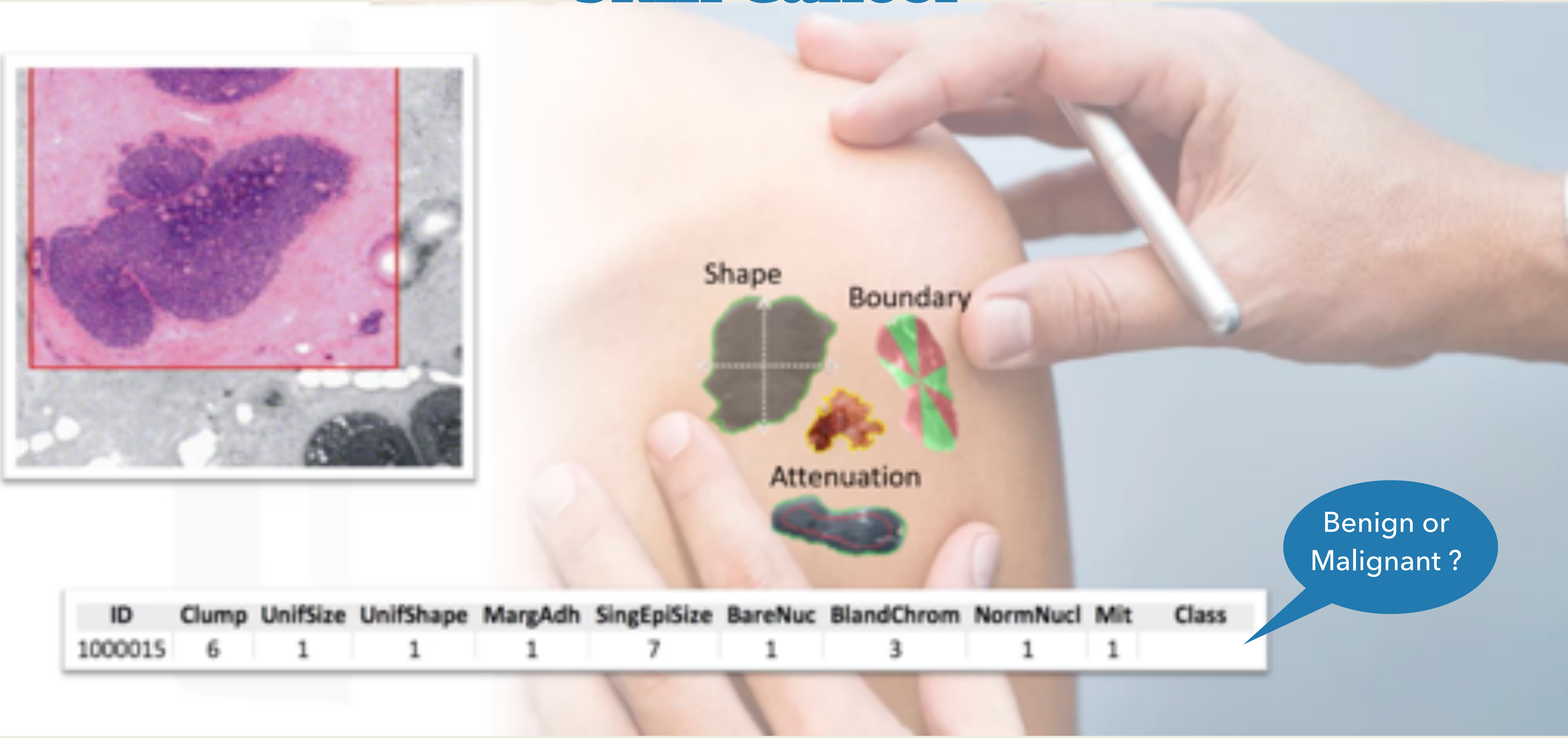
JAVIER GALEANO, ECOFLOR

Skeptical notes on the Machine Learning

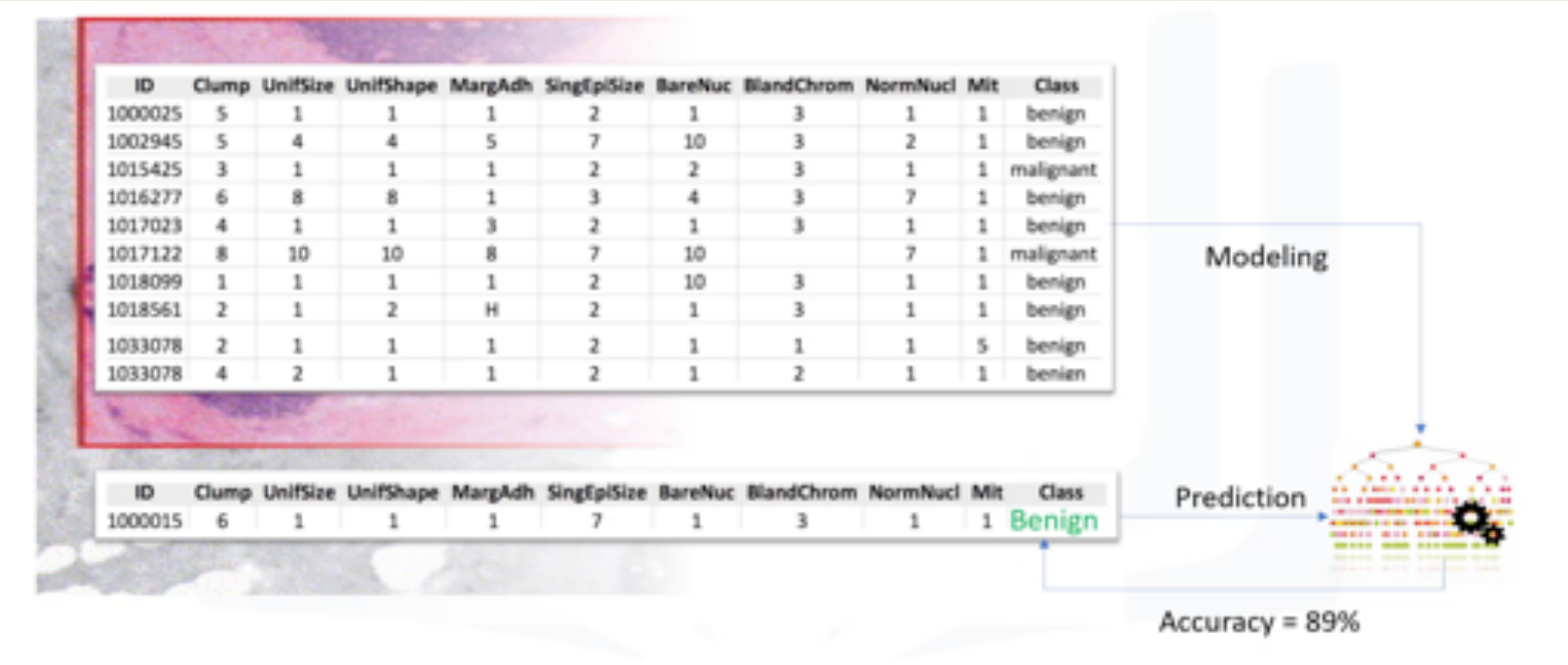
using Orange3

First example in Machine Learning

Skin Cancer



ID	Clump	UnifSize	UnifShape	MargAdh	SingEpiSize	BareNuc	BlandChrom	NormNucl	Mit	Class
1000015	6	1	1	1	7	1	3	1	1	



ID	Clump	UnifSize	UnifShape	MargAdh	SingEpiSize	BareNuc	BlandChrom	NormNucl	Mit	Class
1000025	5	1	1	1	2	1	3	1	1	benign
1002945	5	4	4	5	7	10	3	2	1	benign
1015425	3	1	1	1	2	2	3	1	1	malignant
1016277	6	8	8	1	3	4	3	7	1	benign
1017023	4	1	1	3	2	1	3	1	1	benign
1017122	8	10	10	8	7	10		7	1	malignant
1018099	1	1	1	1	2	10	3	1	1	benign
1018561	2	1	2	H	2	1	3	1	1	benign
1033078	2	1	1	1	2	1	1	1	5	benign
1033078	4	2	1	1	2	1	2	1	1	benien

ID	Clump	UnifSize	UnifShape	MargAdh	SingEpiSize	BareNuc	BlandChrom	NormNucl	Mit	Class
1000015	6	1	1	1	7	1	3	1	1	Benign

First definition of ML

Machine Learning is the subfield of computer science that gives computers the ability to learn without being explicit programmed

Arthur Samuel, coin the term machine learning in 1959 at IBM

Examples in our daily life.

"Our lives are completely run by algorithms"

Marcus du Sautoy in The Creativity code

Examples of ML today

Some ideas

Differences between

- Artificial Intelligence
- Machine Learning
- Deep Learning

Artificial Inteligence

AI tries to make computers intelligent so that they mimic the cognitive functions of humans.

