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Evaluation Metrics

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN}$$
$$Precision = \frac{TP}{TP+FP}$$
$$Recall = \frac{TP}{TP+FN}$$
$$Specificity = \frac{TP}{TN+FP}$$
$$Fscore = \frac{2 \cdot Precision \cdot Recall}{Precision + Recall}$$
$$error\ rate = 1 - accuracy$$
$$macro\ average = \frac{1}{n}\sum_{i=1}^{n} avg_i$$

Activation Functions

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

Hyperbolic tangent : $\frac{e^x - e^{-x}}{e^x + e^{-x}}$

Relu : $\begin{cases} 0 & \text{si } x < 0 \\ x & \text{si } x \geq 0 \end{cases}$

Gaussian : e^{-x^2}

Softmax : $\frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}}$

Neural Network

Structure

Biais : b, An extra weight that can be learned using a learning algorithm. The purpose is to replace threshold.
Input : I, Input vector
Weights : W, Vector of weights

Learning algorithm

1. Randomly initialize weights
2. Compute the neuron's output for a fiven input vector X
3. Update weights : $W_j(t+1) = W_j(t) + \eta\,(\hat{y_i} - y)\,x$ with η the learning rate and $\hat{y_i}$ the desired output.
4. Repeat steps 2 and 3 for the number of epochs you need or until the error is smaller than a threshold.

KNN

Hyperparameters :

- Number of neighbours k
- Distance metric
- normalization type
- strategy if no majority

Big k :

Bayes

$$P(C_k|x) = \frac{P(x|C_k) \cdot P(C_k)}{P(x)}$$

où

- C_k : Classe ciblée
- x : Évidence
- $P(C_k)$: Probabilité a priori de la classe C_k
- $P(x|C_k)$: probability of observing x given class j
- $P(C_k|x)$: Probabilité a posteriori de la classe C_k après observation de x
- $P(x)$: Probabilité de l'évidence x

avec

$$P(x) = \sum_{\text{toutes classes } C_k} P(x|C_k) \cdot P(C_k)$$

Classifier H/F:

- $P(C_f) = \frac{4}{70}, P(C_g) = \frac{66}{70}$
- $p(x|C_g) = 0.8, p(x|C_f) = 0.2$
- Calcul de $p(x)$:

$$p(x) = 0.2 \times \frac{4}{70} + 0.8 \times \frac{66}{70}$$

- Calcul de $P(C_f|x)$ et $P(C_g|x)$:

$$P(C_f|x) = \frac{0.2 \times \frac{4}{70}}{p(x)}, \quad P(C_g|x) = \frac{0.8 \times \frac{66}{70}}{p(x)}$$

(+)Can deal with imbalanced dataset, prior can be changed

Linear Regression

Soit un tableau de données :
x = Surface(g) , y = Price(cm) , $x \cdot y$, x^2

$$X = [1, Surface]$$

$$X^T X = \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} = \begin{bmatrix} 7 & 38.5 \\ 38.5 & 218.95 \end{bmatrix}$$

$$X^T y = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix} = \begin{bmatrix} 348 \\ 1975 \end{bmatrix}$$

$$\hat{\theta} = (X^T X)^{-1} X^T y = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} -2.67 \\ 9.51 \end{bmatrix}$$

$$\hat{y} = \theta_0 + \theta_1 x$$

Matrix Inversion (2x2)

Logistic Regression

$$h_\theta(x_n) = \sigma(x\theta^T)$$

- $h_\theta(x_n)$: predicted value
- θ : model's parameters
- X : input vector

Goal : Find the θ that maximizes the likelihood of the data.
Loss :

$$J(\beta) = -\frac{1}{n}\sum_{i=1}^{n} y_i \log(h_\theta(x_n)) + (1-y_i)\log(1-h_\theta(x_n))$$

Normalization

Min-max [0,1] : $x' = \frac{(x - x_{min})}{(x_{max} - x_{min})}$

Min-max [-1,1] : $x' = 2 \cdot min\_max(x) - 1$
min-max doesn't handle outliers.

