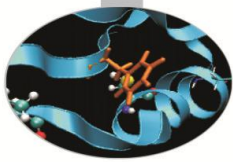
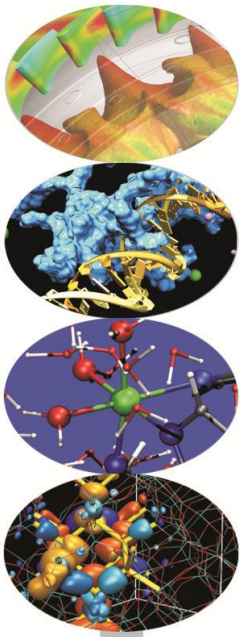
CINECA SCAI
SuperComputing Applications and Innovation



Machine Learning with Spark



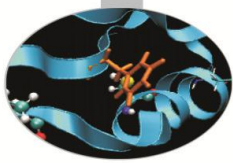
Giorgio Pedrazzi, *CINECA-SCAI*

Tools and techniques for massive data analysis

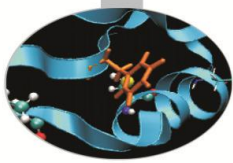
Roma, 15/12/2016

CINECA

Agenda



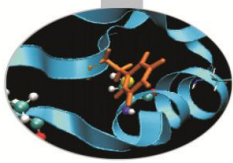
- Cluster Analysis
  - Basic concept
  - Main clustering algorithms
  - Distance measures
- Association rules and sequential patterns
  - Association Rules mining
  - Sequential Patterns mining
- Supervised learning: Classification
  - Training and test
  - Evaluation metrics
  - Decision tree
  - Naïve Bayes
- Examples with Spark MLlib in Scala and Python



Cluster analysis

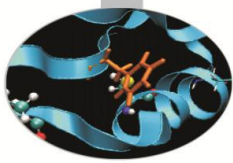
- Cluster analysis
  - no predefined classes for a training data set
  - find *similarities* between data according to characteristics underlying the data and grouping similar data objects into clusters
  - two general tasks: identify the “natural” clustering number and properly grouping objects into “sensible” clusters
- Cluster: A collection/group of data objects/points
  - similar (or related) to one another within the same group
  - dissimilar (or unrelated) to the objects in other groups
- Typical applications
  - as a stand-alone tool for data exploration
  - as a precursor to other supervised learning methods

Typical applications



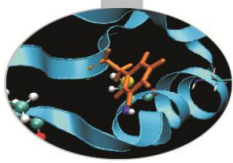
- Scientific applications
  - **Biology**: discover genes with similar functions in DNA microarray data.
  - **Seismology**: grouping earthquake epicenters to identify dangerous zone.
  - …
- Business applications
  - **Marketing:** discover distinct groups in customer bases (insurance, bank, retailers) to develop targeted marketing programs.
  - **Behavioral analysis**: identifying driving styles.
  - …
- Internet applications
  - **Social network analysis:** in the study of social networks, clustering may be used to recognize communities within a network.
  - **Search result ordering:** grouping of files or web pages to create relevant sets of search results.
  - …

Data representation



The problem must be formulated in a mathematical way as, for example, a data matrix containing information on N objects (cases or observations ; rows of the matrix) specified by the values assigned to V variables (columns of the matrix)

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$



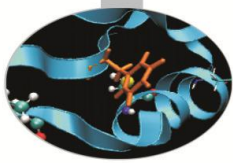
Cluster Analysis steps

- Variable selection
- Preprocessing
- Select a clustering algorithm
- Select a distance or a similarity measure (*)
- Determine the number of clusters (*)
- Validate the analysis

Changing one parameter may result in complete different cluster results.

