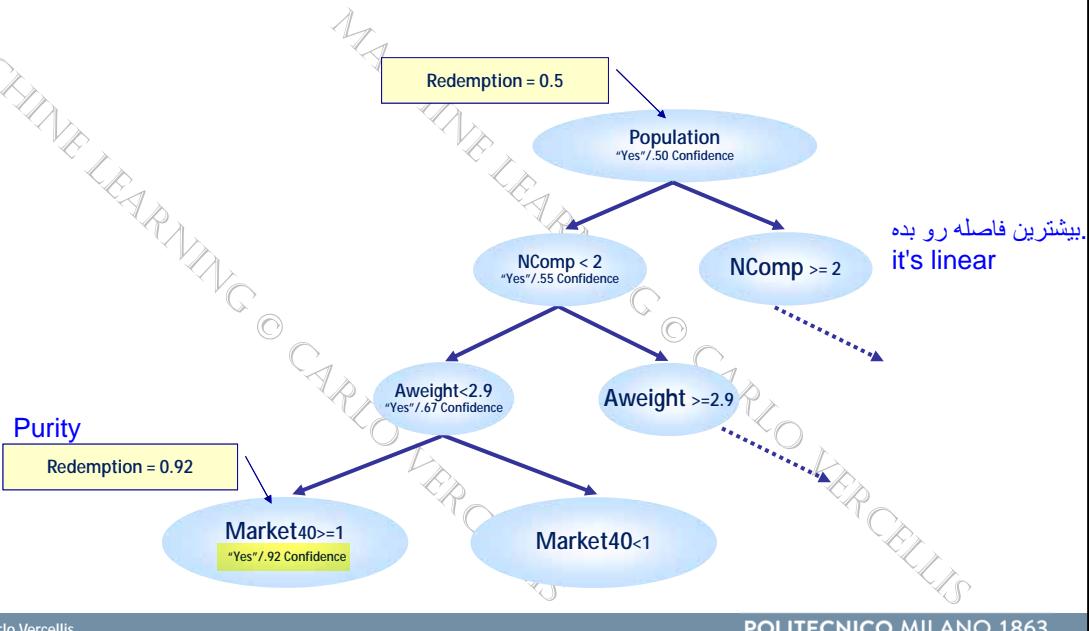
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Session Oct 16th

Business case automotive – customer acquisition



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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.

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Classification trees

- Classification trees are distinguished in:

- binary trees

- general trees

and in

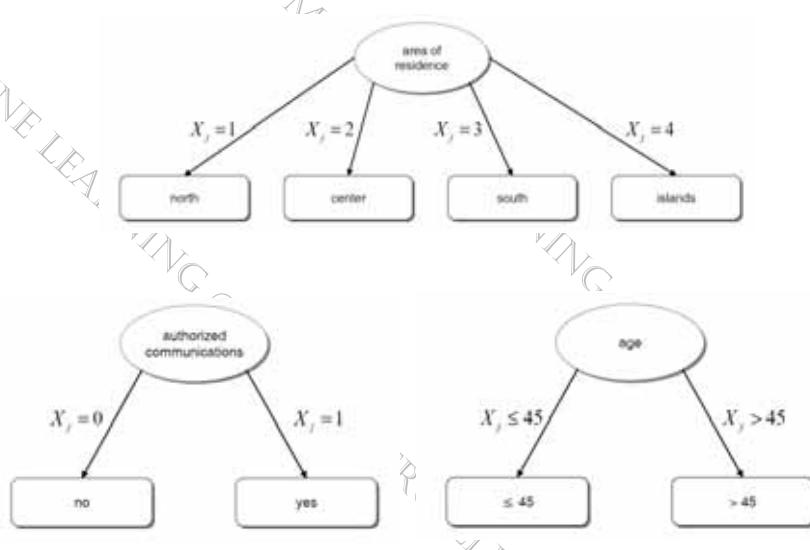
- univariate trees (or axis parallel)

$$\Rightarrow X_j \leq b$$

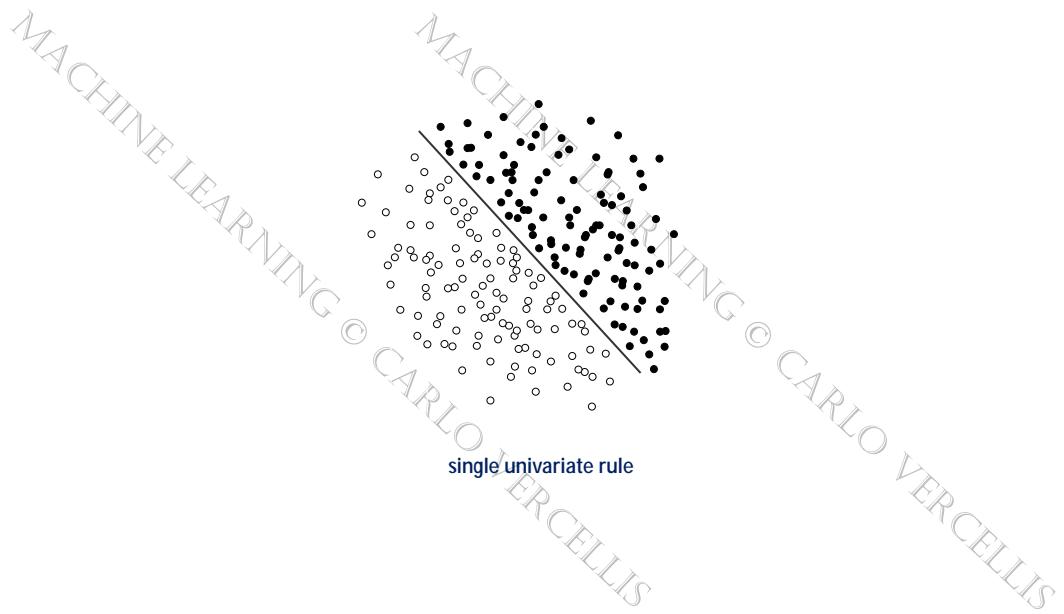
- multivariate trees (or oblique)

