POLIMI GRADUATE SCHOOL OF MANAGEMENT

EXECUTIVE PROGRAM IN DIGITAL TRANSFORMATION FLEX

BIG DATA, MACHINE LEARNING AND AI

ABOUT ME

- Researcher at DI-UNIMI
  - mauricioabel.soto@polimi.it
- Previous
  - Mathematical Engineering - U. of Chile
  - PhD. Computer Science - U. of Paris
  - Researcher - U. of Orléans, U. of Chile, UNIMIB
  - Researcher at DIG-POLIMI
- Research interests
  - Graph theory
  - Evolutionary networks
  - Data representation (NLP)

AGENDA

1. Day 1
   - Pre-processing
   - Classification
   - Regression
   - Assignment

2. Day 2
   - PCA
   - Clustering

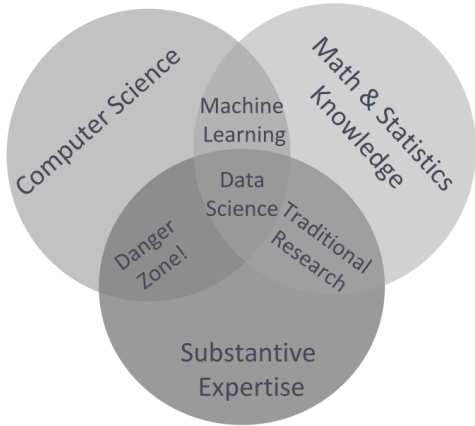
All the material can be found at:
https://github.com/mauriciosotogomez/FLEX_BD_ML_AI

QUESTION TIME

Go to https://pollev.com/mauriciosoto

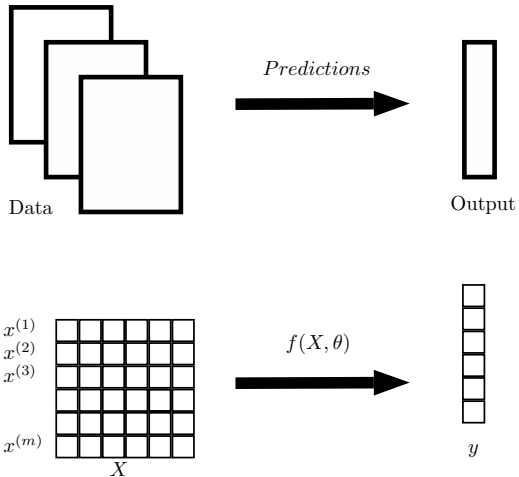
DATA SCIENCE

- Drew Conway, 2010



@manudellavalle - http://emanueledellavalle.org

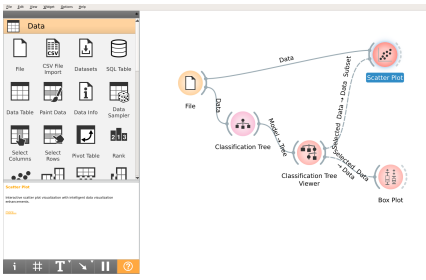
THE OBJECTIVE



PROGRAMMING TOOLS

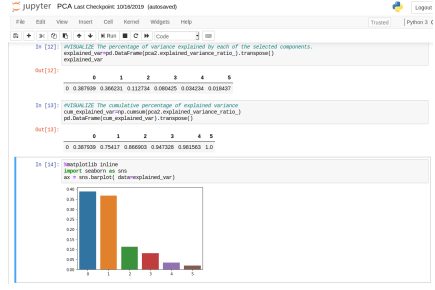
1. Orange

https://orange.biolab.si/



2. Jupyter-Notebook (Anaconda)

https://www.anaconda.com/



scikit learn

A library featuring various ML algorithms designed to inter-operate with the Python numerical and scientific libraries e.g. NumPy, Pandas.

https://scikit-learn.org/stable/

AN EXAMPLE: BANK TELEMARKETING

Attribute		Type	Description/Values
Personal	age	num	Age of the potential client
	job	cat	admin., blue- collar, entrepreneur, housemaid,... ,unknown
	marital_status	cat	divorced, married, single, unknown
	education	cat	basic.4y, basic.6y, basic.9y, high.school,.. unknown
Bank	default	cat	The client has credit in default: no,yes,unknown
	housing	cat	The client has a housing loan contract: no,yes,unknown
	loan	cat	The client has a personal loan: no,yes,unknown
Campain	contact	cat	Communication type: cellular,telephone
	month	cat	Last month contacted: jan, feb ,..., dec
	day_of_week	cat	Last contact day : mon, tue,..., fri
	duration	num	Last contact duration (in seconds)
	campain	num	Number of contacts performed during this campaign
	pdays	num	Number of days that passed by after last contact
	previous	num	Number of contacts performed before this campaign
	poutcome	cat	Outcome of the previous marketing campaign: failure,nonexistent,success
Economical	emp.var.rate	num	Employment variation rate in the last quarter
	cons.price.idx	num	Consumer price index in the last month
	cons.conf.idx	num	Monthly consumer confidence index
	euribor3m	num	Dayly Euro Interbank Offered Rate
	nr.employed	num	Number of employed citizens in the last quarter (thousands)
Target	**success**	**target**	**0: no, 1: yes**

[1] A data-driven approach to predict the success of bank telemarketing. S. Moroa, P. Cortez, P. Rita.Decision Support Systems, 62:22-31, 2014.

SUPERVISED LEARNING EXAMPLE

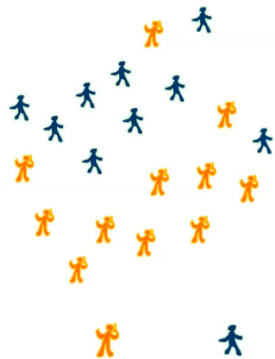
Features

Target

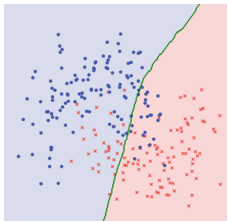
Observations/Clients

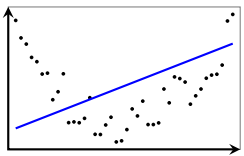
id	Age	Job	⋯	nr.employed	success
1	50	admin.	⋯	0.31	**1**
2	22	housemaid	⋯	0.23	**0**
3	34	unknown	⋯	0.16	**1**
⋮	⋮	⋮	⋱	⋮	⋮
n	20	blue-collar	⋯	0.65	**1**

id	Age	Job	⋯	nr.employed	success
$n+1$	30	blue-collar.	⋯	0.61	**?**
$n+22$	21	unknown	⋯	0.16	**?**
$n+33$	66	housemaid	⋯	0.45	**?**
⋮	⋮	⋮	⋱	⋮	⋮
$n+k$	28	blue-admin.	⋯	0.35	**?**