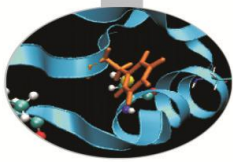
(*) if needed by the method used

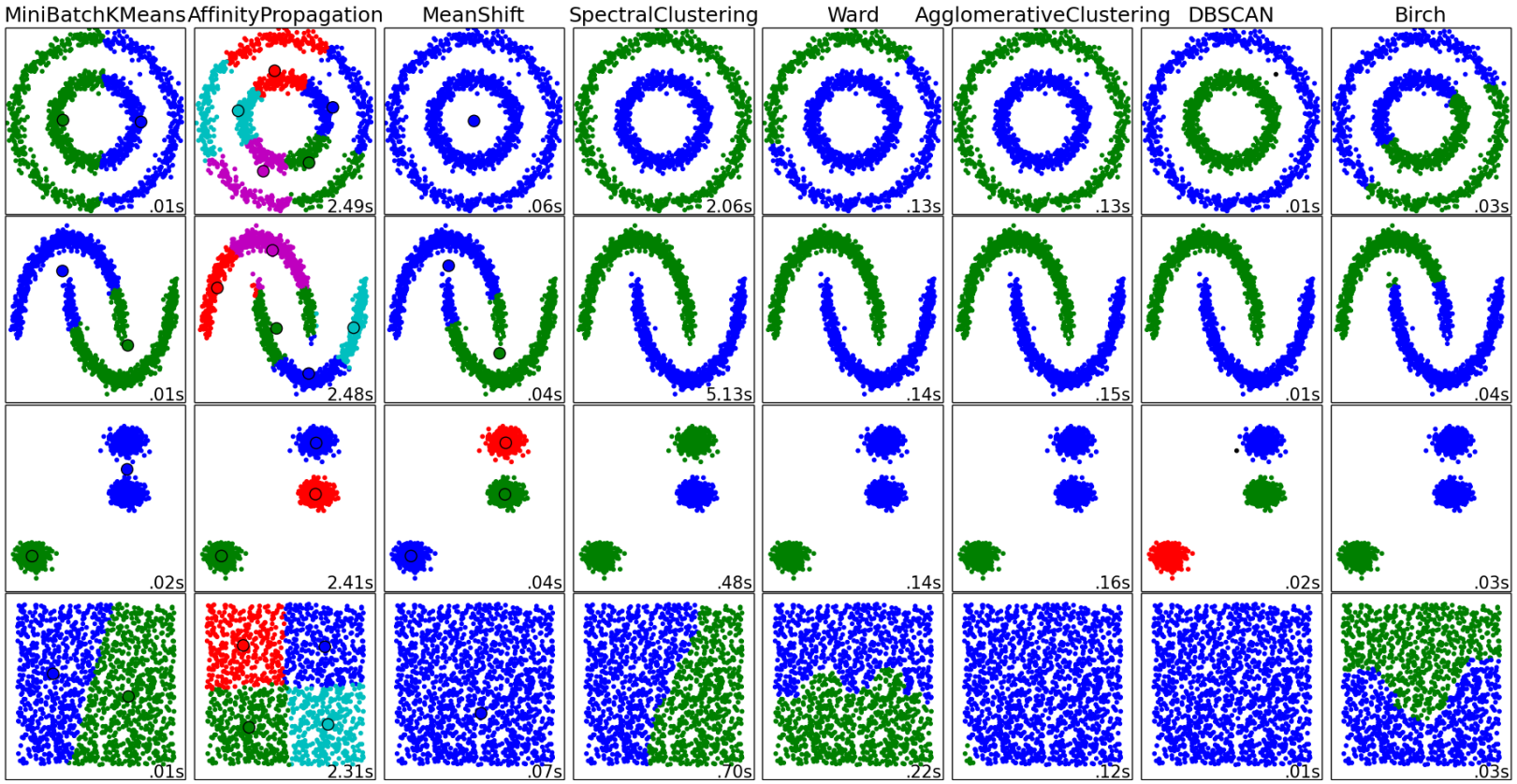
Classifications of methods



- Types of clustering (1)
  - Distance-based
  - Density based
  - Model based
  - Spectral clustering
  - …
  - Combination of methods
- Types of clustering (2)
  - Partitional vs. Hierarchical
  - Complete vs. Partial
  - Exclusive vs. Fuzzy vs. Overlapping
- …

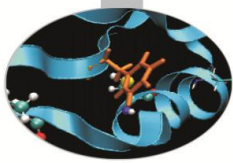
Comparison of methods





http://scikit-learn.org/stable/modules/clustering.html

Distance measure



Different distance metrics give different clusters.

Minkowski distance (L_p Norm)

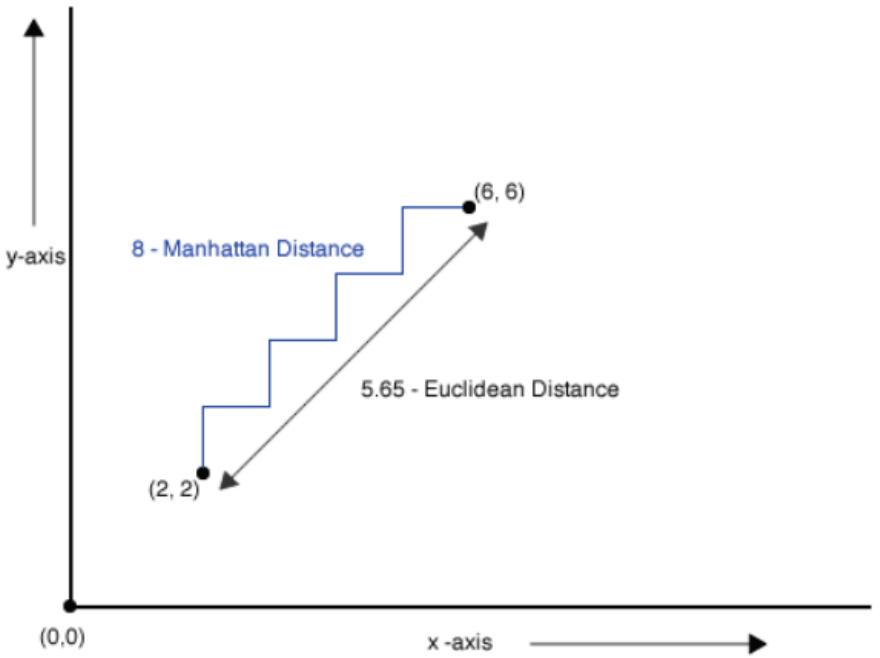
$$d(i,k) = \left[\sum_{j=1}^{d} | x_{ij} - x_{kj} |^{p} \right]^{1/p}$$

Euclidean distance (L_2 Norm)

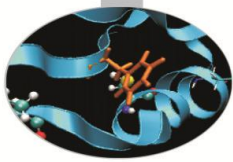
$$d(i,k) = \left[\sum_{j=1}^{d} (x_{ij} - x_{kj})^{2} \right]^{1/2}$$

Manhattan distance (city block distance)

$$d(i,k) = \sum_{j=1}^{d} | x_{ij} - x_{kj} |$$



Distance Measures



- Cosine Measure (Similarity vs. Distance)

For $\mathbf{x} = (x_1\ x_2 \cdots x_n)$ and $\mathbf{y} = (y_1\ y_2 \cdots y_n)$

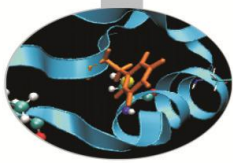
$$\cos(\mathbf{x},\mathbf{y}) = \frac{\mathbf{x} \bullet \mathbf{y}}{\|\mathbf{x}\|\,\|\mathbf{y}\|} = \frac{x_1 y_1 + \cdots + x_n y_n}{\sqrt{x_1^2 + \cdots + x_n^2}\,\sqrt{y_1^2 + \cdots + y_n^2}}$$

$$d(\mathbf{x},\mathbf{y}) = 1 - \cos(\mathbf{x},\mathbf{y}) = 1 - \frac{\mathbf{x} \bullet \mathbf{y}}{\|\mathbf{x}\|\,\|\mathbf{y}\|}$$

$$0 \le d(\mathbf{x},\mathbf{y}) \le 2$$

  - Cosine similarity is a common similarity metric in text analysis.
  - It measures the smallest angle between two vectors
  - It can be turned into a pseudo distance by subtracting it from 1.0

