POLIMI GRADUATE SCHOOL OF MANAGEMENT

INFRAMODULO 1 - MACHINE LEARNING

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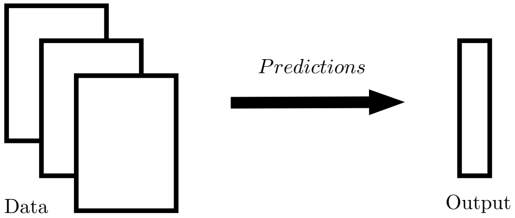
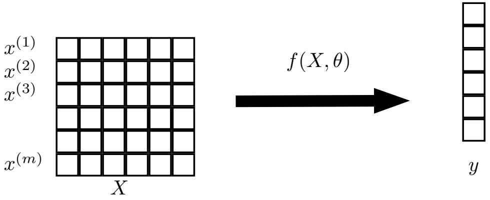
SUPERVISED LEARNING





CLASSIFICATION PROBLEM

attributes

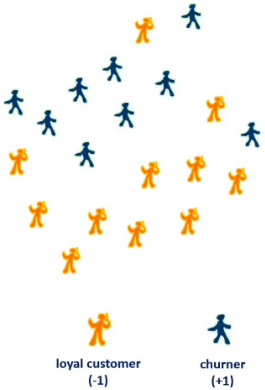
customers

Area	Pothers	Pmob	...	NumSMS	Class
2	0.14	0.59	...	18	1
3	0.26	0.35	...	9	-1
1	0.37	0.23	...	1	1
⋮	⋮	⋮	⋮	⋮	⋮
4	0.41	0.27	...	64	-1

past data

Area	Pothers	Pmob	...	NumSMS	Class
1	0.27	0.67	...	36	?
4	0.44	0.22	...	50	?
4	0.31	0.47	...	14	?
⋮	⋮	⋮	⋮	⋮	⋮
2	0.31	0.14	...	49	?

future data

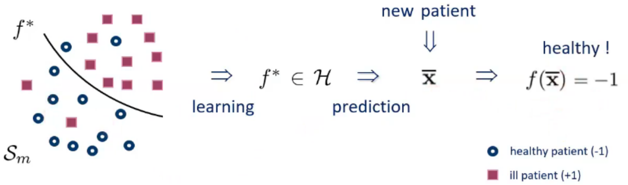


CLASSIFICATION FORMULATION

$\mathcal{S}_m = \{(\mathbf{x}_i, y_i),\ i \in \mathcal{M}\}$: **training set, where** $\mathbf{x}_i \in \Re^n$ **and** $y_i \in \mathcal{D}$

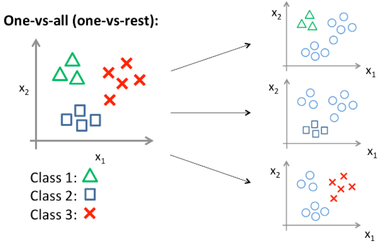
$\mathcal{H}$ **denotes a set of functions** $f(\mathbf{x}) : \Re^n \mapsto \mathcal{D}$

Classification problem: define a hypotheses space $\mathcal{H}$ **and a function** $f^* \in \mathcal{H}$ **which optimally describes the relationship between** $\mathbf{x}_i$ **and** y_i



MULTI-CLASS CLASSIFICATION

1. **One-vs-Rest** We perform $|H|$ different binary classifications: one for every class.



[1]

   We decide based on a majority vote.

2. **One-vs-One** We perform $|H|(|H-1|)/2$ binary classifications: one for every pair of classes. We decide based on a majority vote.

[1] Image via www.cc.gatech.edu

CLASSIFICATION MODELS

- Heuristics Methods
  - Nearest Neighbours
  - Classification Trees
- Regression Methods
  - Logistic regression
- Separation Methods
  - Support vector machine
  - Perceptron
  - Neural Networks
- Probabilistic Methods
  - Bayesian Methods
- Ensemble Methods

EVALUATION DIMENSIONS

- Prediction accuracy
- Speed
- Robustness
- Scalability
- Intepretability
- Rules effectiveness