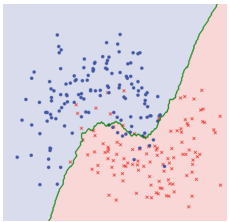


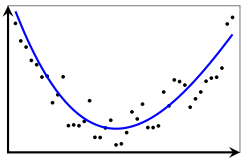
SUPERVISED LEARNING GOAL



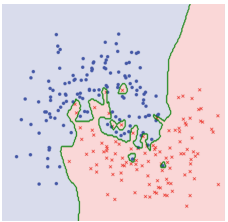


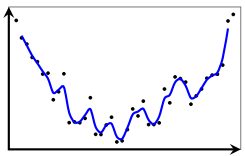
Underfitting





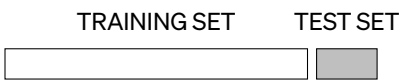
Balance

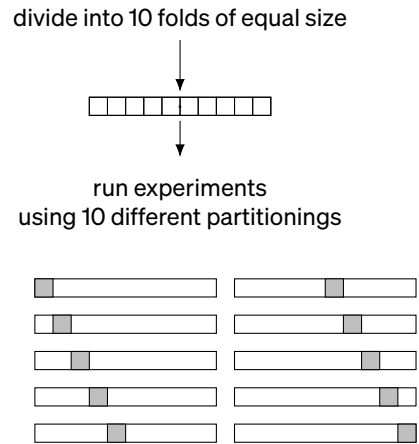




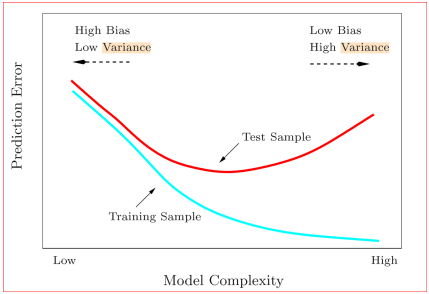
Overfitting

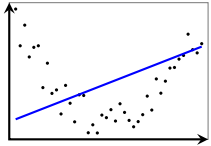
HOLD OUT METHOD / CROSS VALIDATION



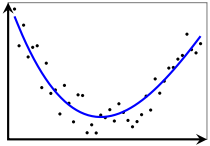


UNDER/OVER-FITTING





Underfitting



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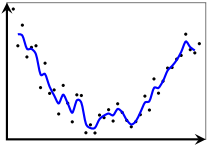
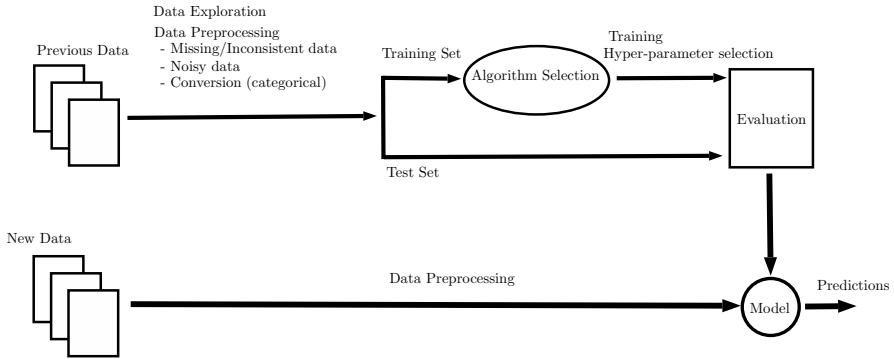
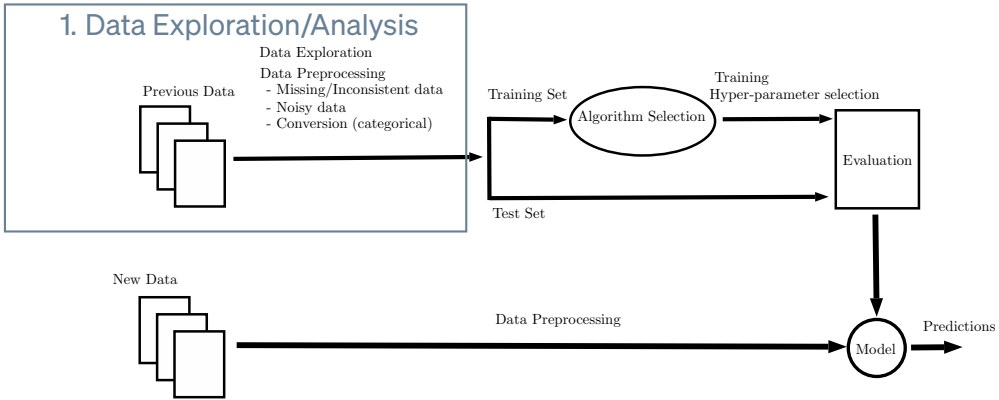


Overfitting

WORKFLOW


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

WORKFLOW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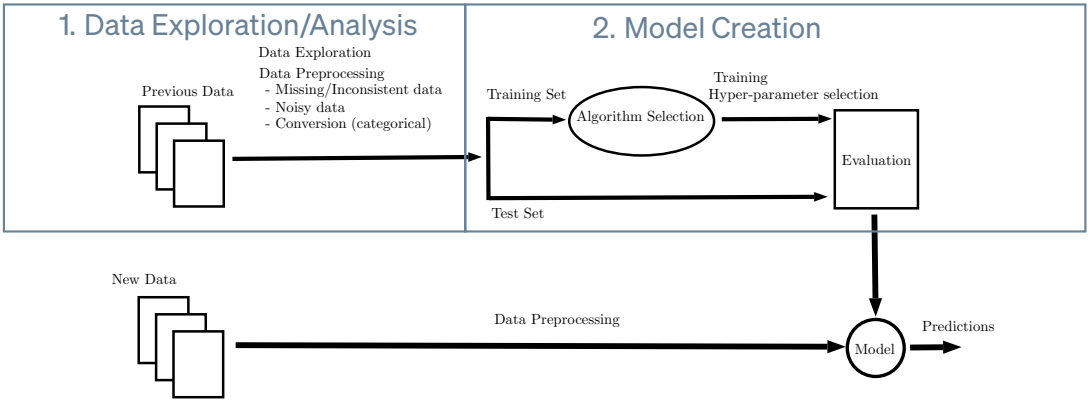
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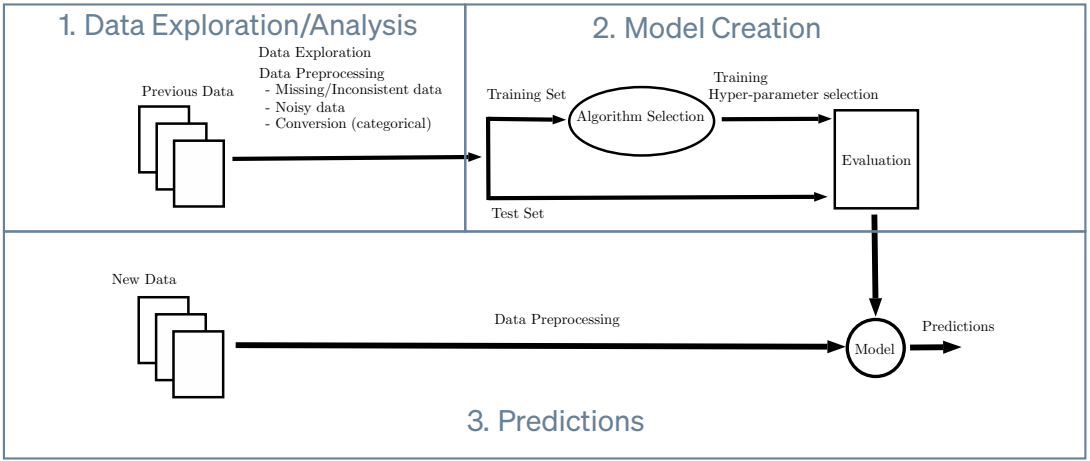
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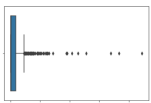
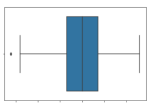
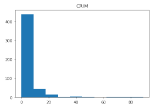
3. Predictions

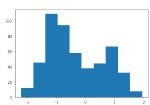
DATA EXPLORATION/ANALYSIS

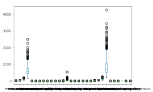
1. Data Validation
   - Incomplete data (identify, drop, replace)
   - Noisy data (Outliers)
2. Data transformation
   - Standardization
   - Discretization
   - Dummy variables
   - Feature construction
3. Data reduction
   - Sampling
   - Discretization
   - Feature/Dimensionality Reduction (PCA)

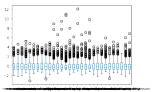






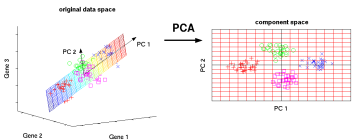




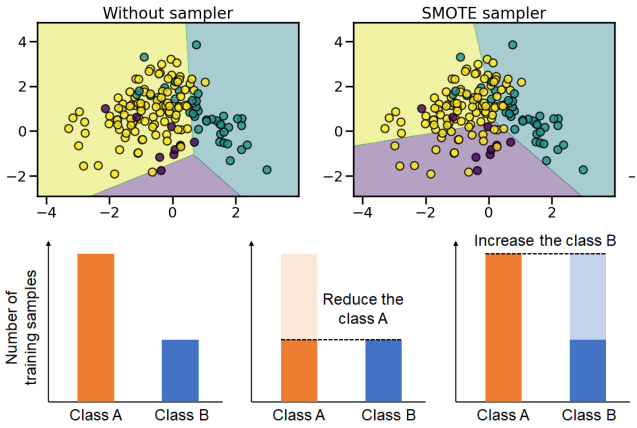


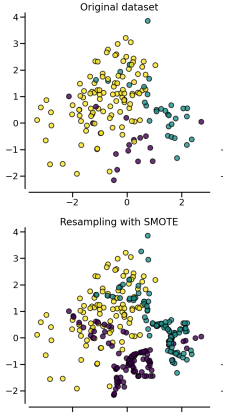
	type_of_food
0	fruit
1	vegetable
2	fruit
3	meat
4	fruit
5	vegetable

	fruit	meat	vegetable
0	1	0	0
1	0	0	1
2	1	0	0
3	0	1	0
4	1	0	0
5	0	0	1



DATA UNBALANCE





https://imbalanced-learn.org/

FEATURE SELECTION

1. Filter Methods

- Model independent
- Simple and Fast
- Ex. Uni/Multi-variate correlation

2. Wrapper methods

- Model determine the variable set quality
- Slow
- Ex. Greedy Forward

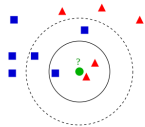
3. Embbeded Methods

- Model determine the variable set
- Slow
- Ex. Tree models

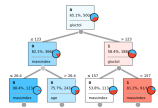
SUPERVISED LEARNING: CLASSIFICATION

CLASSIFICATION MODELS

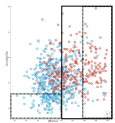
- Heuristics Methods
  - Nearest Neighbours
  - Classification Trees
- Probabilistic Methods
  - Bayesian Methods
- Regression Methods
  - Logistic regression
- Separation Methods
  - Support vector machine
  - Perceptron
  - Neural Networks