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

Classification trees



Classification trees

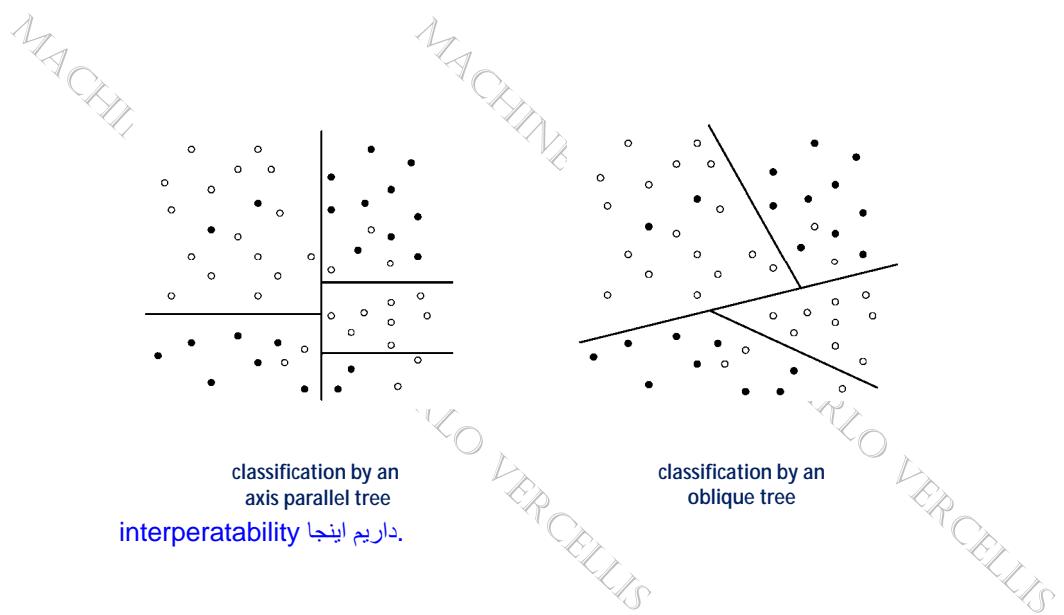


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Classification trees



classification by an
axis parallel tree

interpretability
داریم اینجا

classification by an
oblique tree

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

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Classification trees

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

- Main criteria for splitting

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

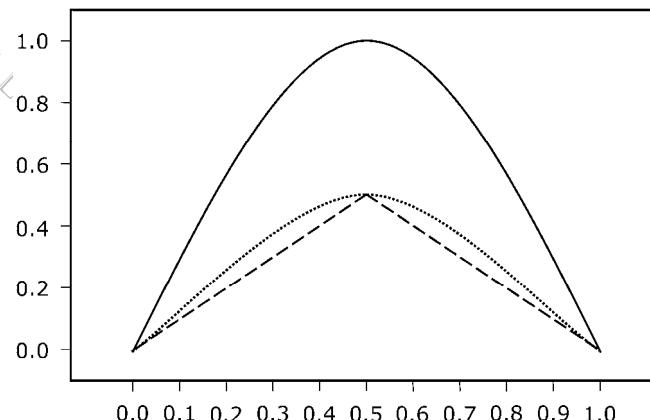
- entropy index $\text{Entropy}(q) = - \sum_{h=1}^H p_h \log_2 p_h$

- 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

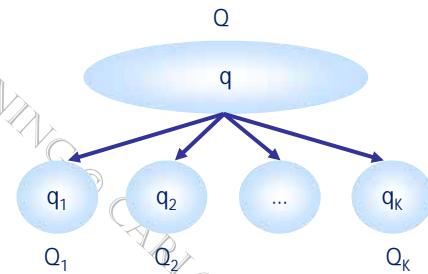
- Impurity of a splitting rule

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

- 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

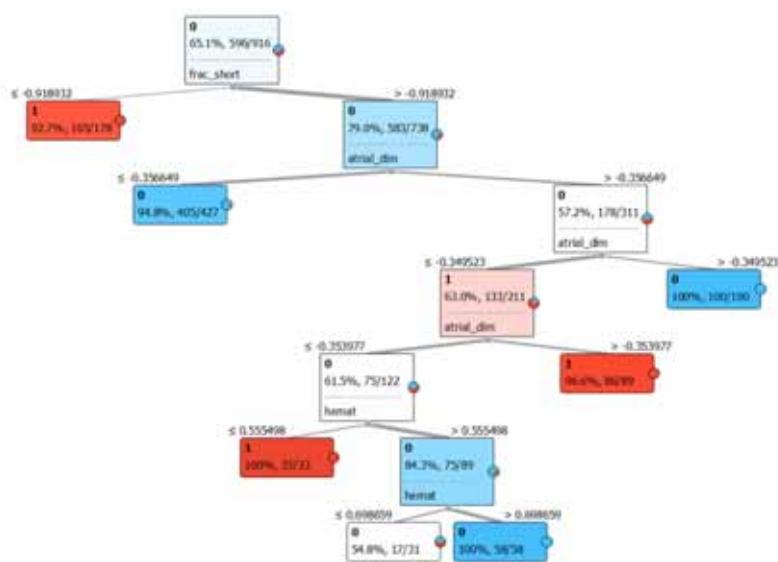
$$I_G(q) = \text{Gini}(q) = 1 - \left(\frac{13}{23}\right)^2 - \left(\frac{10}{23}\right)^2 = 0.491.$$

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

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

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

Classification tree for the Heart dataset



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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