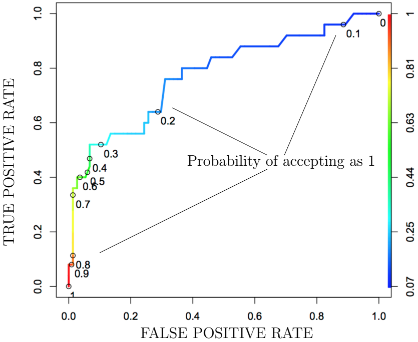
QUALITY MEASURES - CONFUSION MATRIX

Prediction outcome

Actual value	**0**	**1**
0	True Negative	False Positive
1	False Negative	True Positive

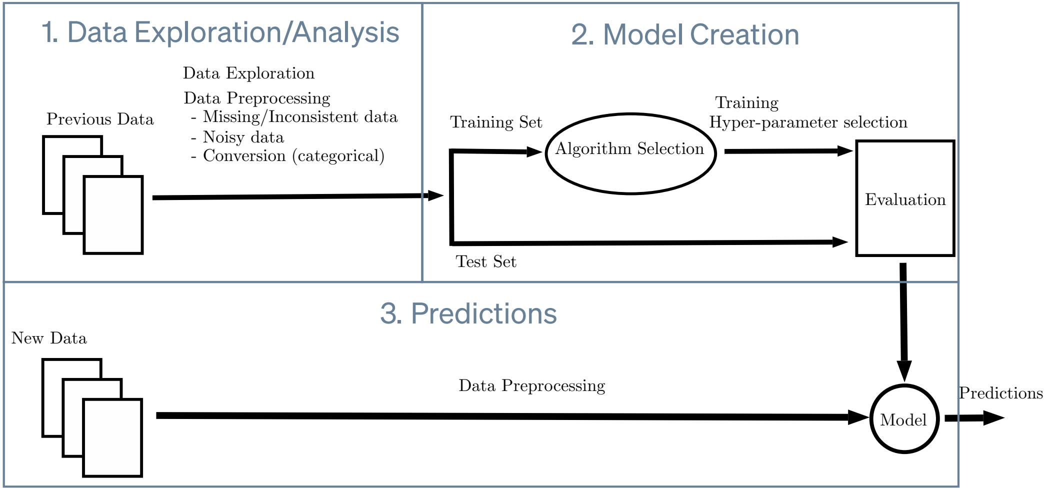
- Precision = $\frac{TP}{TP+FP}$
  *"proportion of true positives among **positive predictions**"*
- False Positive rate = $\frac{FP}{FP+TN}$
  *"proportion of false positives among **actual negatives**"*
- Recall (True Positive rate)=$\frac{TP}{FN+TP}$
  *"proportion of true positives among **actual positive**"*
- Geom. mean=$\sqrt{\text{Precision} \times \text{Recall}}$
- F-score=$\frac{(\beta^2+1)}{\beta^2} \frac{1}{\frac{1}{\text{Precision}}+\frac{1}{\text{Recall}}}$

QUALITY MEASURES - ROC CURVE & AUC



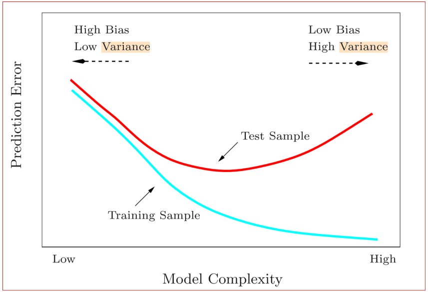
- If we accepting even with small probability then $TPR = FPR = 1$
- If we accepting just with high probability then $TPR = FPR = 0$
- The perfect classificator is the the point $(0, 1)$
- $AUC \in [0.5, 1]$ area under the curve is a quality measure of our algorithm.