Z-norm : $x' = \frac{(x-\mu)}{\sigma}$

Support Vector Machine

Concept : SVM finds the hyperplane that best separates different classes by maximizing the margin between the closest points of different classes (support vectors).
hw(x) = sign(b + wx)

Formulation

$$\max_{\omega,b} \frac{1}{\|\omega\|} \quad \text{s.t.} \quad y_i(\omega \cdot x_i + b) \geq 1\,\forall i$$

where

- ω : Normal vector to the hyperplane
- b : Bias term
- x_i, y_i : Training data points and labels

Kernel Trick

SVM can be extended to non-linearly separable data using kernel functions, which implicitly map input space to a higher-dimensional feature space

Common Kernels

- Linear : $\langle x, x' \rangle$
- Polynomial : $(\gamma\langle x, x' \rangle + r)^d$
- Gaussian (RBF) : $e^{(-\gamma\|x-x'\|^2)}$

(+) Effective in high-dimensional spaces, Memory efficient, Versatile (different kernel functions)

(-) Sensitive to the choice of kernel and regularization parameters, Not suitable for very large datasets
hinge loss : $max(0, 1 - y_i(w \cdot x_i + b))$ (0 if correct classification) (1 if falls on the hyperplane) (>1 if misclassified)

Objective function to min

$$\min_{\omega,b} \quad \frac{1}{2}\|\omega\|^2 + C\sum_{i=1}^{n} \max(0, 1 - y_i(\omega \cdot x_i + b))$$

where C nutch the hinge loss term (how far are we predicting from ground truth) and regularization term (impeach big value, min w => maximize margin)

Similarity Measures

$$Pearson = R^2 = 1 - \frac{\sum_1^n (y_i - \hat{y}_i)^2}{\sum_1^n (y_i - \overline{y_i})^2}$$

$$Euclidian = \sqrt{\sum (I_1 - I_2)^2}$$

$$Manhattan = \sum |I_1 - I_2|$$

$$MSE = \frac{1}{N} \sum_1^n (y_i - \hat{y}_i)^2$$

$$cosine\ similarity = \frac{A \cdot B}{\|A\| \cdot \|B\|}$$

$WSS = \sum_{i=1}^{k} \sum_{x \in C_i} d(x, \mu_i)^2$ Within-cluster-sum (distortion) is the sum of the squared distances between each point in a cluster x_j and its cluster center.

K-Means

1. Initialize k centroids randomly.
2. Assign each point to the nearest centroid.
3. Recompute centroids as the mean of assigned points.
4. Repeat steps 2-3 until convergence.

minimize distortion : $J = \sum_{i=1}^{k} d(x_n, \mu_c)$

(+) Will converge
(-) Sensitive to initial conditions(size, density, distribution), Finds a local optimum

Mean Shift Clustering

1. Choose bandwidth and initialize centroids.
2. Shift each centroid to the mean of points within the bandwidth.
3. Repeat until centroids converge.

(+) Can find clusters of arbitrary shape; robust to outliers.
(-) Computationally intensive; bandwidth parameter can be tricky to set.

DB-Scan

1. Classify points as core, border, or noise based on density.
2. Form clusters around core points.
3. Assign border points to clusters or mark as noise.

(+) Identifies clusters of varying shapes; robust to noise.
(-) Sensitive to parameters; struggles with varying density clusters.

Hierarchical Clustering

Algorithm (Agglomerative) :

1. Start with each point as a separate cluster.
2. Merge the closest pair of clusters.
3. Repeat step 2 until desired number of clusters is reached.

(+) No need to specify the number of clusters; intuitive dendrogram representation.
(-) Computationally expensive for large datasets; sensitive to outliers.

Clustering

Clustering partitions data into clusters with high intra-class similarity and low inter-class similarity.
Needs : distance measure, criterion, algorithm.

Partitions

Distortion : How close are we to a "centroid" defining the partition ?
Connectivity of points : How close are points to each other ?

Elbow Method

Heuristic used in determining the number of clusters in a data set. It selects the value of k that corresponds to the elbow of the curve (#cluster, WSS)

Silhouette Coefficient

$$s = \frac{b - a}{\max(a, b)}$$

- a is the mean distance between a sample and all other points in the same class (cohesion)
- b is the mean distance between a sample and all other points in the next nearest cluster (isolation)

s range is $[-1, 1]$. A high value indicates that the object is well matched to its own cluster and poorly matched to neighboring clusters.

Davies-Bouldin Index

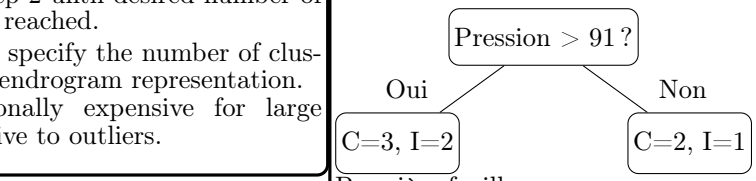
$$DB = \frac{1}{k} \sum_{i=1}^{k} \max_{j \neq i} \frac{R_i + R_j}{d(C_i, C_j)}$$

- R_i is the average distance between a point in cluster C_i and all points in C_i (cluster diameter))
- $d(C_i, C_j)$ is the distance between the centroids of C_i and C_j

zero is the lowest possible score. Values closer to zero indicate a better partition.

Decision Tree

A flowchart-like structure in which each internal node represents a test on a feature. Each leaf node represents a class label(decision taken after computing all features).