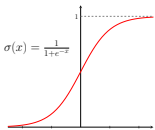


KNN

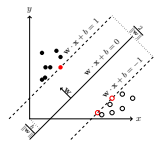


Classification Tree

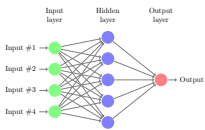




Logistic Regression

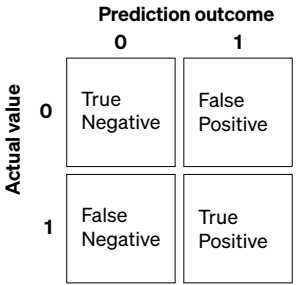


SVM



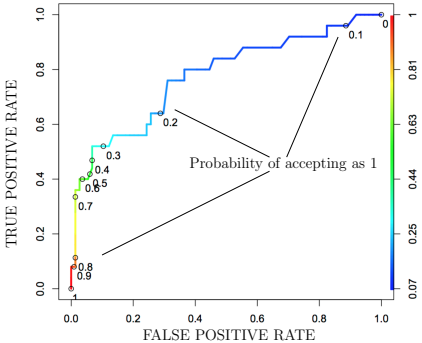
Neural Network

QUALITY MEASURES - CONFUSION MATRIX



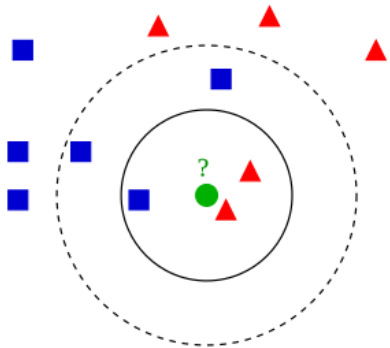
- Precision = $\frac{TP}{TP+FP}$
  ``*proportion of true positives among **positive predictions***''
- False Positive rate= $\frac{FP}{FP+TN}$
  ``*proportion of false positives among **actual negatives***''
- Recall (True Positive rate)= $\frac{TP}{FN+TP}$
  ``*proportion of true positives among **actual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

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.

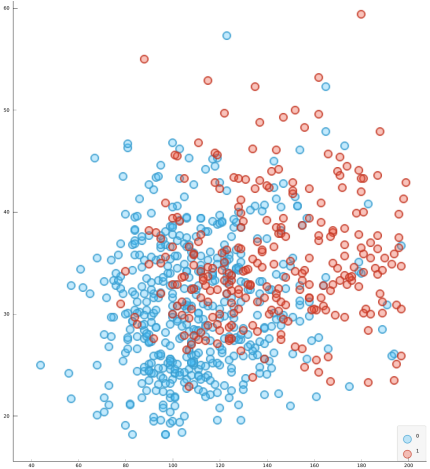
KNN K-NEAREST NEIGHBOURS



Main Parameters

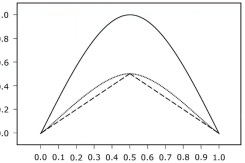
- k : number of neighbours
- neighbour weights
- distances

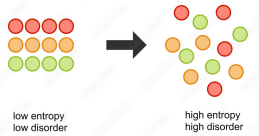
CLASSIFICATION TREE



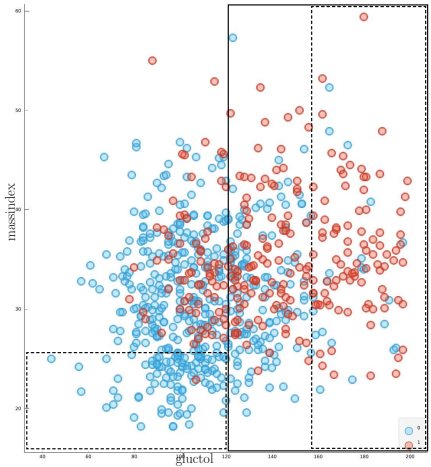
Split criteria

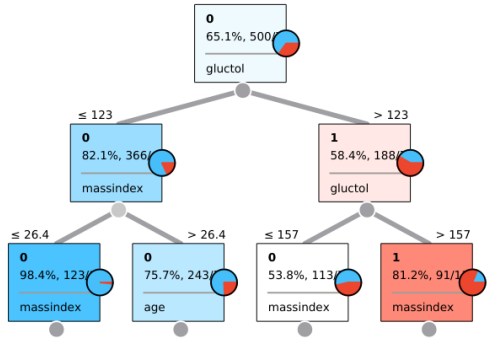
- Entropy index
- Gini index
- Miss-classification index



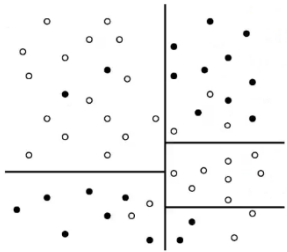


CLASSIFICATION TREE

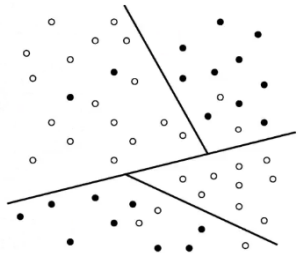




UNI/MULTI-VARIATE CLASSIFICATION TREE



classification by an
axis parallel tree



classification by an
oblique tree

NAIVE BAYESIAN CLASSIFIER

- Bayes Theorem ``**Predict future probabilities based on history"**

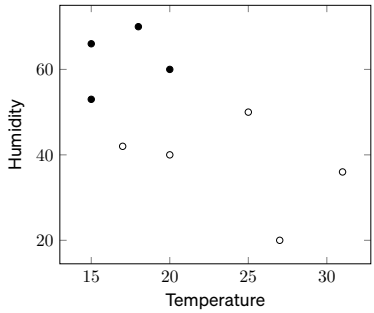
$$P(y|\mathbf{x}) = \frac{P(\mathbf{x}|y)P(y)}{P(\mathbf{x})} = \frac{P(\mathbf{x}|y)\,P(y)}{\sum_{l=1}^{H} P(\mathbf{x}|y)\,P(y)}$$

- Naive (Independence) - **Strong hypothesis**

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

LOGISTIC REGRESSION - EXAMPLE

Temp. [C]	20	31	15	18	27	15	20	25	17
Humidity [%]	60	36	53	70	20	66	40	50	42
Rain	1	-1	1	1	-1	1	-1	-1	-1



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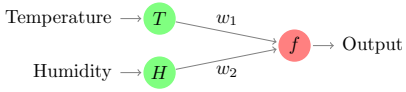
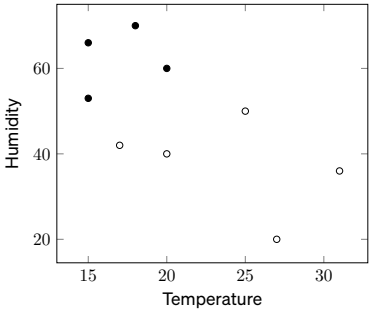
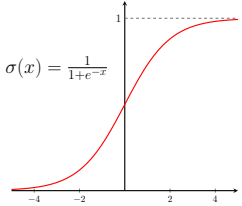


$$P(y = 1|T, H; w) = \underbrace{\sigma}_{\text{sigmoid function}}(w_0 + w_1 \cdot T + w_2 \cdot H)$$



Maximize Likelihood

$$\max_w L(w \mid y; x) = \Pr(Y \mid X; w) = \prod_i \Pr(y_i \mid x_i; w)$$



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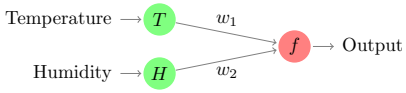

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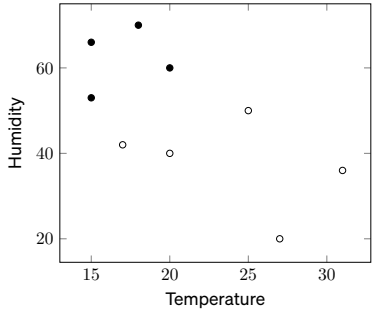