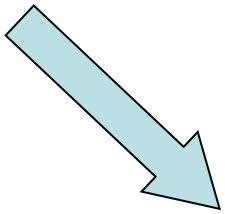
Similarity measures

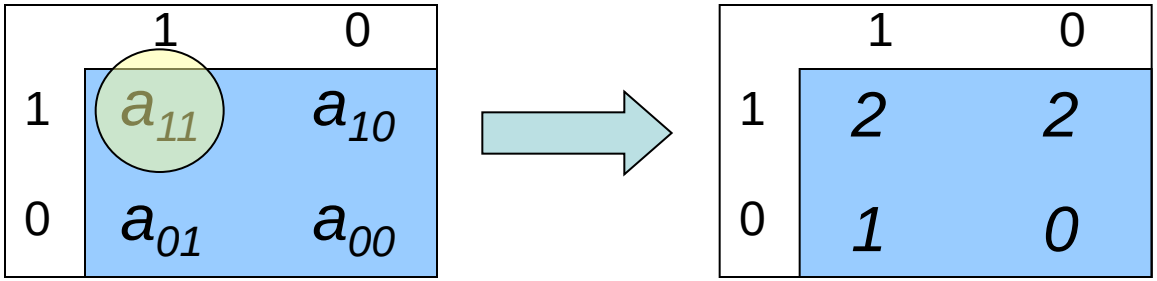


Correspondent 1's

x_k: 0 1 1 0 1

x_j: 1 1 0 1 1



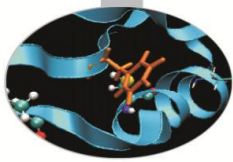


Jaccard: $d(i,k) = (a_{11}) / (a_{11} + a_{10} + a_{01})$

Condorcet: $d(i,k) = a_{11} / [a_{11} + 0.5(a_{10} + a_{01})]$

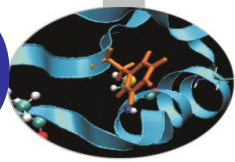
Dice bis: $d(i,k) = a_{11} / [a_{11} + 0.25(a_{10} + a_{01})]$

Distance based (Partitioning)



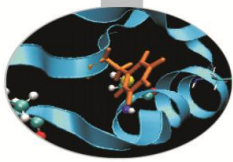
- Partitioning method: Construct a partition of a database ***D*** of ***n*** objects into a set of ***k*** clusters
- Given a *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means*: Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM: Each cluster is represented by one of the objects in the cluster

Distance based (Hierarchical)



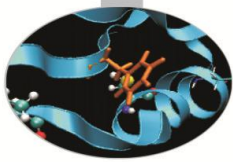
- Agglomerative (bottom-up):
  - Start with each observation being a single cluster.
  - Eventually all observations belong to the same cluster.
- Divisive (top-down):
  - Start with all observations belong to the same cluster.
  - Eventually each node forms a cluster on its own.
  - Could be a recursive application of k-means like algorithms
- Does not require the number of clusters *k* in advance
- Needs a termination/readout condition

Hierarchical Agglomerative Clustering

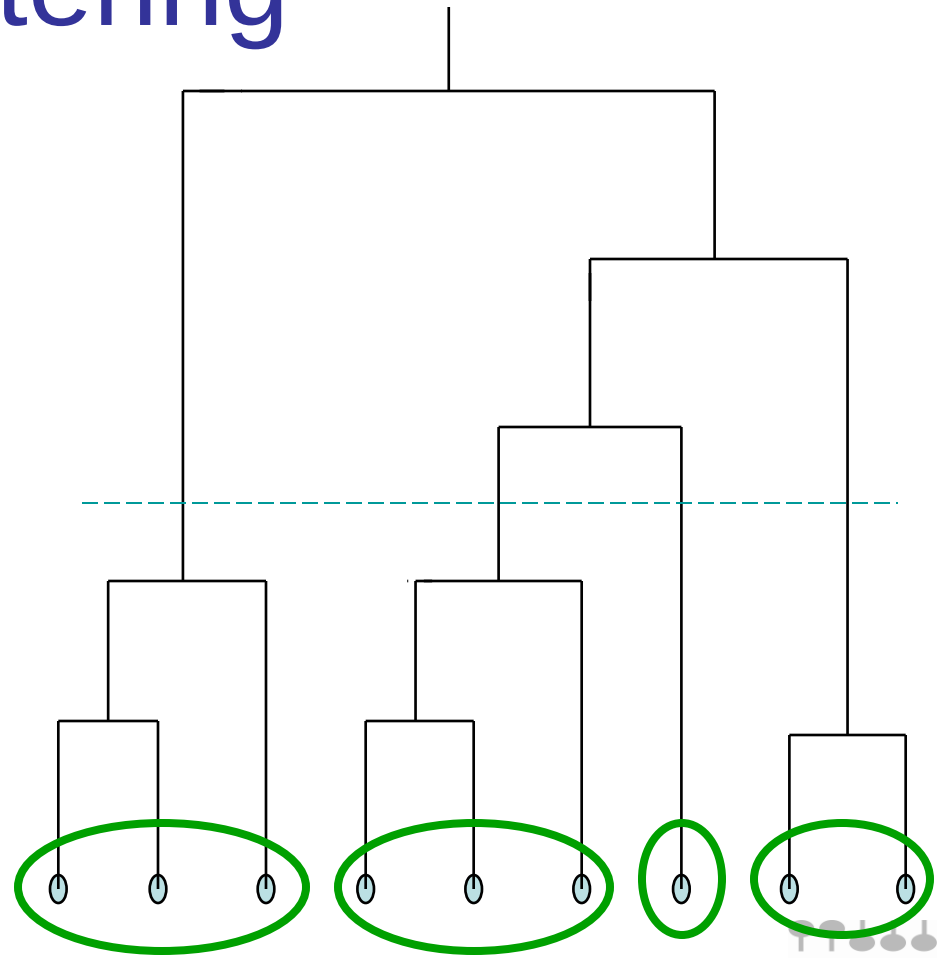


- Assumes a similarity function for determining the similarity of two instances.
- Starts with all instances in a separate cluster and then repeatedly joins the two clusters that are most similar until there is only one cluster.
- The history of merging forms a binary tree or hierarchy.