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

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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

$$\begin{aligned} P(\text{area} = 1 | \text{churner} = 0) &= \frac{5}{13}, & P(\text{area} = 1 | \text{churner} = 1) &= \frac{1}{10}, \\ P(\text{area} = 2 | \text{churner} = 0) &= \frac{2}{13}, & P(\text{area} = 2 | \text{churner} = 1) &= \frac{3}{10}, \\ P(\text{area} = 3 | \text{churner} = 0) &= \frac{5}{13}, & P(\text{area} = 3 | \text{churner} = 1) &= \frac{2}{10}, \\ P(\text{area} = 4 | \text{churner} = 0) &= \frac{1}{13}, & P(\text{area} = 4 | \text{churner} = 1) &= \frac{4}{10}. \end{aligned}$$

Pothers

$$\begin{aligned} P(\text{Pothers} = 1 | \text{churner} = 0) &= \frac{2}{13}, & P(\text{Pothers} = 1 | \text{churner} = 1) &= \frac{5}{10}, \\ P(\text{Pothers} = 2 | \text{churner} = 0) &= \frac{3}{13}, & P(\text{Pothers} = 2 | \text{churner} = 1) &= \frac{4}{10}, \\ P(\text{Pothers} = 3 | \text{churner} = 0) &= \frac{3}{13}, & P(\text{Pothers} = 3 | \text{churner} = 1) &= 0, \\ P(\text{Pothers} = 4 | \text{churner} = 0) &= \frac{5}{13}, & P(\text{Pothers} = 4 | \text{churner} = 1) &= \frac{1}{10}. \end{aligned}$$

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

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

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

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

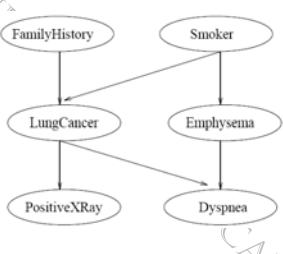
$$= 0.81 \cdot 10^{-5} \cdot 0.56 = 0.46 \cdot 10^{-5},$$

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

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

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

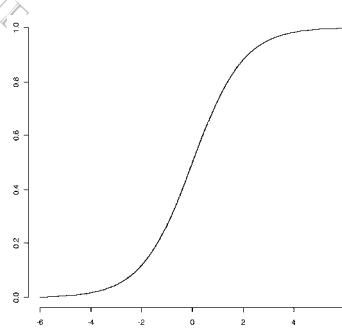
- A logistic function (sigmoid)

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

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:

$$\beta_1 = 0.17$$

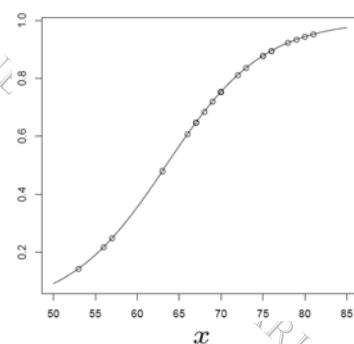
$$\beta_0 = -10.8 \text{ (intercept)}$$

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)

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

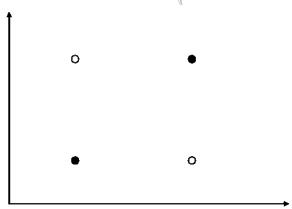
↓ ↓
loss function regularizer

Classification and statistical learning theory

Probabilistic upper bound on the expected risk (structural risk)

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

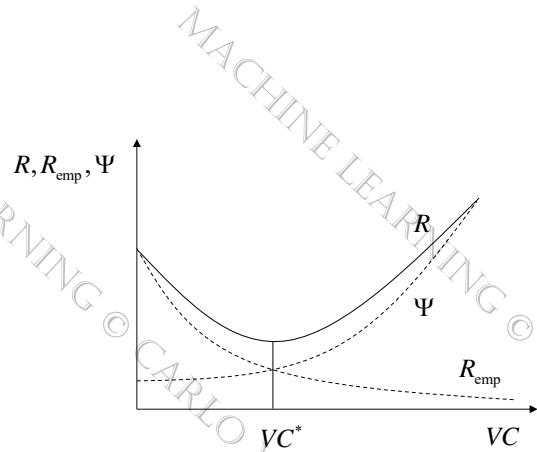
γ is the VC-dimension (Vapnik-Chervonenkis) expressing the complexity of the hypothesis space \mathcal{F}