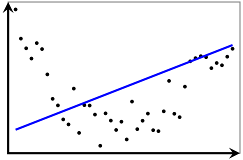
WORKFLOW



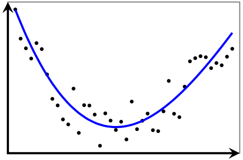
1. Data Exploration/Analysis
Data Exploration
Data Preprocessing
- Missing/Inconsistent data
- Noisy data
- Conversion (categorical)
Previous Data
2. Model Creation
Training Set
Algorithm Selection
Training
Hyper-parameter selection
Evaluation
Test Set
3. Predictions
New Data
Data Preprocessing
Model
Predictions

UNDER/OVER-FITTING

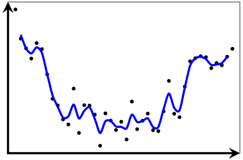




Underfitting

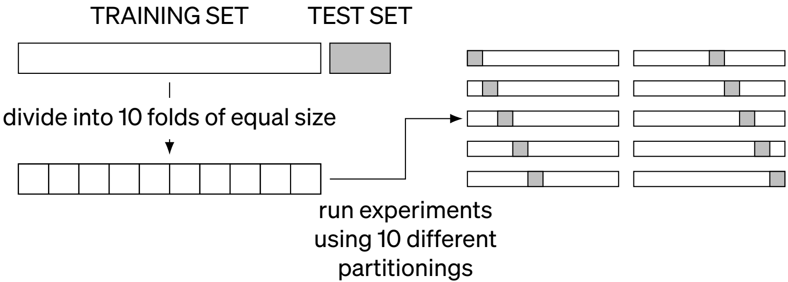


Balance



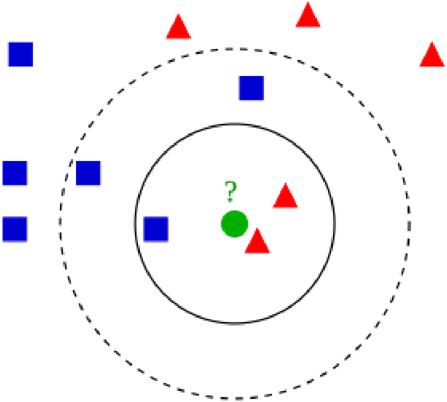
Overfitting

CROSS VALIDATION



THE ALGORITHMS

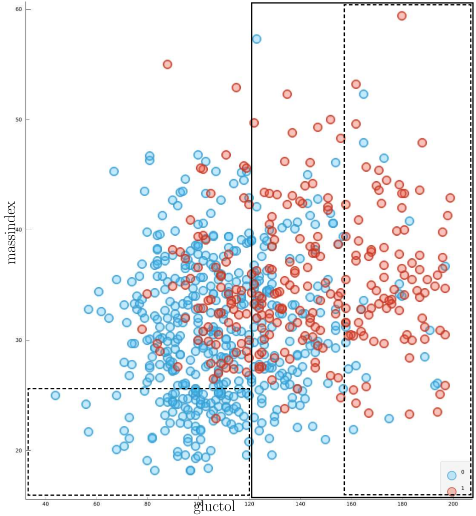
KNN K-NEAREST NEIGHBOURS

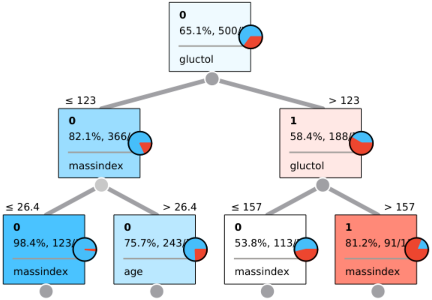


Main Parameters

- k : number of neighbours
- neighbour weights
- distances

CLASSIFICATION TREE

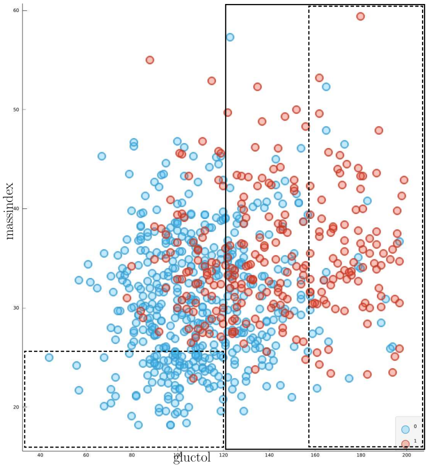


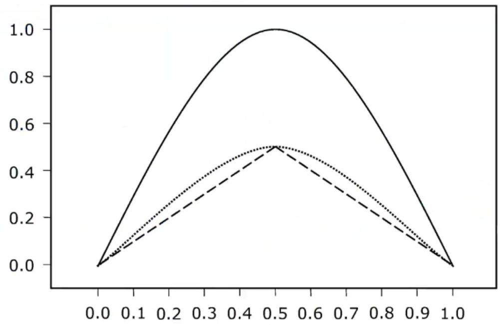


Tree types

- Binary tree (zero/two descendants)
- General trees
- Uni-variate tree ($X_j < b$)
- Multi-variate tree ($\sum_{j=1}^{n} w_j x_j = b$)