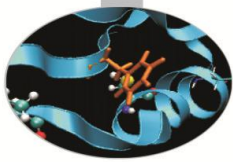
Dendogram: Hierarchical Clustering



- Clustering obtained by cutting the dendrogram at a desired level: each connected component forms a cluster.



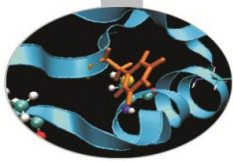
Hierarchical Agglomerative Clustering (HAC)



- Starts with each observation in a separate cluster
  - then repeatedly joins the *closest pair* of clusters, until there is only one cluster.
- The history of merging forms a binary tree or hierarchy.

How to measure distance of clusters??

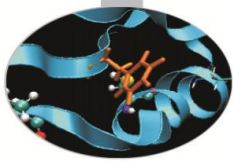
Closest pair of clusters



Many variants to defining closest pair of clusters

- Single-link
  - Distance of the *"closest" points* (single-link)
- Complete-link
  - Distance of the "furthest" points
- Centroid
  - Distance of the centroids (centers of gravity)
- Average-link
  - Average distance between pairs of elements

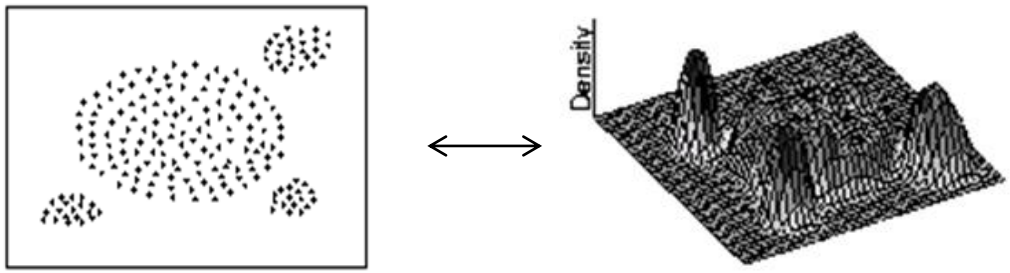
Density based approach



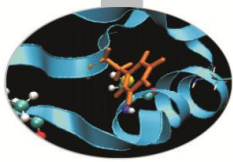
DBSCAN is a density-based clustering algorithm: given a set of points in some space, it groups together points that are closely packed together (points with many nearby neighbors), omitting as outliers points that lie alone in low-density regions (whose nearest neighbors are too far away).

The number of clusters is determined by the algorithm.

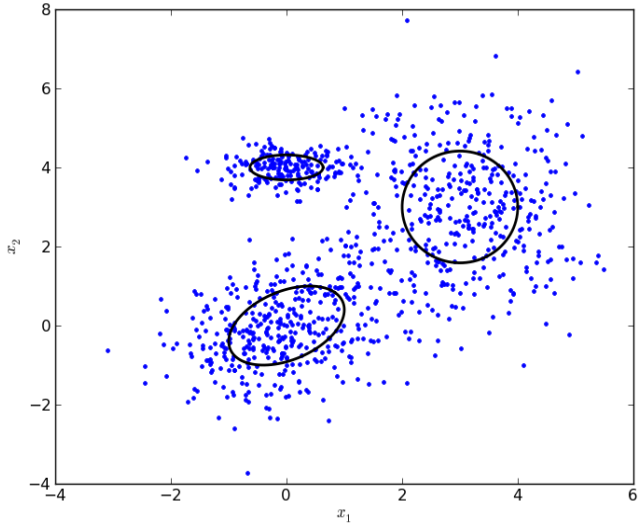
DBSCAN does not produce a complete clustering



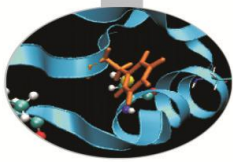
Model-based Approach



- Probabilistic model-based clustering
  - In model-based clustering, it is assumed that the data are generated by a mixture of underlying probability distributions in which each component represents a different group or cluster.
  - Cluster: Data points (or objects) that most likely belong to the same distribution
  - Clusters are created so that they will have a maximum likelihood fit to the model by a mixture of K component distributions (i.e., K clusters)



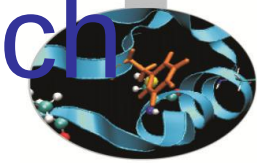
Spectral Clustering Approach



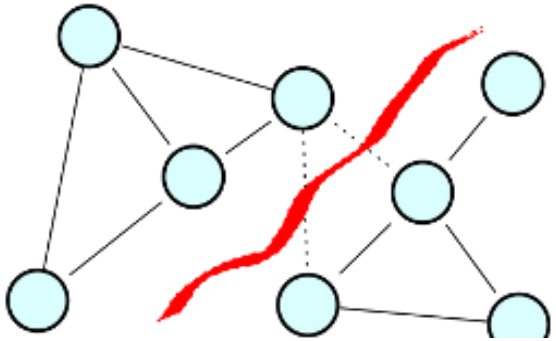
- In multivariate statistics, spectral clustering techniques make use of eigenvalue decomposition (spectrum) of the similarity matrix of the data to perform dimensionality reduction before clustering in fewer dimensions. The similarity matrix is provided as an input and consists of a quantitative assessment of the relative similarity of each pair of points in the dataset.