- 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

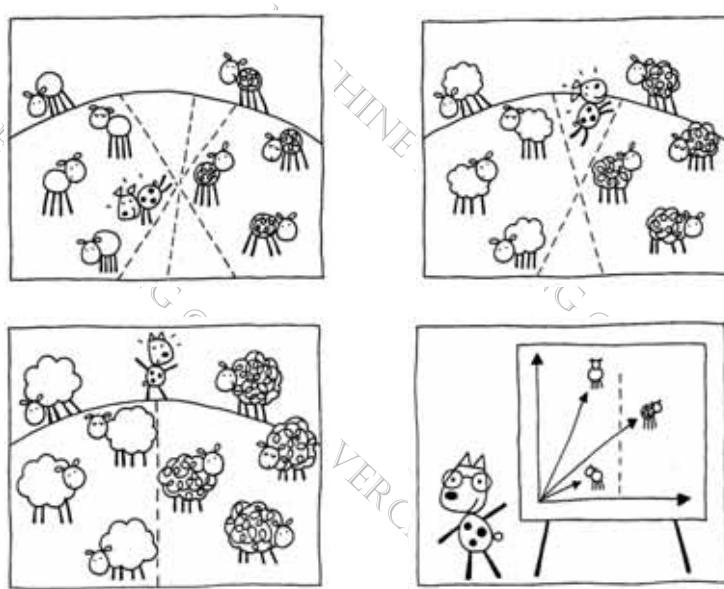


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Accuracy vs. generalization

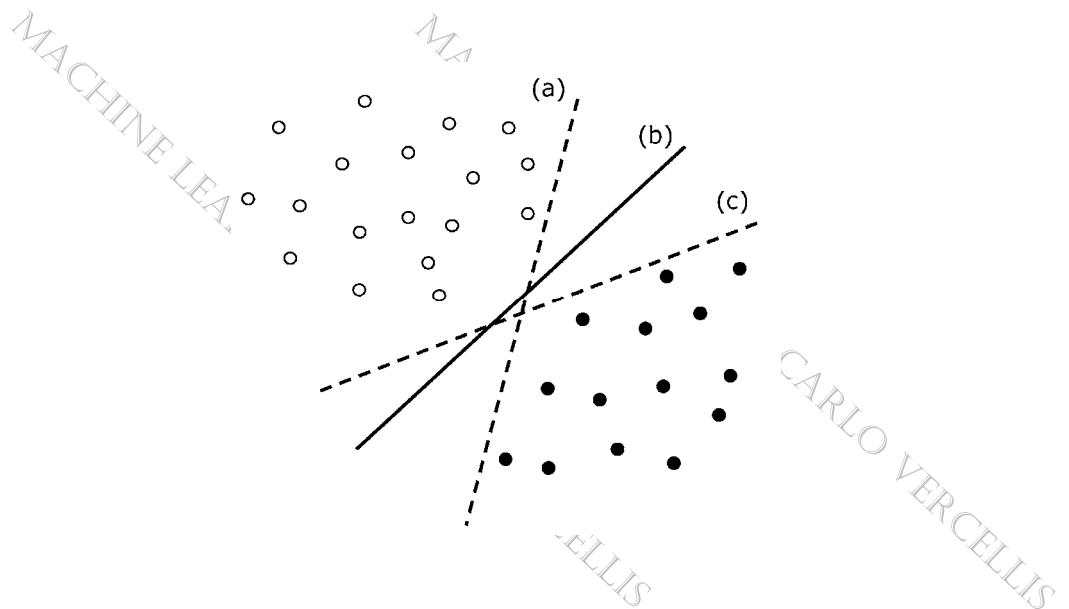


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Support vector machines

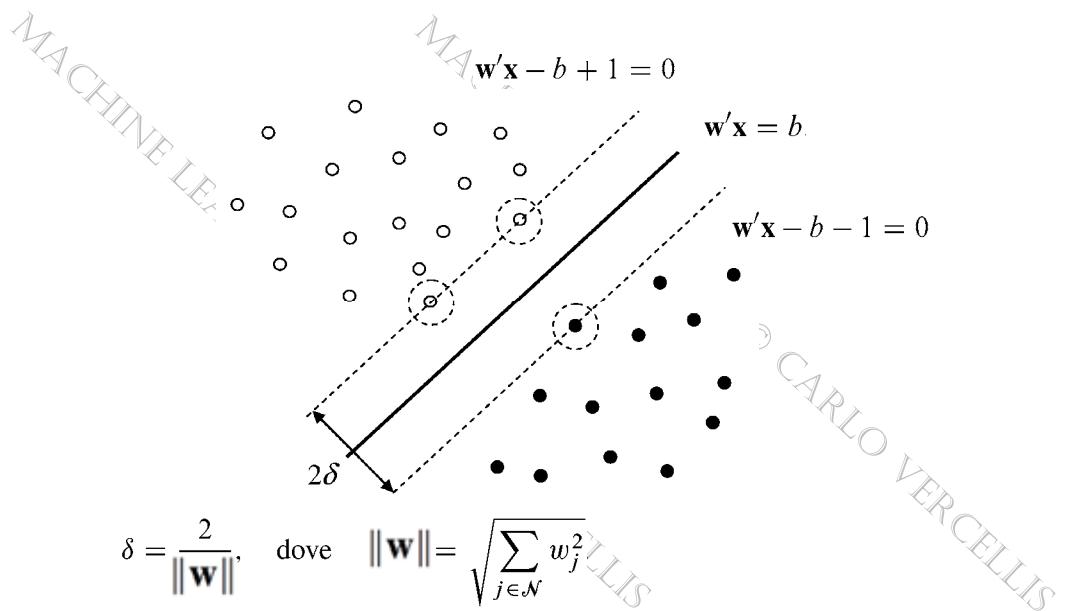


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Support vector machines



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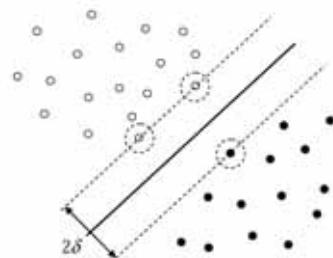
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Support vector machines: SVM formulation

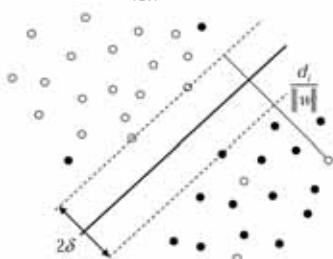
$$\text{MACH}_{\text{SVM}} \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2^2$$

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



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

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



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Support vector machines

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

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

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

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

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

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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

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

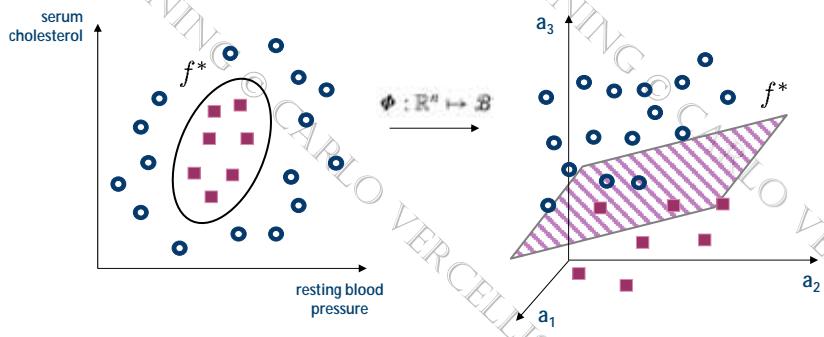
Prediction

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

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



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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