CLASSIFICATION TREE

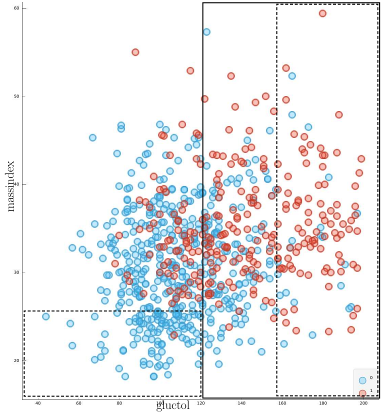


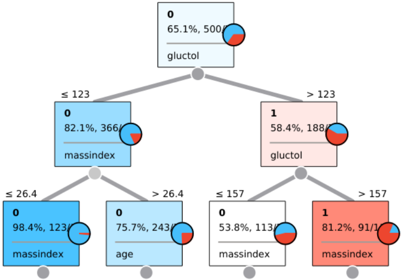


Split criteria

- **Gini index:** $1 - \sum_{h=1}^{H} f_h^2$
- **Entropy index:** $-\sum_{h=1}^{H} f_h \log_2 f_h$
- **Miss-classification index:** $1 - \max_h f_h$

CLASSIFICATION TREE

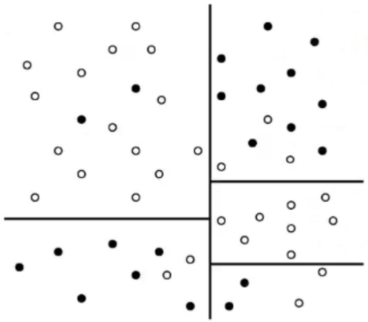




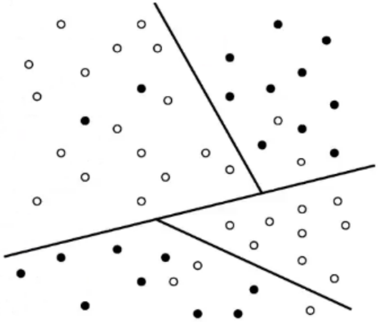
Main Parameters

- impurity measure: “gini”, “entropy”
- max_depth
- min_samples_split: minimum number of samples to split an internal node
- min_sample_leaf: minimum number of samples required to be at a leaf node

CLASSIFICATION TREE

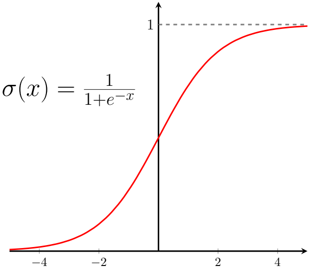


classification by an
axis parallel tree



classification by an
oblique tree

LOGISTIC REGRESSION



$$\sigma(x) = \frac{1}{1+e^{-x}}$$

The model postulates that

$$\log\left[\frac{P(y=1|x)}{P(y=0|x)}\right] = w^T x$$

then if $p = P(y=1|x)$:

$$\frac{p}{1-p} = e^{w^T x}$$

$$\Rightarrow p = P(y=1|x) = \frac{e^{w^T x}}{1+e^{w^T x}} = \frac{1}{1+e^{-w^T x}},$$

$$P(y=0|x) = 1-p = \frac{1}{1+e^{w^T x}} = \frac{e^{-w^T x}}{1+e^{-w^T x}}$$

NAIVE BAYESIAN CLASSIFIER

- Bayes Theorem

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

- Maximum a posteriori hypothesis

$$y_{MAP} = \operatorname*{arg\,max}_{y \in \mathcal{H}} P(y|\mathbf{x}) = \operatorname{arg\,max} \frac{P(\mathbf{x}|y)P(y)}{P(\mathbf{x})}$$

- Independence (Naive)