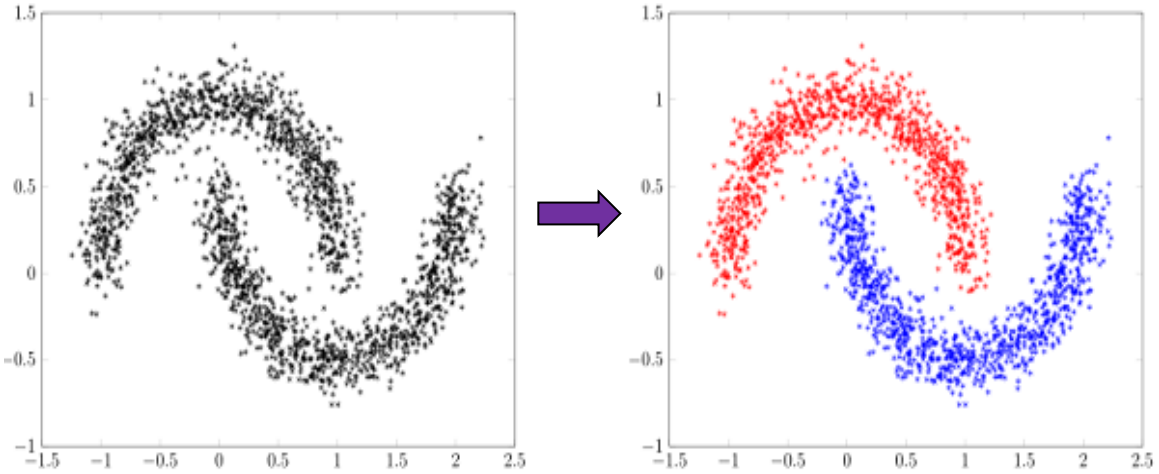
- In application to image segmentation, spectral clustering is known as segmentation-based object categorization.

Spectral Clustering Approach

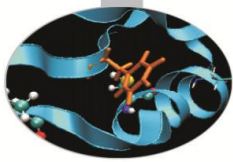


- Convert data set into weighted graph (vertex, edge), then cut the graph into sub-graphs corresponding to clusters via spectral analysis
- Typical methods: Normalised-Cuts ……





Combination of methods

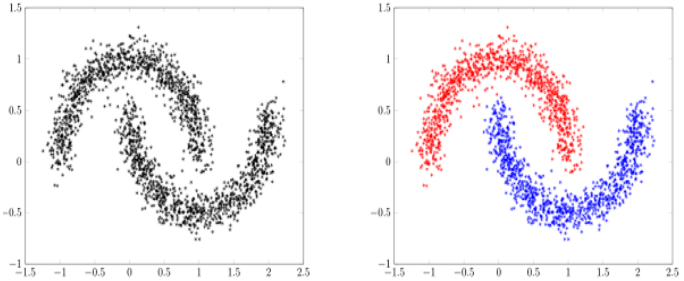


Using different methods can be useful for overcome the drawbacks of a single methods.

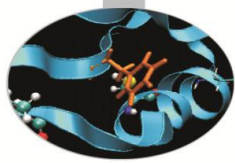
For example it is possible to generate a large number of clusers with K-means and then cluster them together using a hierarchical method.

It is important using the “single-link” method, in which the distance between two clusters is defined by the distance between the two closest data points we can find, one from each cluster.

This method has been applied to find cluster in non-convex set.

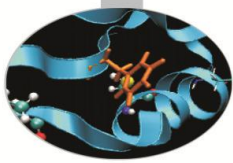


Cluster validation



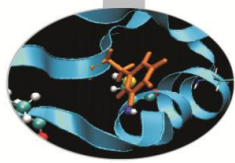
- In supervised classification, the evaluation of the resulting model is an integral part of model developing process
- For cluster analysis, the analogous question is how to evaluate the “goodness” of the resulting clusters with the aim of:
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Cluster validation



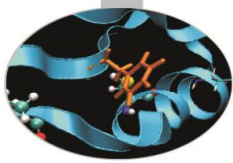
- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - e.g.: Entropy $e_i = -\sum_q \rho_{ij} \log_2 \rho_{ij}$.
  - Internal Index: Used to measure the goodness of a clustering structure *without* respect to external information.
    - e.g.: Sum of Squared Error (SSE) $WSS = \sum_i \sum_{x \in C_i} (x - m_i)^2$
  - Relative Index: Used to compare two different clusterings or clusters.
    - Often an external or internal index is used for this function, e.g., SSE or entropy
- Sometimes these are referred to as criteria instead of indices
  - However, sometimes criterion is the general strategy and index is the numerical measure that implements the criterion.

Spark MLlib



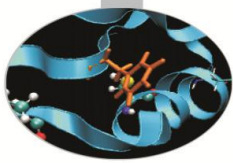
- MLlib is a Spark subproject providing machine learning primitives:
- MLlib's goal is to make practical machine learning (ML) scalable and easy. Besides new algorithms and performance improvements that we have seen in each release, a great deal of time and effort has been spent on making MLlib *easy*.

Spark MLlib



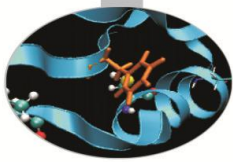
- MLlib algorithms
  - classification: logistic regression, naive Bayes, decision tree, ensemble of trees (random forests)
  - regression: generalized linear regression (GLM)
  - collaborative filtering: alternating least squares (ALS)
  - clustering: k-means, gaussian mixture, power iteration clustering, latent Dirichelet allocation
  - decomposition: singular value decomposition (SVD), principal component analysis, singular value decompostion
- Spark packages availables for machine learning at http://spark-packages.org

Association Rules mining



- Association rule mining is used to find objects or attributes that frequently occur together.
- For example, products that are often bought together during a shopping session (market basket analysis), or queries that tend to occur together during a session on a website's search engine.
- The unit of "togetherness" when mining association rules is called a transaction. Depending on the problem, a transaction could be a single shopping basket, a single user session on a website, or even a single customer.
- The objects that comprise a transaction are referred to as items in an itemset.