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

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Support vector machines

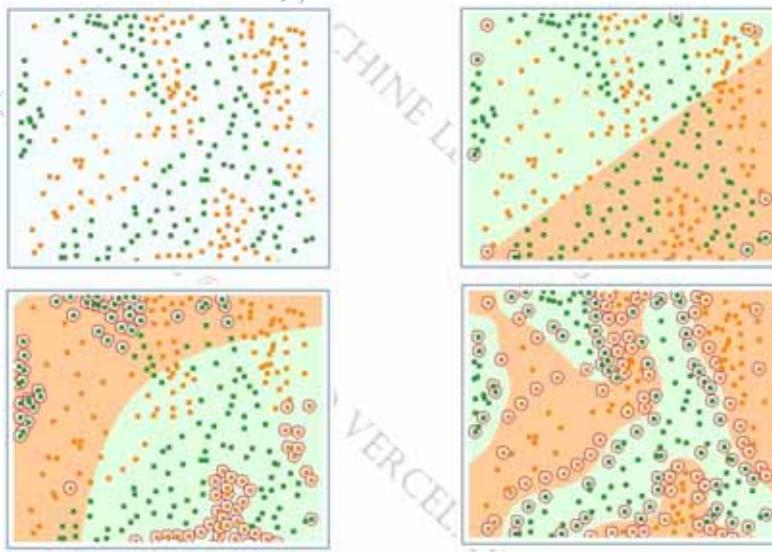
- complementarity conditions (KKT theorem)

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

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

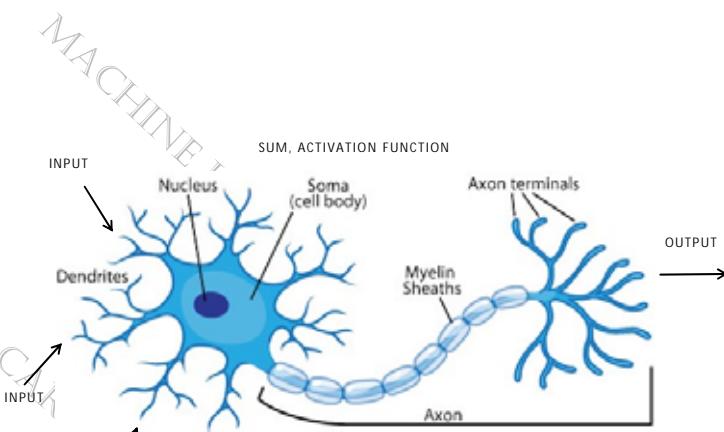
- the observations for which $0 < \alpha < \lambda$ are at distance $\frac{1}{\|\mathbf{w}\|}$ from separating hyperplane and therefore lie on the canonical hyperplanes: **support vectors**

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.

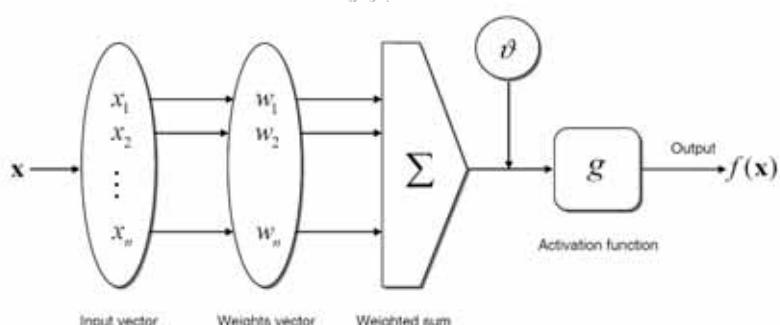


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Neural networks (artificial): perceptron



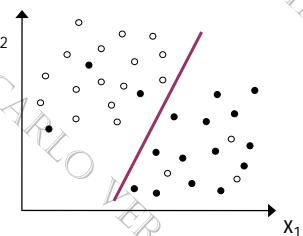
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Neural networks

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

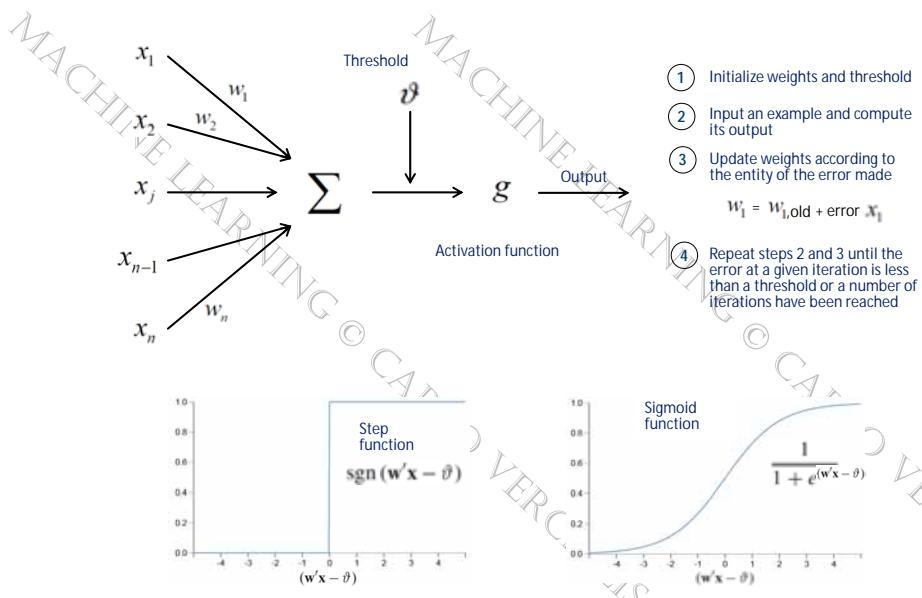


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Rosenblatt's Perceptron



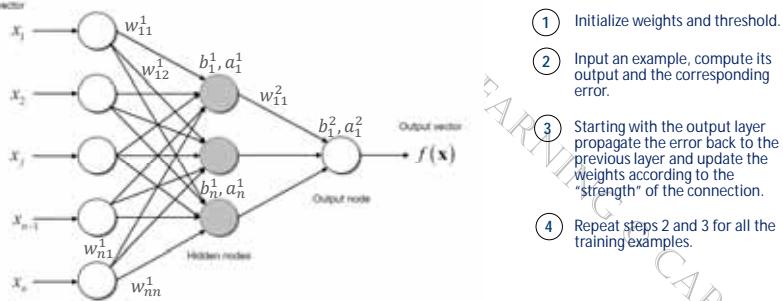
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Multi-layer feed-forward neural networks

Each hidden unit can be considered as a single perceptron.