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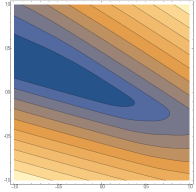

$$P(\text{rain}) = \sigma(-0.044 - 0.633 \times T + 0.235 \times H)$$

$$w^* = (-0.044, -0.633, 0.235)$$

LOGISTIC REGRESSION - EXAMPLE

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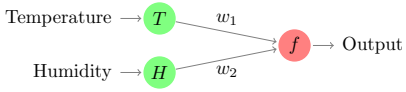

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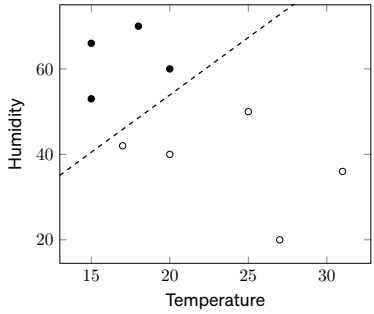

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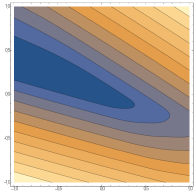

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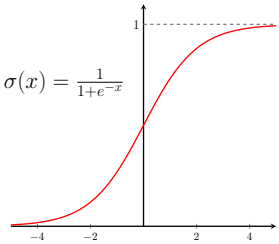
LOGISTIC REGRESSION



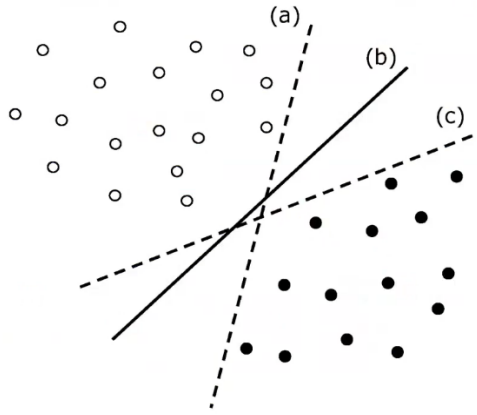
$$\min_{w} \underbrace{\frac{1}{2}||w||^2}_{\text{regularization}} + C \underbrace{\sum_{i=1}^{n} \log(1 + \exp(-y_i\,(w^T x_i)))}_{\text{error}}$$

Main Parameters

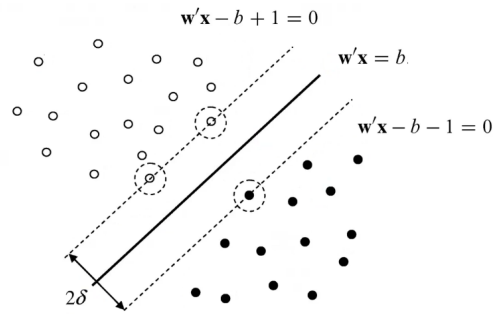
- C: Inverse of regularization strength

$$P(y = 1|x; w) = \sigma(w_0 + w_1 x_1 + \cdots + w_n x_n)$$

SUPPORT VECTOR MACHINE - LINEARLY SEPARABLE



SVM - LINEARLY SEPARABLE

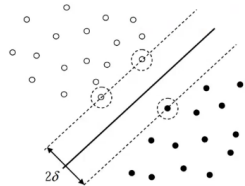


$$\delta = \frac{2}{\|w\|}, \qquad \|w\| = \sqrt{\sum_{j \in \mathcal{N}} w_j^2}$$

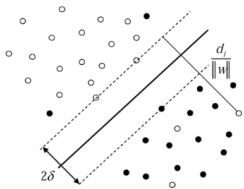
$$\min_{\mathbf{w},b} \quad \frac{1}{2}\|\mathbf{w}\|_2^2$$
$$\text{s.t.} \quad y_i(\mathbf{w}'\mathbf{x}_i - b) \geq 1 \quad i \in \mathcal{M}$$

SVM - GENERAL CASE

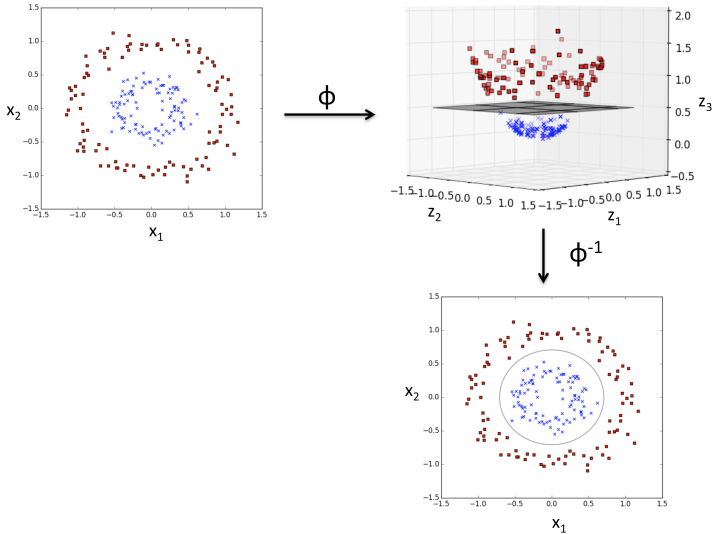
$$\begin{aligned} \min_{\mathbf{w},b} \quad & \frac{1}{2}\|\mathbf{w}\|_2^2 \\ \text{s.t.} \quad & y_i(\mathbf{w}'\mathbf{x}_i - b) \geq 1 \quad i \in \mathcal{M} \end{aligned}$$



$$\begin{aligned} \min_{\mathbf{w},b,d} \quad & \frac{1}{2}\|\mathbf{w}\|_2^2 + \lambda \sum_{i=1}^{m} d_i \\ \text{s.t.} \quad & y_i(\mathbf{w}'\mathbf{x}_i - b) \geq 1 - d_i \quad i \in \mathcal{M} \\ & d_i \geq 0 \quad i \in \mathcal{M} \end{aligned}$$

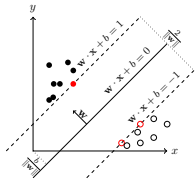


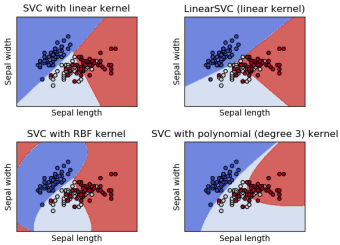
SVM - KERNELS



Try yourself: https://dash.gallery/dash-svm/

SVM - GENERAL CASE





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

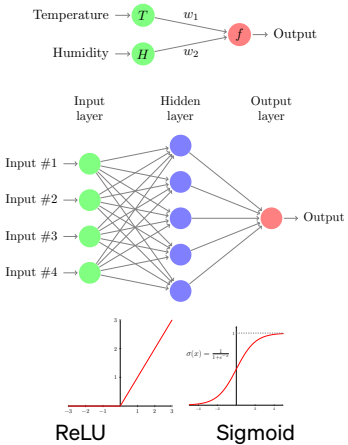
$$\text{subject to } y_i(w^T \underbrace{\phi(x_i)}_{\text{kernel}} - b) \geq 1 - d_i,$$

$$d_i \geq 0$$

Main Parameters

- C: Inverse of regularization strength
- kernel:
  - linear: $x'x$
  - poly: $(\gamma x'x + r)^d$
  - rbf: $exp(-\gamma||x - x'||^2)$
  - sigmoid: $\tanh(\gamma x'x + r)$

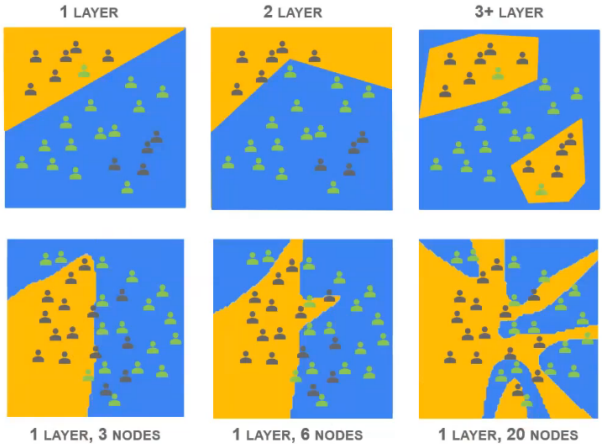
MULTI-LAYER PERCEPTRON



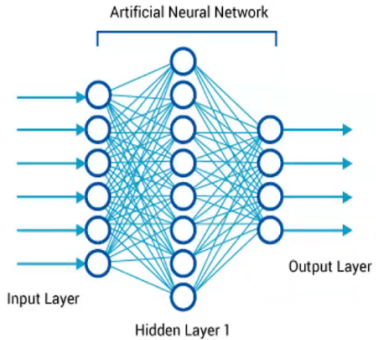
Main Parameters

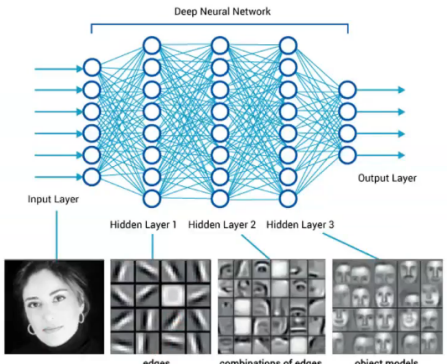
- hidden_layer_sizes: $(n_1, n_2, \ldots, n_L)$
- activation: identity, logistic, tanh, relu
- alpha regularization term parameter
- Resolution algorithm parameters: tol, max_iter.