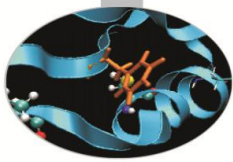
Market Basket Analysis



- Basket data consist of collection of transaction date and items bought in a transaction
- Retail organizations interested in generating qualified decisions and strategy based on analysis of transaction data
  - what to put on sale, how to place merchandise on shelves for maximizing profit, customer segmentation based on buying pattern
- Examples.
  - Rule form: LHS $\rightarrow$ RHS [confidence, support].
  - diapers $\rightarrow$ beers [60%, 0.5%]
  - “90% of transactions that purchase bread and butter also purchase milk”
  - bread and butter $\Rightarrow$ milk [90%, 1%]

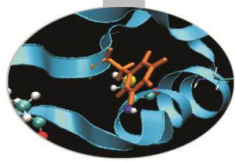
- https://www.youtube.com/watch?v=N5WurXNec7E&feature=player_embedded

Association rule discovery problem



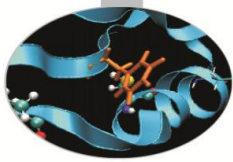
- Two sub-problems in discovering all association rules:
  - Find all sets of items (itemsets) that have transaction support above minimum support → Itemsets with minimum support are called *large itemsets*, and all others small itemsets.
  - Generate from each large itemset, rules that use items from the large itemset.
    - Given a large itemset *Y*, and *X* is a subset of *Y*
    - Take the support of *Y* and divide it by the support of *X*
    - If the ratio is at least *minconf*, then $X \Rightarrow (Y - X)$ is satisfied with confidence factor c

Discovering Large Itemsets



- Algorithm for discovering large itemsets make multiple passes over the data
  - In the first pass: count the support of individual items and determine which of them are large.
  - In each subsequent pass:
    - start with a set of itemsets found to be large in the previous pass.
    - This set is used for generating new potentially large itemsets, called *candidate* itemsets
    - counts the actual support for these candidate itemsets during the pass over the data.
  - This process continues until no new large itemsets are found.

Generate rules from large itemsets

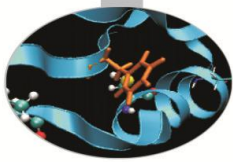


Y = {Bread, Butter, Milk}, X = {Bread, Butter}

conf = support(Y) / support(X) = {Bread, Butter, Milk} / {Bread, Butter}

if *conf* $\geq$ *minconf* then the rule {Bread, Butter} $\Rightarrow$ Milk holds

Sequential Pattern Mining



- Given a set of sequences and support threshold, find the complete set of *frequent* subsequences

A *sequence* : <(ef)(ab)(df)cb>

A *sequence database*

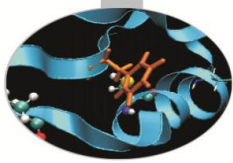
SID	sequence
10	<a(abc)(ac)d(cf)>
20	<(ad)c(bc)(ae)>
30	<(ef)(ab)(df)cb>
40	<eg(af)cbc>

An element may contain a set of items. Items within an element are unordered and we list them alphabetically.

<a(bc)dc> is a *subsequence* of <a(abc)(ac)d(cf)>

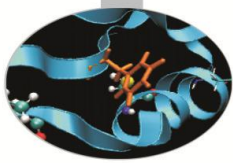
Given *support threshold* *min_sup* =2, <(ab)c> is a *sequential pattern*

Applications of sequential pattern mining



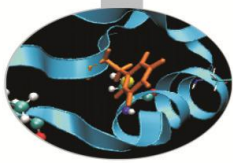
- Customer shopping sequences:
  - First buy computer, then CD-ROM, and then digital camera, within 3 months.
- Medical treatments, natural disasters (e.g., earthquakes), science & eng. processes, stocks and markets, etc.
- Telephone calling patterns, Weblog click streams
- DNA sequences and gene structures

Supervised learning: classification



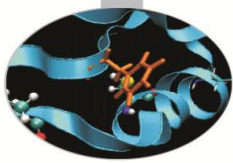
- Human learning from past experiences.
- A computer does not have “experiences”.
- A computer system learns from data, which represent some “past experiences” of an application domain.
- Learn a target function that can be used to predict the values of a discrete class attribute,
- The task is commonly called: Supervised learning, classification, or inductive learning.

Two-Step Process (1)

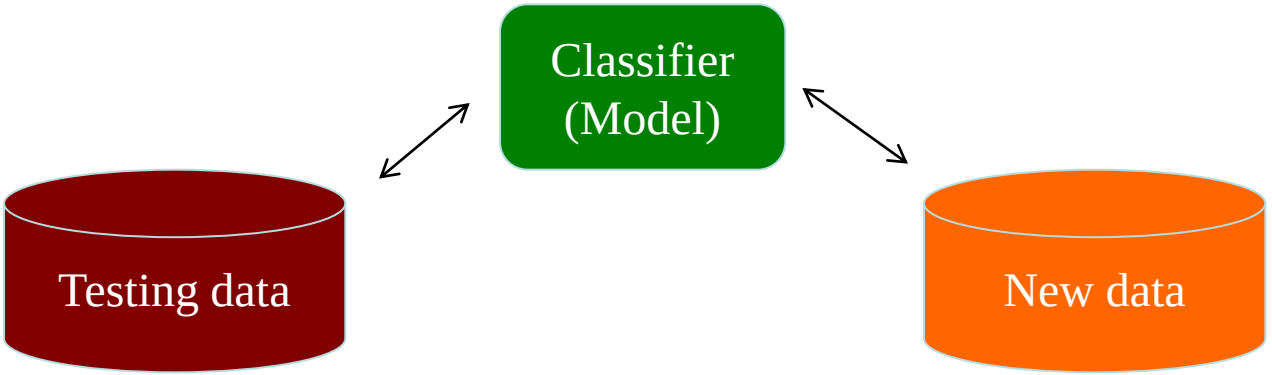


- Model construction
  - The set of samples used in this step is training data
  - Each sample belongs to a predefined class, suggested by its class label
  - The model is represented as classification rules, decision trees, or other functions

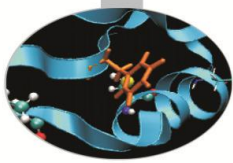
Two-Step Process (2)



- Model usage: classifying new objects
  - Estimate model accuracy
    - The set of samples for testing accuracy is testing data
    - Accuracy rate is the percentage of correctly classified samples
    - Testing data is independent of training data
  - If the accuracy is acceptable, apply it to new data