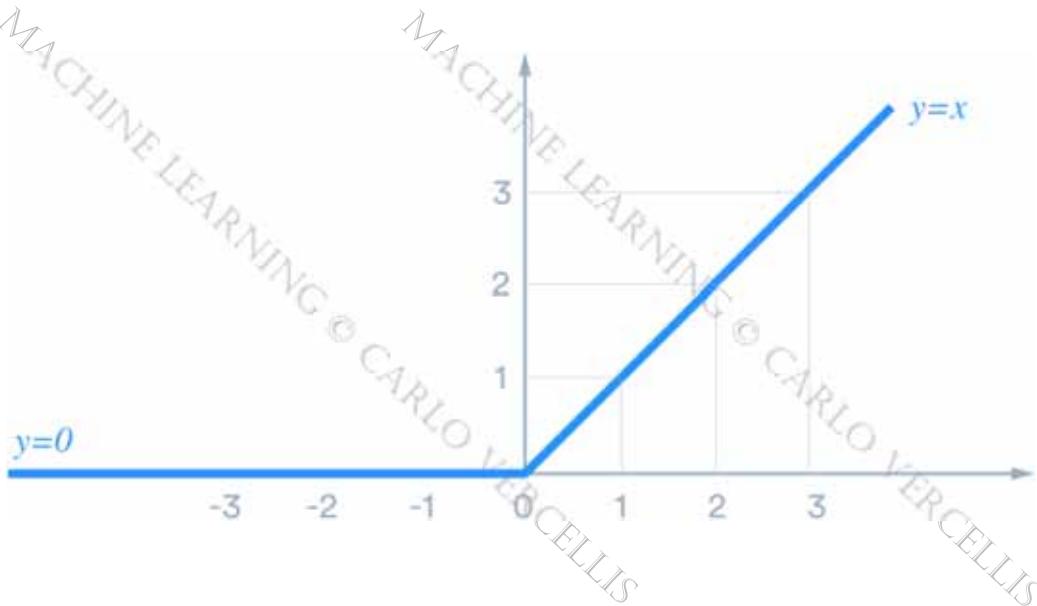


- 1 Initialize weights and threshold.
- 2 Input an example, compute its output and the corresponding error.
- 3 Starting with the output layer propagate the error back to the previous layer and update the weights according to the "strength" of the connection.
- 4 Repeat steps 2 and 3 for all the training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

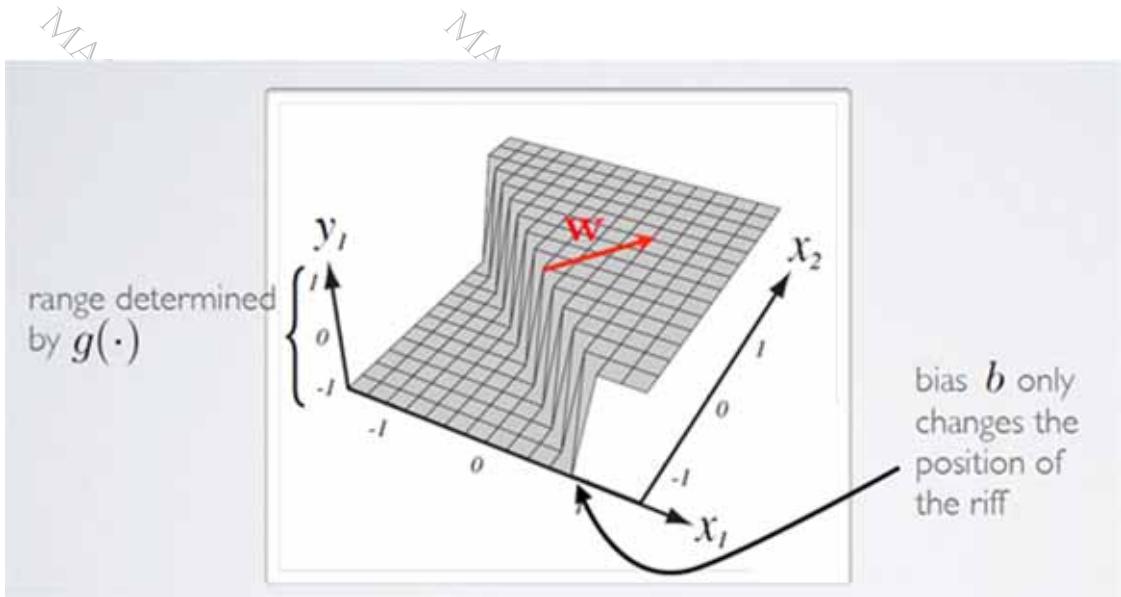
$$w_j^{(k+1)} = w_j^{(k)} + \lambda(y_i - \hat{y}_i^{(k)})x_{ij}$$