Première feuille :

$$Gini = 1 - \left(\frac{3}{3+2}\right)^2 - \left(\frac{2}{3+2}\right)^2 = \frac{12}{25}$$

Deuxième feuille :

$$Gini = 1 - \left(\frac{2}{2+1}\right)^2 - \left(\frac{1}{2+1}\right)^2 = \frac{4}{9}$$

CART Algorithm :

- Select the best attribute using IG or Gini
- Make that attribute a decision node and break the dataset into smaller subsets
- Recursively repeat the process on each subset until you find leaf nodes in all the branches of the tree

Pruning : Pruning is a technique in machine learning and search algorithms that reduces the size of decision trees by removing sections of the tree that provide little power to classify instances.

(+) Easy to interpret and explain, Can handle both numerical and categorical data, Requires little data preparation, Able to handle multi-output problems, Uses a white box model, Can be used for feature selection, Performs well even if its assumptions are somewhat violated by the true model from which the data were generated

(-) Overfitting, Can be unstable because small variations in the data might result in a completely different tree being generated, Not suitable for large datasets, Unbalanced datasets where one class is dominant, Biased trees if some classes dominate

Gini Impurity

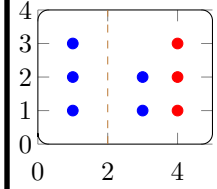
Gini Set :$G(X) = 1 - \sum_{i=1}^{n} p(x_i)^2$ where

- $p(x_i)$: is the proportion of points in a set that belongs to a class i : $\frac{N_i}{N}$.
- G = 0.5 : maximum value of impurity, classes are balanced in the set.
- G = 0 : minimum value of impurity, all the values belong to a single class.

Gini Split :$\sum_{i=1}^{n} \frac{N_i}{N} G(X_i)$

Gini Gain :$Gini_{set} - Gini_{split}$

Example



Gini set :

$$Gini = 1 - \left(\frac{5}{10}\right)^2 - \left(\frac{5}{10}\right)^2 = \frac{1}{2}$$

Left Set :

$$Gini = 1 - \left(\frac{3}{3}\right)^2 - \left(\frac{0}{3}\right)^2 = 0$$

Right Set :

$$Gini = 1 - \left(\frac{2}{7}\right)^2 - \left(\frac{5}{7}\right)^2 = \frac{20}{49}$$

Gini Split :

$$Gini = \frac{3}{10} \times 0 + \frac{7}{10} \times \frac{20}{49} = \frac{2}{7}$$

Gini Gain :

$$Gini = \frac{1}{2} - \frac{2}{7} = \frac{3}{14}$$

Entropy

$$H(X) = -\sum_{i=1}^{n} p(x_i) \log_2 p(x_i)$$

where

— $p(x_i)$: Probability of class x_i

Information Gain :

$$IG(X, Y) = H(X) - H(X|Y)$$

where

— $H(X)$: Entropy of the parent node
— $H(X|Y)$: Entropy of the child node

Principal Component Analysis

Kmeans

Hierarchical clustering

Autoencoders

Kmeans

Hierarchical clustering

Convolutional Neural Networks

Recurrent Neural Networks

Dimensionality Reduction

Reinforcement Learning

Computational Complexity of ML Algorithms

Algorithm	**Assumption**	**Train Time/Space**	**Inference Time/Space**
KNN (Brute Force)	Similar things exist in close proximity	$O(knd)$ / $O(nd)$	$O(knd)$ / $O(nd)$
KNN (KD Tree)	Similar things exist in close proximity	$O(nd\log(n))$ / $O(nd)$	$O(k\log(n)d)$ / $O(nd)$
Naive Bayes	Features are conditionally independent	$O(ndc)$ / $O(dc)$	$O(dc)$ / $O(dc)$
Logistic Regression	Classes are linearly separable	$O(nd)$ / $O(nd)$	$O(d)$ / $O(d)$
Linear Regression	Linear relationship between variables	$O(nd)$ / $O(nd)$	$O(d)$ / $O(d)$
SVM	Classes are linearly separable	$O(n^2d^2)$ / $O(nd)$	$O(kd)$ / $O(kd)$
Decision Tree	Feature selection by information gain	$O(n\log(n)d)$ / $O(\text{nodes})$	$O(\log(n))$ / $O(\text{nodes})$
Random Forest	Low bias and variance trees	$O(kn\log(n)d)$ / $O(\text{nodes}\times k)$	$O(k\log(n))$ / $O(\text{nodes}\times k)$
GBDT	High bias, low variance trees	$O(Mn\log(n)d)$ / $O(\text{nodes}\times M+\gamma_m)$	$O(M\log(n))$ / $O(\text{nodes}\times M+\gamma_m)$