NEURAL NETWORK



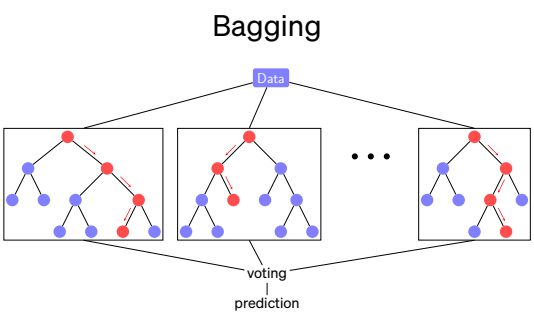
DEEP LEARNING

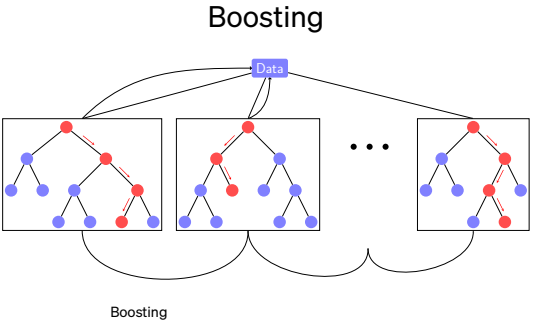




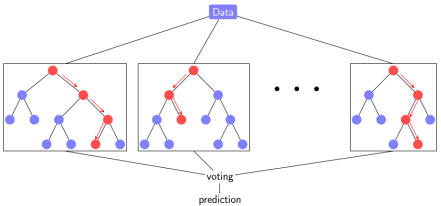
Try yourself: https://adamharley.com/nn_vis/

ENSEMBLE METHODS





RANDOM FOREST

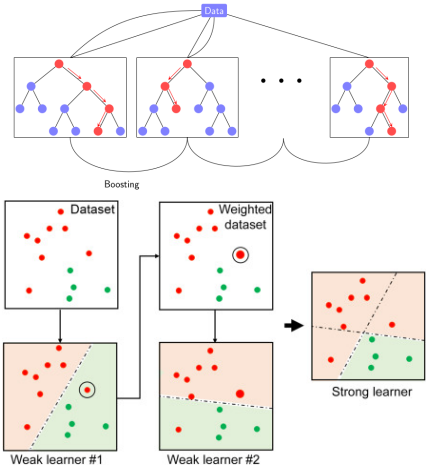


1. Create different (simple) tree models (stumps)
2. Each model is created with a subset of observation/features ($\sim$2m/3)
3. We combine the prediction of all trees

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
2. For $k = 1, \dots, K$
   - 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 according to its error.
   - Update sample weights
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)

BANK TELEMARKETING RESULTS

Model	AUC	CA	F1	Precision	Recall
AdaBoost	1.000	1.000	1.000	1.000	1.000
kNN	1.000	1.000	1.000	1.000	1.000
Logistic Regression	0.937	0.875	0.712	0.756	0.672
Naive Bayes	0.834	0.791	0.599	0.535	0.681
Neural Network	0.956	0.899	0.793	0.747	0.844
Random Forest	0.969	0.915	0.808	0.844	0.775
SVM	0.932	0.852	0.630	0.738	0.549
Tree	0.945	0.884	0.750	0.744	0.757

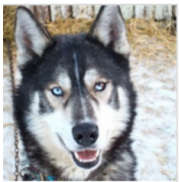
Model	AUC	CA	F1	Precision	Recall
AdaBoost	0.785	0.846	0.668	0.663	0.673
kNN	0.741	0.825	0.607	0.630	0.586
Logistic Regression	0.938	0.877	0.714	0.767	0.668
Naive Bayes	0.847	0.807	0.627	0.566	0.703
Neural Network	0.935	0.879	0.748	0.716	0.784
Random Forest	0.937	0.877	0.720	0.758	0.686
SVM	0.931	0.854	0.636	0.745	0.554
Tree	0.932	0.880	0.740	0.739	0.741

MODEL EXPLAINABILITY

Predicted: wolf
True: wolf

Predicted: husky
True: husky

Predicted: wolf
True: wolf



Predicted: wolf
True: husky

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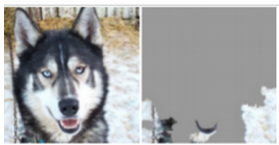

Predicted: wolf
True: husky

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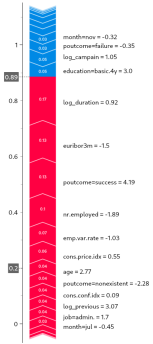
True: husky

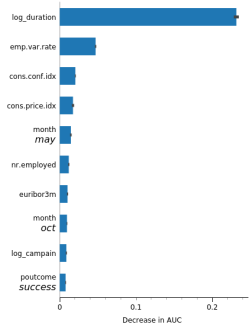
Predicted: wolf
True: wolf

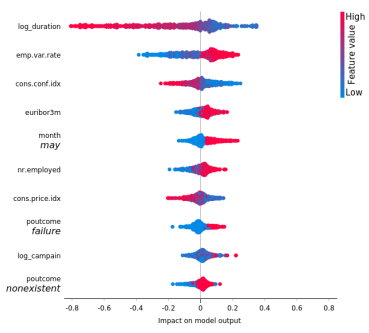
MODEL EXPLAINABILITY

SHAP: SHapley Additive exPlanation

``Marginal contribution of the feature in the prediction"







$$\phi_A = \sum_{S \subseteq F \setminus \{A\}} \frac{|S|!(|F| - |S| - 1)!}{|F|!} [f(S \cup \{A\}) - f(S)]$$

CASE STUDY - HEALTH INSURANCE CROSS SELLING

Variable	Definition
id	Unique ID for the customer
Gender	Gender of the customer
Age	Age of the customer
Driving_License	0 : Customer does not have DL, 1 : Customer already has DL
Region_Code	Unique code for the region of the customer
Previously_Insured	1 : Customer already has Vehicle Insurance, 0 : Customer doesn't have Vehicle Insurance
Vehicle_Age	Age of the Vehicle
Vehicle_Damage	1 : Customer got his/her vehicle damaged in the past. 0 : Customer didn't get his/her vehicle damaged in the past.
Annual_Premium	The amount customer needs to pay as premium in the year
PolicySalesChannel	Anonymized Code for the channel of outreaching to the customer ie. Different Agents, Over Mail, Over Phone, In Person, etc.
Vintage	Number of Days, Customer has been associated with the company
Response	**1 : Customer is interested, 0 : Customer is not interested**

CASE STUDY - INSURANCE FRAUD

- months_as_customer
- age
- policy_number
- policy_bind_date
- policy_state
- policy_csl
- policy_deductable
- policy_annual_premium
- umbrella_limit
- insured_zip
- insured_sex
- insured_education_level
- insured_occupation
- insured_hobbies
- insured_relationship
- capital-gains
- capital-loss
- incident_date
- incident_type
- collision_type
- incident_severity
- authorities_contacted
- incident_state
- incident_city
- incident_location
- incident_hour_of_the_day
- number_of_vehicles_involved
- property_damage
- bodily_injuries
- witnesses
- police_report_available
- total_claim_amount
- injury_claim
- property_claim
- vehicle_claim
- auto_make
- auto_model
- auto_year
- fraud_reported
- _c39

ASSIGNMENT: THE $50K/YR BASED ON CENSUS DATA

The prediction task is to determine whether a person makes over $50K a year from the data in 1994 Census bureau database.