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

ReLU activation function



Nonlinear learning

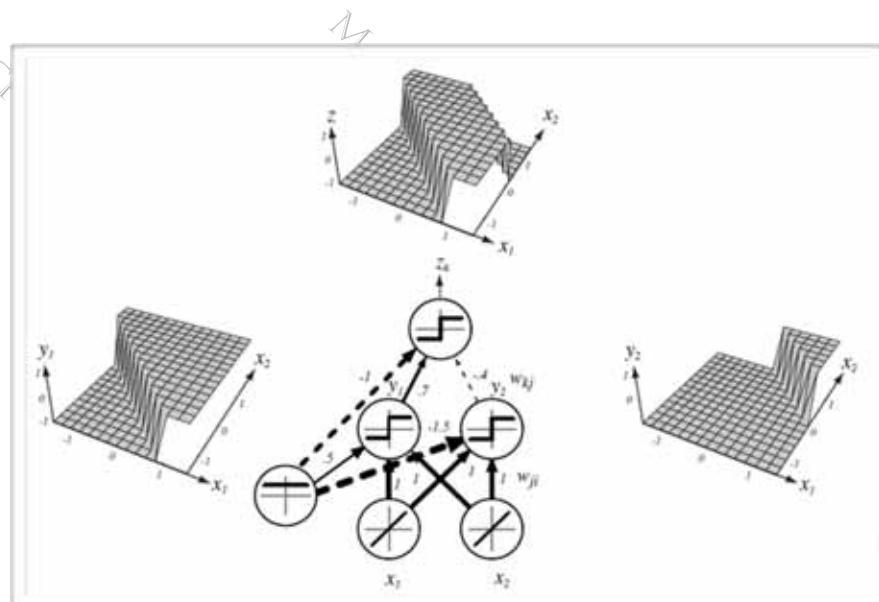


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Nonlinear learning

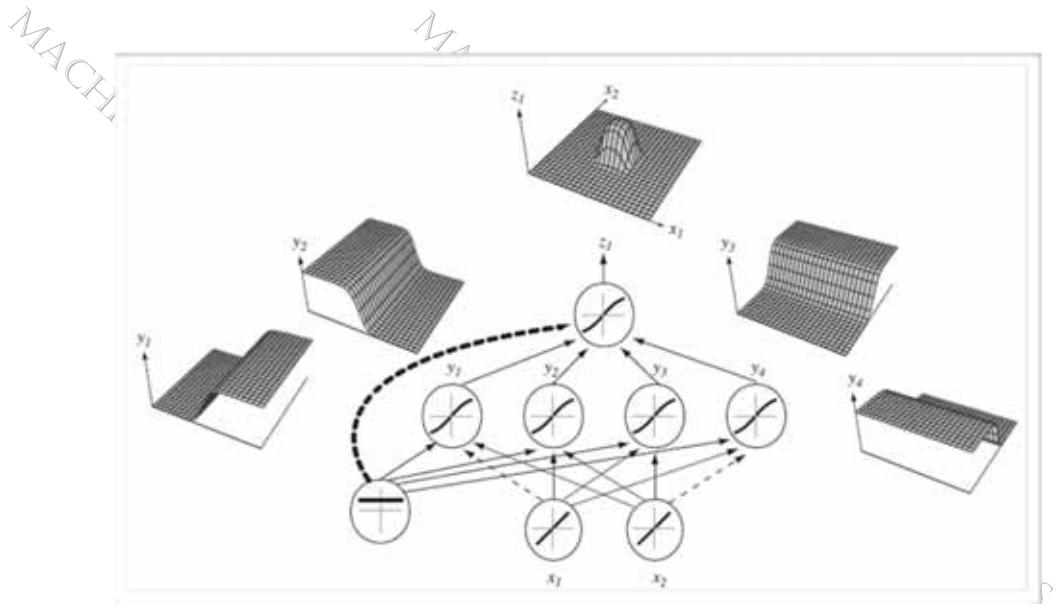


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Nonlinear learning

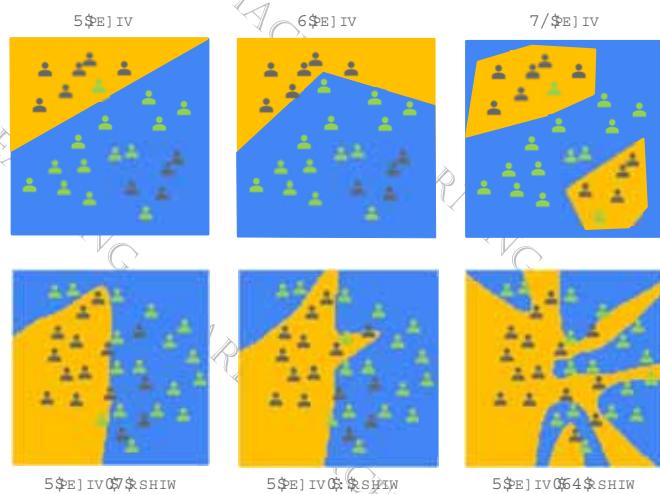


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Nonlinear learning



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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



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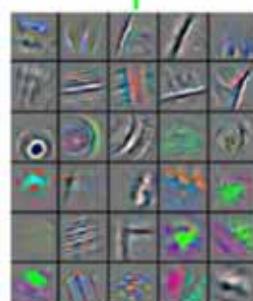
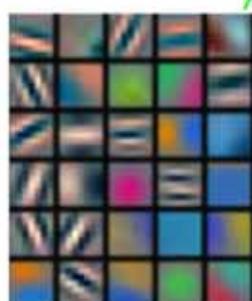
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Deep Learning as Hierarchical Feature Learning

ML

ML

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



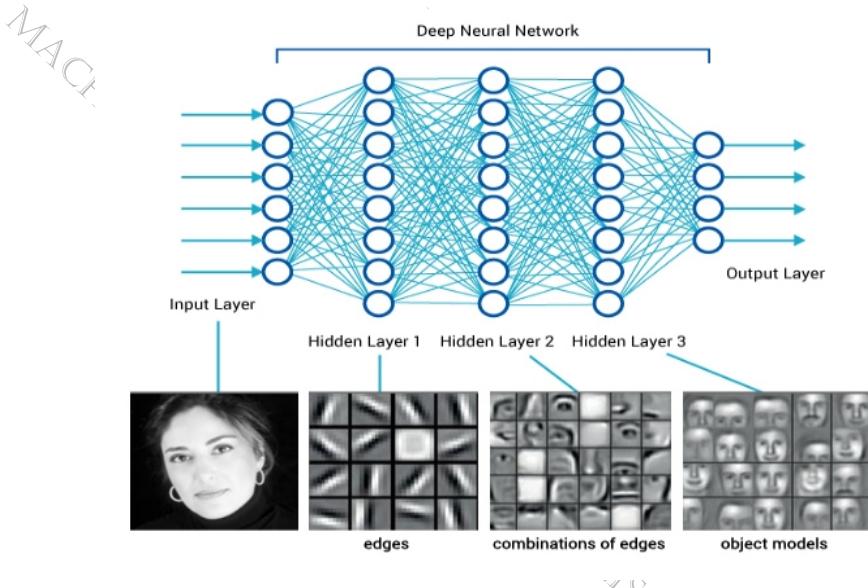
Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