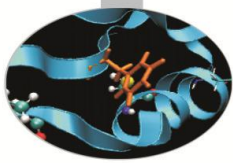


Typical applications



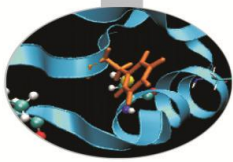
- Scientific applications
  - **Medical Diagnosis**: Given the symptoms exhibited in a patient and a database of anonymized patient records, predict whether the patient is likely to have an illness.
  - …
- Business applications
  - **Credit Card Fraud Detection**: Given credit card transactions for a customer in a month, identify those transactions that were made by the customer and those that were not.
  - **Stock Trading**: Given the current and past price movements for a stock, determine whether the stock should be bought, held or sold. A model of this decision problem could provide decision support to financial analysts.
  - …
- Internet applications
  - **Spam Detection**: Given email in an inbox, identify those email messages that are spam and those that are not.
  - …

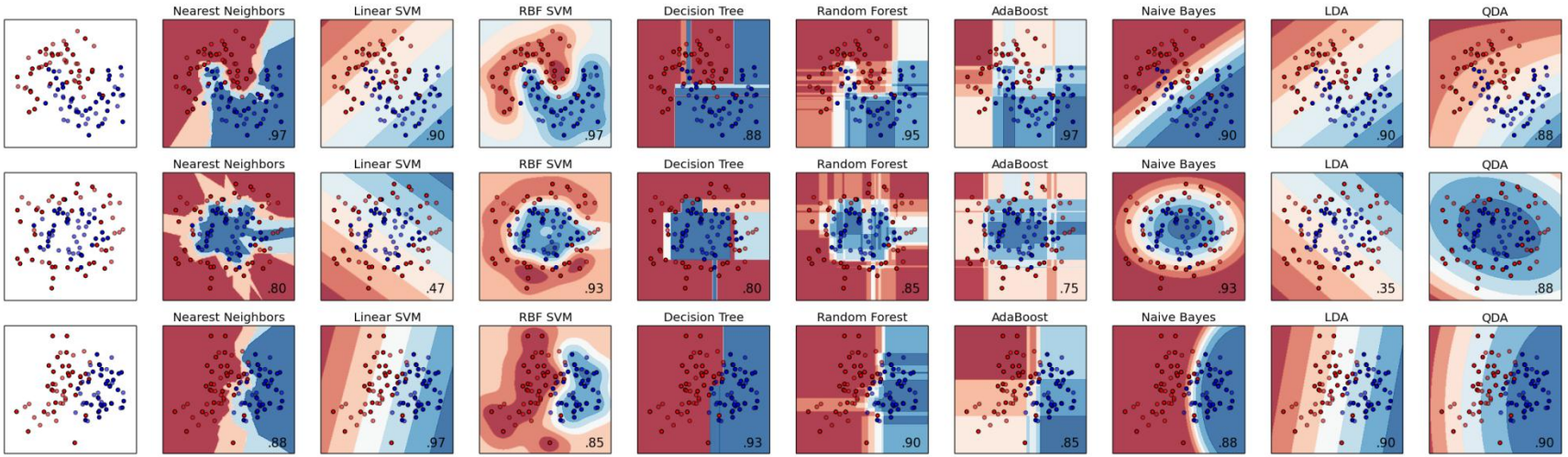
Classification Techniques



- Decision Tree based Methods
- Ensemble methods
- Naïve Bayes and Bayesian Belief Networks
- Rule-based Methods
- Memory based reasoning
- Neural Networks
- Support Vector Machines

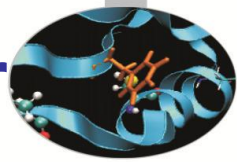
Comparison of algorithms





CINECA

Training and test a classifier

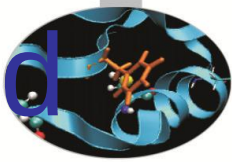


Is the model able to generalize? Can it deal with unseen data, or does it overfit the data? Test on hold-out data:

- **split** data to be modeled in training and test set
- **train** the model on training set
- evaluate the model on the training set
- **evaluate** the model on the test set
- difference between the fit on training data and test

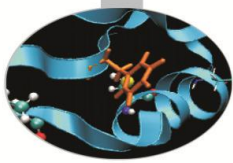
data measures the model's ability to *generalize*

Methods to create training and test data



- Fixed
  - Leave out random N% of the data
- K-fold Cross-Validation
  - Select K folds without replace
- Leave-One-Out Cross Validation
  - Special case of CV
- Bootstrap
  - Generate new training sets by sampling with replacement

Evaluation metrics



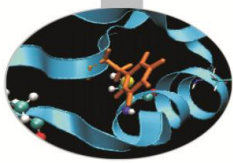
Confusion matrix

The known class of test samples is matched against the class predicted by the model		Predicted labels (model)		
		False	**True**	
Real labels (target)	**False**	TN	FP	Specificity TN / (FP+TN)
	True	FN	TP	Sensitivity TP / (TP+FN)
		Negative Predictive Value TN / (TN + FN)	Positive Predictive Value TP / (TP + FP)	Accuracy (TP+TN) / (TP+FP+TN+FN)

⇨ Recall

⇩ Precision

F-score = 2*Precision*Recall / (Precision + Recall)
Error rate = 1 – Precision
FP rate = 1 – Specificity

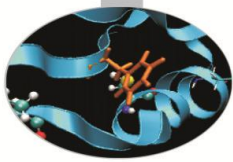


Evaluation metrics

Accuracy baselines

- Base Rate
  - Accuracy of trivially predicting the most-frequent class
- Random Rate
  - Accuracy of making a random class assignment
- Naive Rate
  - Accuracy of some simple default or pre-existing model

Building a Decision Tree

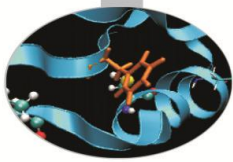


- Choose the attribute with the highest Information Gain
- Create branches for each value of attribute
- Partition examples on the basis of selected attributes
- Repeat with remaining attributes
- Stopping conditions
  - All examples assigned the same label
  - No examples left

Problems

- Expensive to train
- Prone to overfitting
  - perform well on training data, bad on test data
  - pruning can help: remove or aggregate subtrees that provide little discriminatory power