- age: continuous.
- workclass: Private, Self-emp-not-inc, Federal-gov, etc.
- final weight[a]: continuous.
- education level: Bachelors, Some-college, 11th, etc.
- education-num: continuous.
- marital-status: Married-civ-spouse, Divorced, etc.
- occupation: Tech-support, Craft-repair,etc.
- relationship: Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried.
- ethnic : White, Asian-Pac-Islander, Amer-Indian-Eskimo, Other, Black.
- gender: Female, Male.
- capital-gain/capital-loss: continuous.
- hours-per-week: continuous.
- origin-country: United-States, Cambodia, England, etc.

[a] The weights on the Current Population Survey (CPS) files are controlled to independent estimates of the civilian noninstitutional population of the US.

Ron Kohavi, "Scaling Up the Accuracy of Naive-Bayes Classifiers: a Decision-Tree Hybrid", Proceedings of the Second International Conference on Knowledge Discovery and Data Mining, 1996.

ASSIGNMENT: THE $50K/YR BASED ON CENSUS DATA

- `adult_data_model.csv`: il dataset contiene le informazioni di circa 25000 osservazioni con le rispettive variabili esplicative. Dovete usare questi dati per creare e valutare il vostro modello.
- `adult_data_future_with_target.csv`: il dataset contiene le informazioni di 7000 records. Vi viene richiesto di fornire le previsioni per questo set di record.

L'obiettivo è quello di mazimizzare la qualità delle previsioni del modello, misurata in base alla metrica F1.

SUPERVISED LEARNING: REGRESSION

CASE STUDY - HOUSE PRICING

Variable	Definition
CRIM	per capita crime rate by town
ZN	proportion of residential land zoned for lots over 25,000 sq.ft.
INDUS	proportion of non-retail business acres per town
CHAS	Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
NOX	nitric oxides concentration (parts per 10 million)
RM	average number of rooms per dwelling
AGE	proportion of owner-occupied units built prior to 1940
DIS	weighted distances to five Boston employment centres
RAD	index of accessibility to radial highways
TAX	full-value property-tax rate per $10,000
PTRATIO	pupil-teacher ratio by town
B	$1000(Bk - 0.63)2$ where Bk is the proportion of blacks by town
LSTAT	% lower status of the population
MEDV	Median value of owner-occupied homes in $1000's

The Boston house-price data of Harrison, D. and Rubinfeld, D.L. 'Hedonic prices and the demand for clean air', J. Environ. Economics & Management, vol.5, 81-102, 1978.

QUALITY MEASURES - REGRESSION

- Coefficient of determination

$$R^2 = 1 - \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 / \sum_{i}(y_i - \bar{y})^2$$

- Mean Absolute Error :

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

- Mean Squared Error :

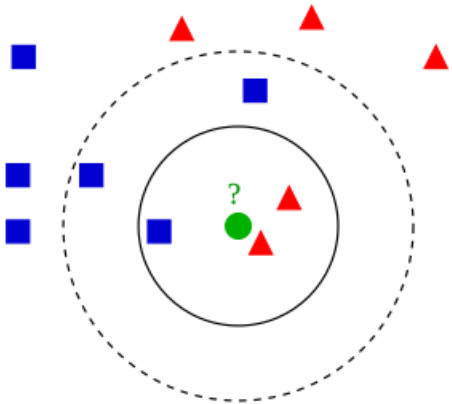
$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- Root Mean Squared Error : $RMSE = \sqrt{MSE}$

REGRESSION MODELS

- Heuristics Methods
  - Nearest Neighbours
  - Regression Trees
- Optimization based Methods
  - Linear models
  - Support vector machine
  - Neural Networks

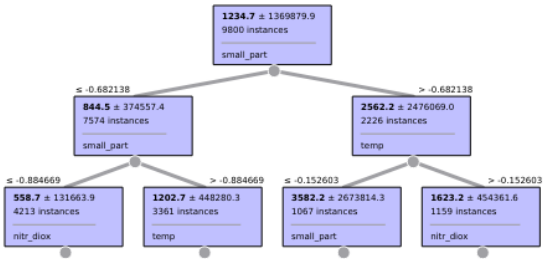
KNN K-NEAREST NEIGHBOURS



Main Parameters

- k : number of neighbours
- neighbour weights
- distances

REGRESSION TREE



Main Parameters

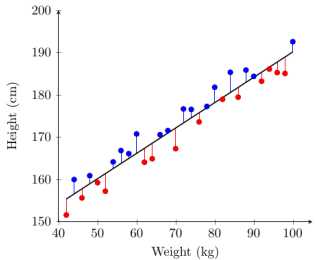
- variability measure: mse (variance from mean), mae (error from median)
- max_depth
- min_samples_split: minimum number of samples to split an internal node
- min_sample_leaf: minimum number of samples required to be at a leaf node

SIMPLE LINEAR REGRESSION

$$y = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n$$

- Least square regression

$$SSE = \sum_{i=1}^{m} e_i^2 = \sum_{i=1}^{m} [y_i - (w\mathbf{x_i} + b)]^2$$



LINEAR MODELS REGULARIZATION

- Ridge:

$$\min_w \lambda||w||^2 + ||e||^2 = \min_w \lambda||w||^2 + (y - Xw)^\top (y - Xw)$$

- Lasso:

$$\min_w \lambda|w| + ||e||^2 = \min_w \lambda|w| + (y - Xw)^\top (y - Xw)$$

GENERAL LINEAR MODELS

- We consider a set of bases functions: polynomials, kernels, etc.

$$Y = \sum_h w_h \, g_h(X_1, X_2, \dots, X_n) + b$$

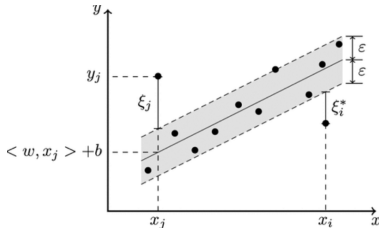
- For example,
  - **quadratic**

$$Y = wX + b = X_1 w_1 + X_2 w_2 + X_1^2 w_3 + X_2^2 w_4 + X_1 X_2 w_5 + b$$

  - **exponential**

$$\log Y = b + wX \qquad \Rightarrow \qquad Y = e^{b+wX}$$

SVR



$$\min_{w,b,\zeta,\zeta^*} \frac{1}{2}\|w\| + C\sum_{i=1}^{n}(\zeta_i + \zeta_i^*)$$

subject to $y_i - w^T\phi(x_i) - b \leq \varepsilon + \zeta_i,$

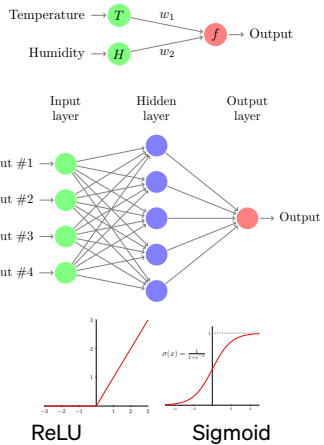
$w^T\phi(x_i) + b - y_i \leq \varepsilon + \zeta_i^*,$

$\zeta_i, \zeta_i^* \geq 0, i = 1, ..., n$

Main Parameters

- C: inverse of regularization strength
- ε: tolerance
- kernel
- Resolution algorithm parameters

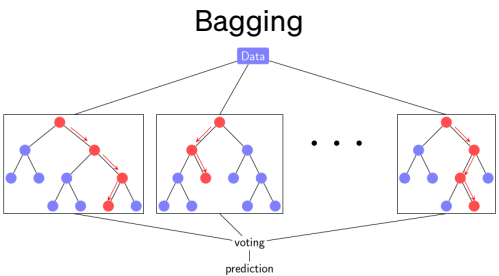
MULTI-LAYER PERCEPTRON

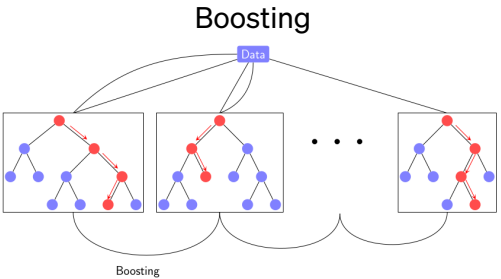


Main Parameters

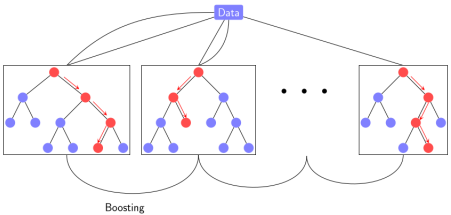
- hidden_layer_sizes: $(n_1, n_2, \ldots, n_L)$
- activation: identity, logistic, tanh, relu
- alpha regularization term parameter
- Resolution algorithm parameters: solver, tol, batch_size, learning_rate, max_iter.