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Image analysis



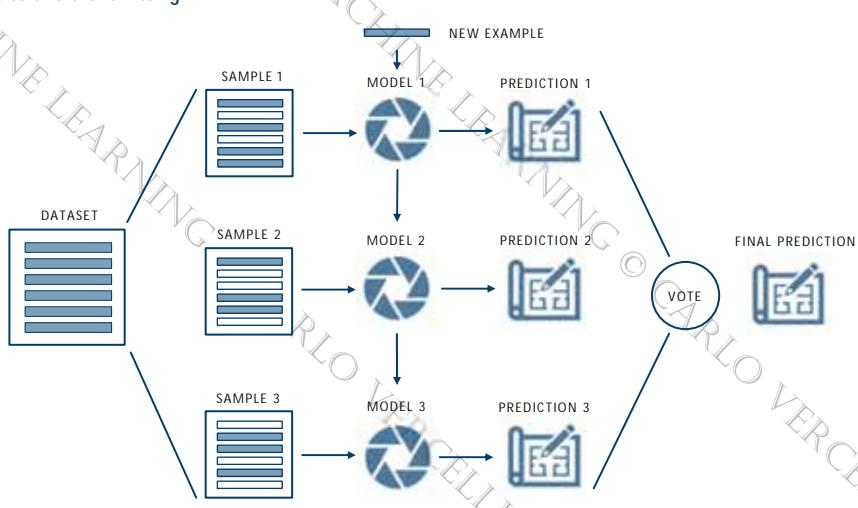
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Ensemble framework: Bagging

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



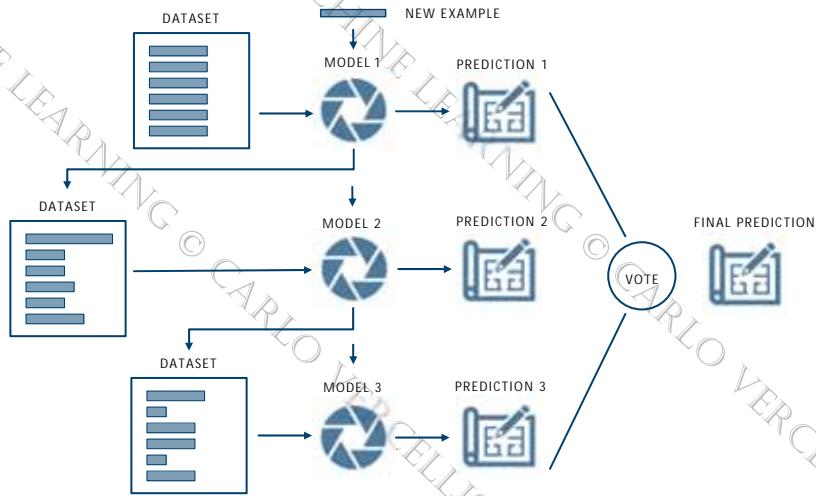
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Ensemble framework : Adaptive Boosting

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



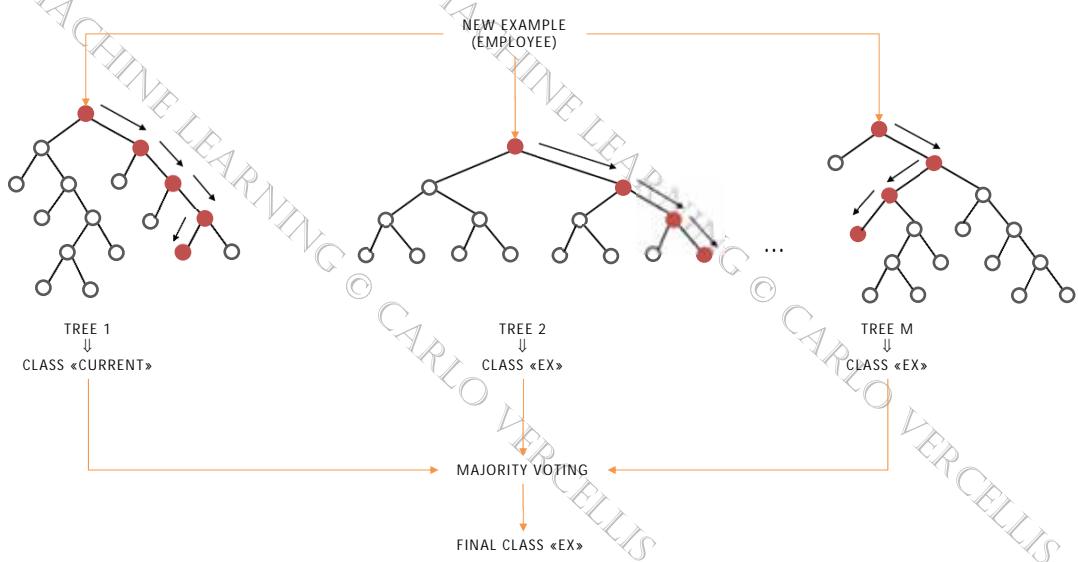
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Random Forest

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



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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 D_i 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:

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

- The weight of classifier M_i 's vote is

$$\log \frac{1 - \text{error}(M_i)}{\text{error}(M_i)}$$