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

NAIVE BAYESIAN CLASSIFIER

- Categorical/discrete attributes

$$P(x_j|y) = P(x_j = r_{jk}|y = v_h)$$

$\rightarrow$ empirical frequency of the observed value on the class v_h

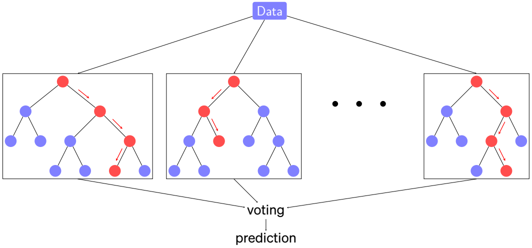
- Numerical attribute

$$P(x_j|y) \sim N(\mu_{jh}, \sigma_{jh})$$

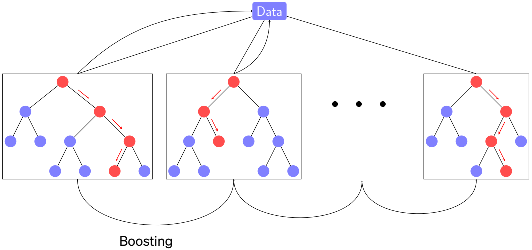
$\rightarrow$ assuming Gaussian density with empirical parameters

ENSEMBLE METHODS

Bagging

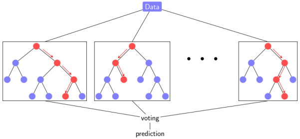


Boosting



*and Stacking

RANDOM FOREST

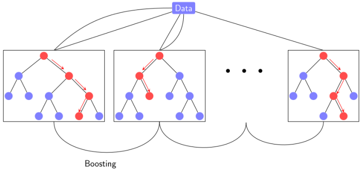


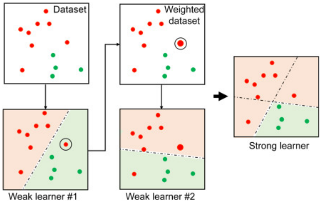
1. Create different (simple) tree models (stumps)
2. Each model is created with a subset of observation/features ($\sim$2m/3)
3. We combine the prediction of all trees

Main Parameters

- n_estimators: Number of trees
- max_features: Number of features selected for the split
- bootstrap=False: Use all samples
- Tree parameters

ADABOOST





1. Assign equal weights to observations $w_i^{(0)} = 1/m$
2. For $k = 1, \ldots, K$
   - Select a sample of observations based on the weights.
   - Create the k-th weak learner and compute predictions $x^{(k)}$
   - Compute the model **weighted** error and assign its coefficient:

$$\alpha^{(k)} = \lambda \times \log((1 - error)/error)$$

   - Update sample weights:

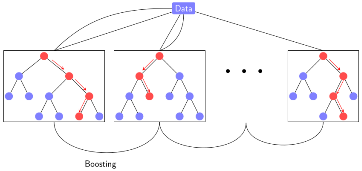
$$w_i^{(k+1)} \propto w_i^{(k)} \times \exp(-\alpha^{(k)} y_i \hat{x}_i^{(k)})$$

3. Final weighted prediction

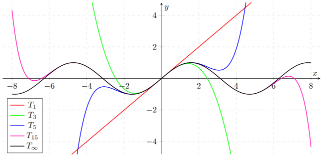
Main Parameters

- n_estimators: Number of estimators (K)
- base_estimator: Weak estimator type
- learning_rate: weights of estimator in final decision (λ)

GRADIENT BOOSTING



$$P_k(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots + \frac{f^{(k)}(a)}{k!}(x-a)^k$$



1. Train a weak learner F_0 and compute predictions $\hat{y}_0 = F_0(x)$
2. For $k = 1, \ldots, K$
   - Compute the difference between the target (y) and the prediction of the current learner ($\hat{y}_{k-1}$)
   - Train e weak learner that minimizes the loss function (error):

$$f_k = \arg\min_f L_m = \arg\min_f \sum_{i=1}^{n} l(y_i, F_{k-1}(x_1) + f(x_i))$$

   - $F_k = F_{k-1} + \lambda f_k$

Main Parameters

- n_estimators: Number of estimators (K)
- base_estimator: Weak estimator type
- learning_rate: weights of estimator in final decision (λ)

THANK YOU