ENSEMBLE METHODS





GRADIENT BOOST



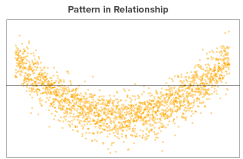
1. Train a weak learner F_0 and compute predictions $x^{(k)}$
2. For $k = 1, \dots, K$
   - Compute the difference between the target y and the predictions of the current learner
   $$\hat{y}_{k-1} = F_{k-1}(x_i)$$
   - Train a weak learner that approximate this difference (error)
   $$f_k = \arg\min_f L_m = \arg\min_f \sum_{i=1}^{n} l(y_i, F_{m-1}(x_i) + f(x_i$$
   - $F_k = F_{k-1} + \lambda f_k$

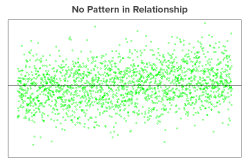
Main Parameters

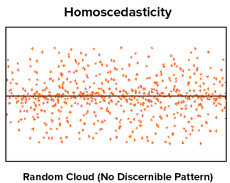
- n_estimators: Number of estimators (K)
- base_estimator: Weak estimator type
- learning_rate: weights of estimator in final decision (λ)

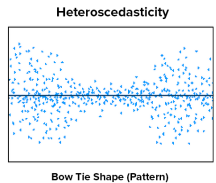
RESIDUAL ASSUMPTIONS

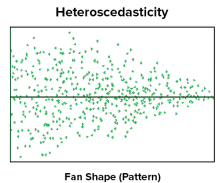
Independence, $E(\varepsilon_i|\mathbf{x_i}) = 0), \qquad Var(\varepsilon_i|\mathbf{x_i}) = \sigma^2$









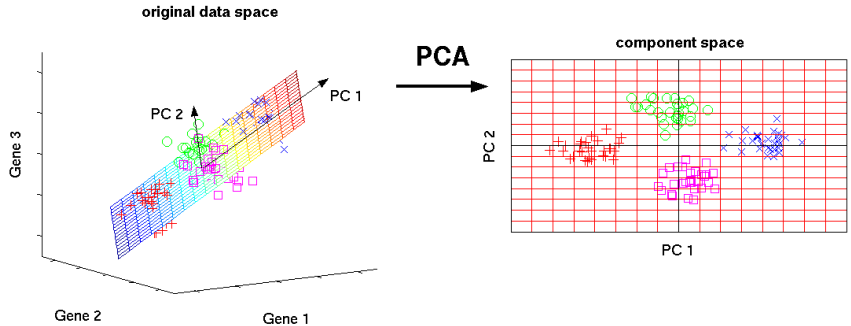


CASE STUDY - MEDICAL INSURANCE COSTS

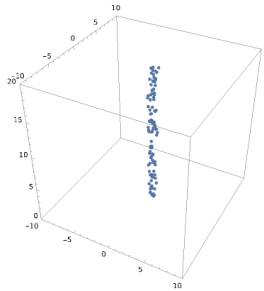
Variable	Definition
age	age of primary beneficiary
sex	insurance contractor gender, female, male
bmi	Body mass index - 18.5 to 24.9
children	Number of children covered by health insurance / Number of dependents
smoker	Smoking
region	the beneficiary's residential area in the US, northeast, southeast, southwest, northwest.
charges	Individual medical costs billed by health insurance

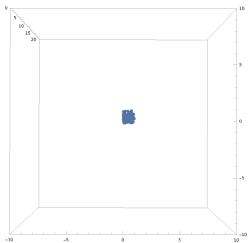
UNSUPERVISED LEARNING

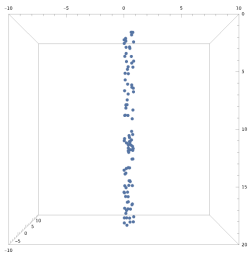
PCA: PRINCIPAL COMPONENT ANALYSIS



PCA-INTUITION



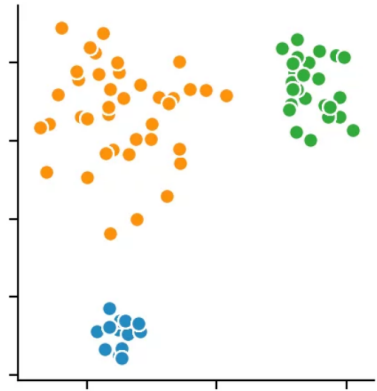




Compute the projection that maximizes the **variance**

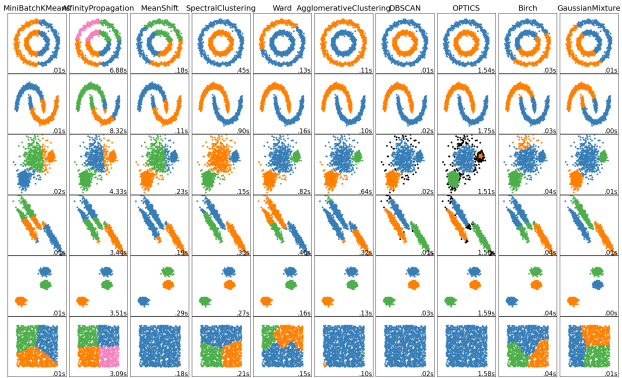
CLUSTERING PROBLEM

- ``Homogeneous" groups of observations
  - observations in the same group should be similar
  - observations in different groups should be dissimilar
- Applications
  - Marketing segmentation
  - Social network analysis
  - Social Science
  - etc



CLUSTERING METHODS

- Stategies
  - Partition
  - Hierarchical
  - Density based
  - Grid
- Classification
  - Exclusive
  - Fuzzy
  - Complete
  - Partial



AFFINITY MEASURES

Based on distances

- Euclidean distance
- Minkowski distance

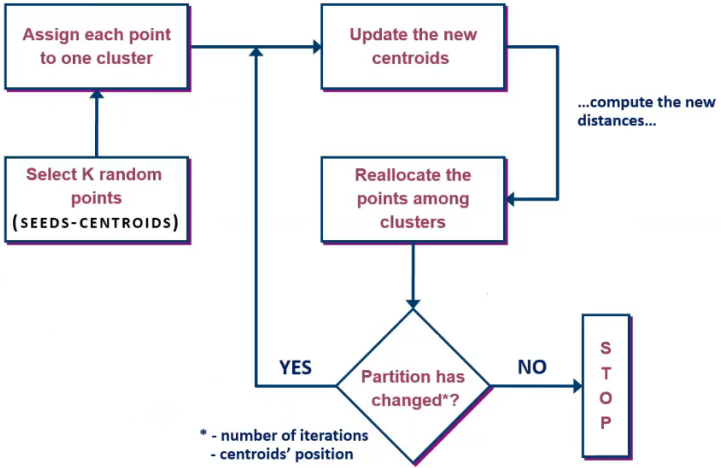
$$\sqrt[q]{\sum_{i=i}^{n} |x_{ij} - x_{kj}|^q}$$

- Mahalanobis distance (consider the covariance)

$$\sqrt{(x_i - x_k)^\top V^{-1} (x_i - x_k)}$$

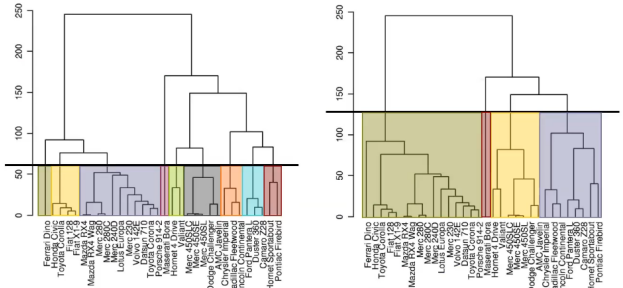
- Cosine distance
- etc.

PARTITION METHODS: K-MEANS



HIERARCHICAL METHODS

- Tree structure
- Based in distances inter/intra-clusters
- No fixed number o clusters



1. Agglomerative algorithms (bottom-up)

- starts with one cluster per observation,
- pairs of closest clusters are merged as one moves up the hierarchy.

2. Divisive algorithms (top-down)

- start with a single cluster
- splits recursively as one moves down the hierarchy.