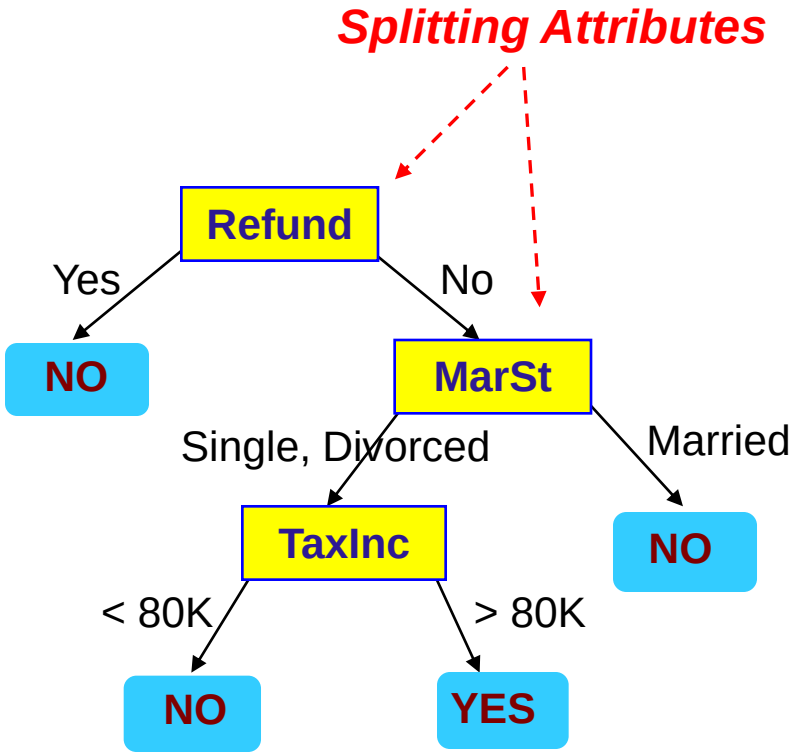
Example of a Decision Tree



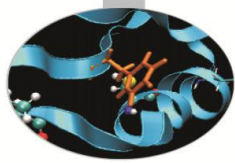
categorical | categorical | continuous | class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data



Model: Decision Tree



Bootstrap

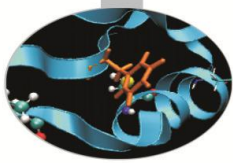
Given a dataset of size N

- Draw N samples with replacement to create a new dataset
- Repeat ~1000 times
- You now have ~1000 sample datasets
  - All drawn from the same population
  - You can compute ~1000 sample statistics
  - You can interpret these as repeated experiments

Very elegant use of computational resources

The bootstrap allows you to simulate repeated statistical experiments

Statistics computed from bootstrap samples are typically unbiased estimators



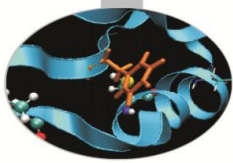
Ensembles

Combining classifiers

The output of a set of classifiers can be combined to derive a stronger classifier

(e.g. average results from different models)

- Better classification performance than individual classifiers
- More resilience to noise
- Time consuming
- Models become difficult to explain



Bagging

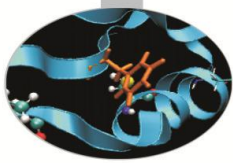
- Draw N bootstrap samples
- Retrain the model on each sample
- Average the results
  - Regression: Averaging
  - Classification: Majority vote

Works great for overfit models

Boosting: instead of selecting data points randomly, favor the misclassified points

- Initialize the weights
- Repeat:
  - Resample with respect to weights
  - Retrain the model
  - Recompute weights

The disadvantage of boosting, relative to big data, is that it's inherently sequential (weights in time t depend from weights in time t-1; while in bagging everything can go parallel)



Random forest

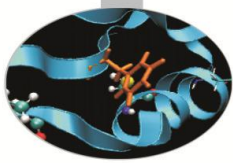
Ensemble method based on decision trees

Repeat k times:

- Draw a bootstrap sample from the dataset
- Train a decision tree

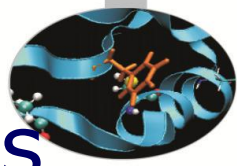
  Until the tree is maximum size
  - Choose next leaf node
  - Select m attributes at random from the p available
  - Pick the best attribute/split as usual
- Measure out-of-bag error
  - Evaluate against the samples that were not selected in the bootstrap
  - Provides measures of strength (inverse error rate), correlation between trees, and variable importance

Make a prediction by majority vote among the k trees



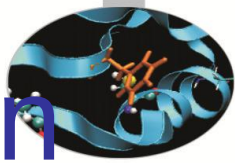
Random Forests

- General and powerful technique
- Easy to parallelize
  - Trees are built independently
- Work on categorical attributes
- Handles “small n big p” problems naturally
  - A subset of attributes are selected by importance
- Avoids overfitting (ensemble of models)



Decision Trees and Random Forests

- Representation
  - Decision Trees
  - Sets of decision trees with majority vote
- Evaluation
  - Accuracy
  - Random forests: out-of-bag error
- Optimization
  - Information Gain or Gini Index to measure impurity and select best attributes



Naïve Bayesian Classfication

Bayes theorem:

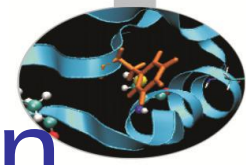
$$P(C|X) = P(X|C) \cdot P(C) / P(X)$$

P(X) is constant for all classes

P(C) = relative freq of class C samples

C such that **P(C|X)** is maximum =
C such that **P(X|C)·P(C)** is maximum

Problem: computing P(X|C) is unfeasible!



Naïve Bayesian Classification

- Here's where the "Naive" comes in. We're going to assume that the different features of the data are *independent* of each other, conditional on *C*=*c*.
- $P(x_1,\ldots,x_k|C) = P(x_1|C)\cdot\ldots\cdot P(x_k|C)$
- By making the decision to completely ignore the correlations between features, this method is blissfully unaware of the primary difficulty of high-dimensional (high-*p*) datasets, and training Naive Bayes classifiers becomes extremely easy.

- If i-th attribute is categorical:
  $P(x_i|C)$ is estimated as the relative freq of samples having value x_i as i-th attribute in class C
- If i-th attribute is continuous:

  $P(x_i|C)$ is estimated thruogh a Gaussian density function