HIERARCHICAL METHODS - INTERCLUSTER DISTANCE

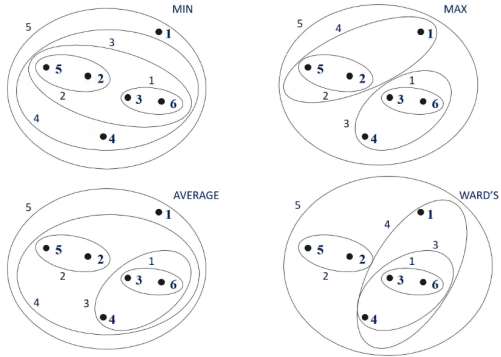
- **Minimum distance:** (Single Linkage)

$$dist(C_a, C_b) = \min_{x_i \in C_a,\, x_j \in C_b} d(x_i, x_j)$$

- **Maximum distance:** (Complete Linkage)

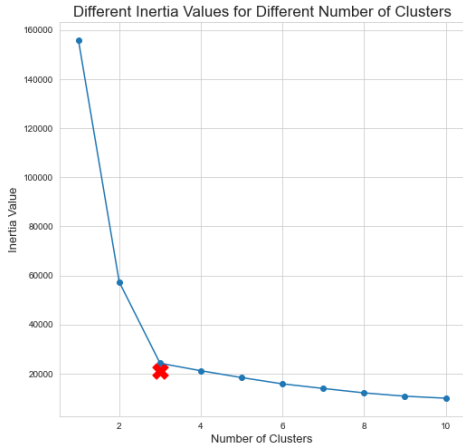
$$dist(C_a, C_b) = \max_{x_i \in C_a,\, x_j \in C_b} d(x_i, x_j)$$

- **Average distance**
- **Ward distance:** Minimizes the within cluster variance

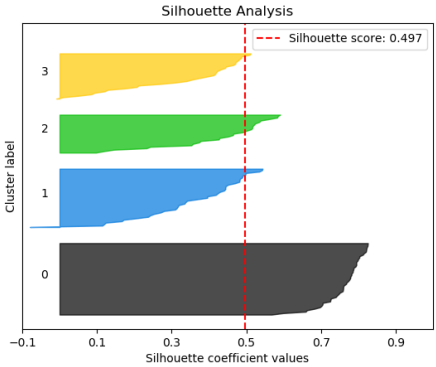


QUALITY MEASURES

- **Inertia** $\sum_{i=1}^{N} (x_i - C_k)^2$
- **Cohesion** of a cluster
  $coes(C) = \sum_{x_i, x_j \in C} d(x_i, x_j)$
- **Separation** between clusters
  $sep(C_a, C_b) = \sum_{x_i \in C_a, x_j \in C_b} d(x_i, x_j)$
- **Overall Cohesion**
  $coes(\mathcal{C}) = \sum_{C \in \mathcal{C}} coes(C)$
- **Overall Separation**
  $sep(\mathcal{C}) = \sum_{C_a, C_b \in \mathcal{C}} sep(C_a, C_b)$



SILHOUETTE

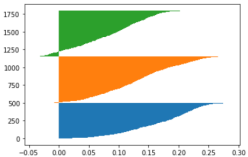
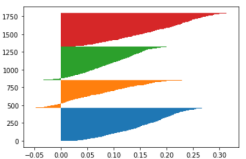
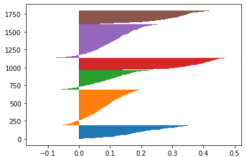
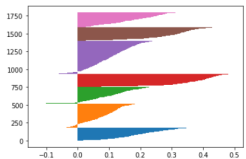
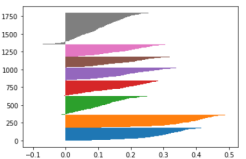
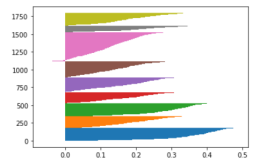
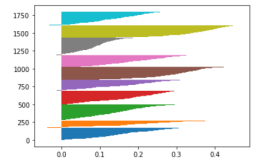
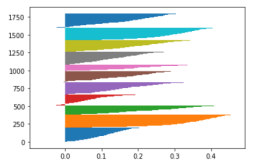


For an observation x_i

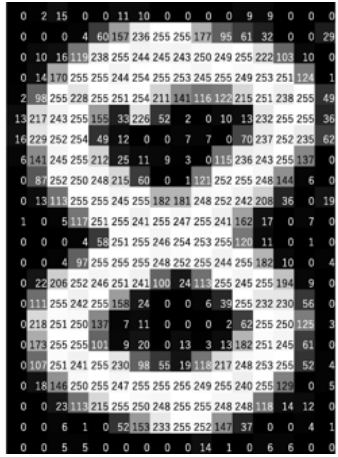
- Compute the average distance u_i of x_i to all the others point in the **same** cluster
- For each of the other clusters C, compute the average distance from x_i to the elements of C
- Compute the minimum of the previous distances v_i

$$silh(x_i) = \frac{v_i - u_i}{\max(u_i, v_i)} \in [-1, 1]$$

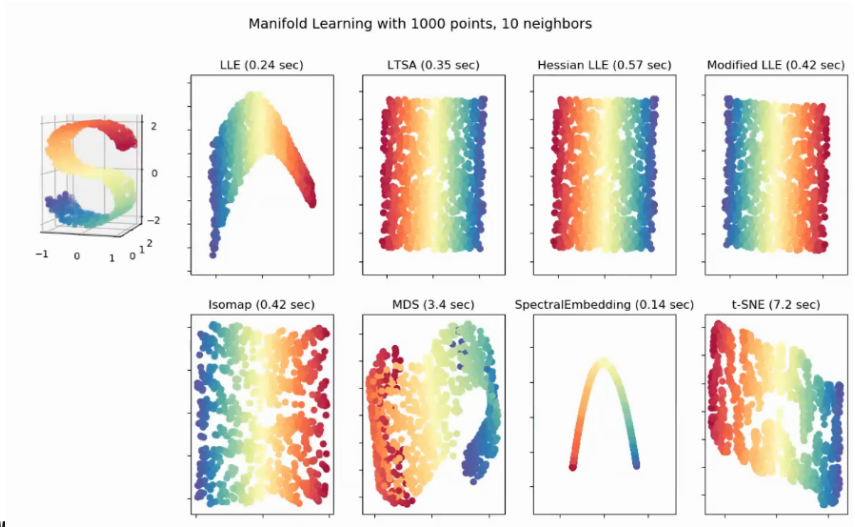
A CLUSTERING EXAMPLE

MNIST DATASET



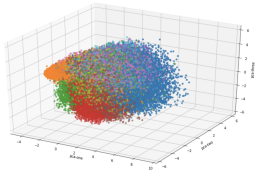
NON-LINEAR REDUCTION



T-SNE: T-DISTRIBUTED STOCHASTIC NEIGHBOUR EMBEDDING

We aim to project observations preserving observation distance.

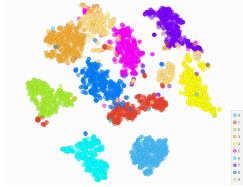
High-Dimensional Space



Distance as Normal Distribution

$$p_{ij} = \frac{\exp\left(-\left\|x_i - x_j\right\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq l} \exp\left(-\left\|x_k - x_l\right\|^2 / 2\sigma_i^2\right)}$$

Low-Dimensional Space



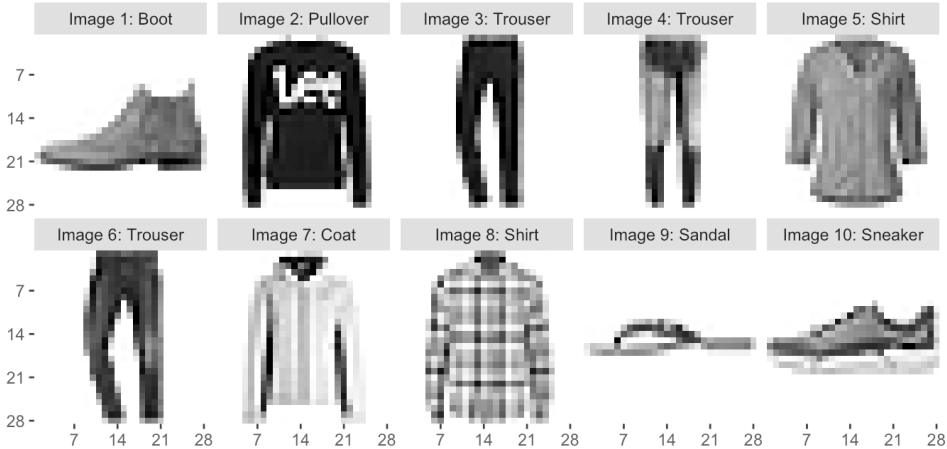
Distance as t-Students Distribution

$$q_{ij} = \frac{\left(1 + \left\|y_i - y_j\right\|^2\right)^{-1}}{\sum_{k \neq l} \left(1 + \left\|y_k - y_l\right\|^2\right)^{-1}}$$

We try to minimize the divergence between the distributions

$$KL(P\|Q) = \sum_i \sum_{j \neq i} p_{ij} \log\left(\frac{p_{ij}}{q_{ij}}\right)$$ (Kullback-Leibler)

MNIST FASHION (ZALANDO)



THANK YOU