Autopilot in Tesla

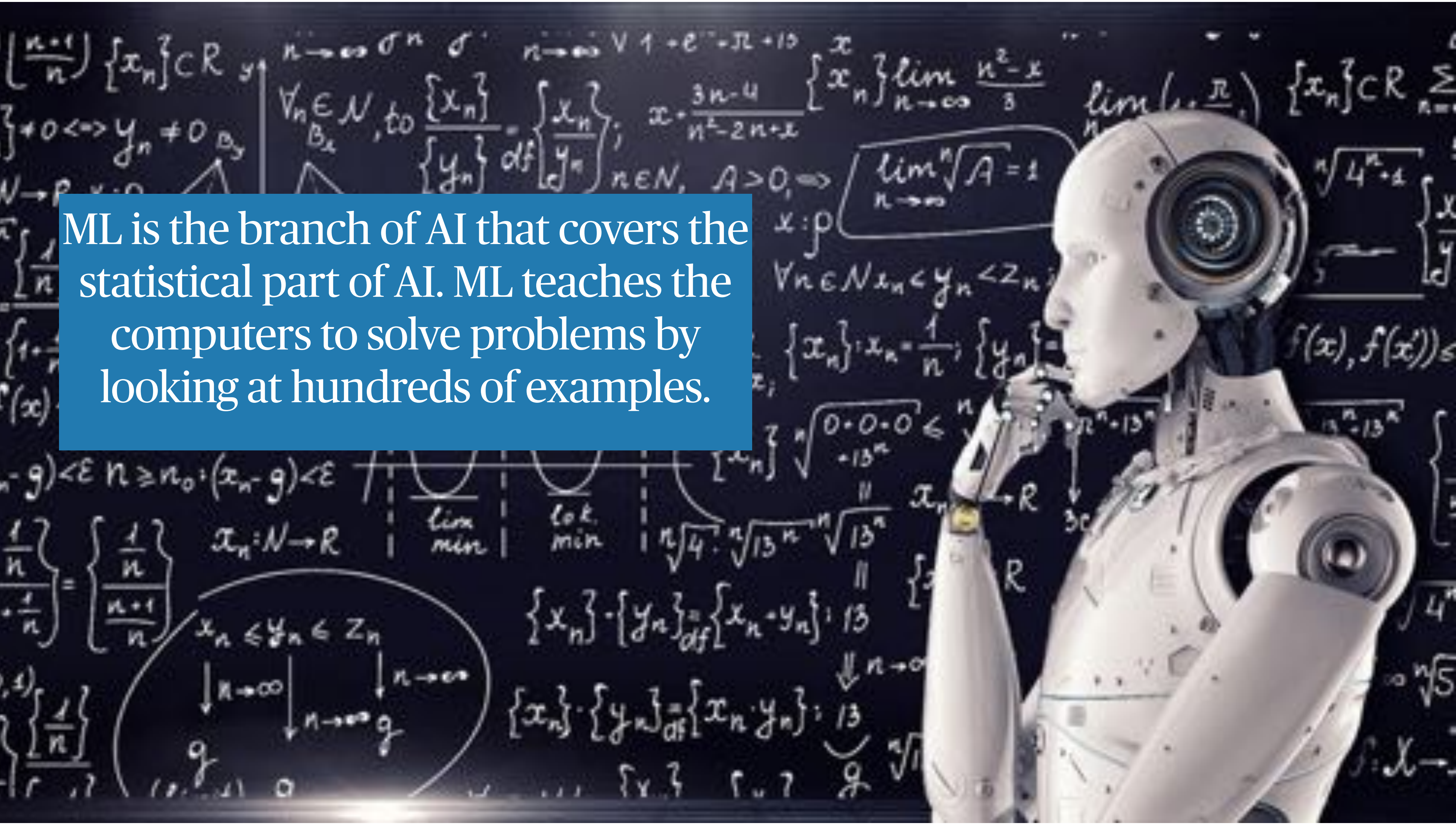
Automatic car driving

Pattern recognition

Using computer vision

Playing games

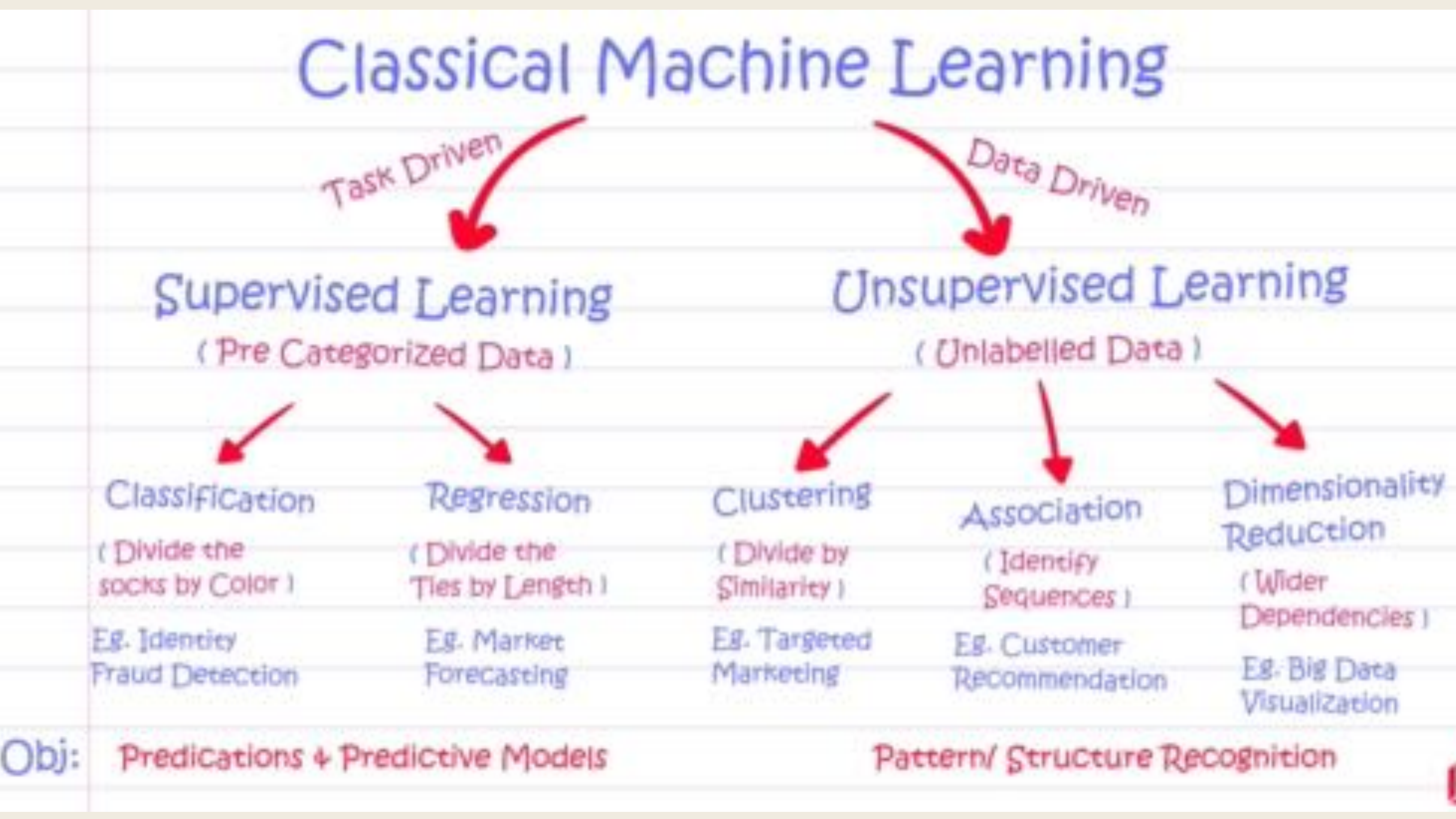
Playing go



ML is the branch of AI that covers the statistical part of AI. ML teaches the computers to solve problems by looking at hundreds of examples.


DEEP
LEARNING

What problem in ML do I have?


Classical Machine Learning
Task Driven
Data Driven
Supervised Learning
(Pre Categorized Data)
Unsupervised Learning
(Unlabelled Data)
Classification
(Divide the socks by Color)
Eg. Identity Fraud Detection
Regression
(Divide the Ties by Length)
Eg. Market Forecasting
Clustering
(Divide by Similarity)
Eg. Targeted Marketing
Association
(Identify Sequences)
Eg. Customer Recommendation
Dimensionality Reduction
(Wider Dependencies)
Eg. Big Data Visualization
Obj:
Predications & Predictive Models
Pattern/ Structure Recognition

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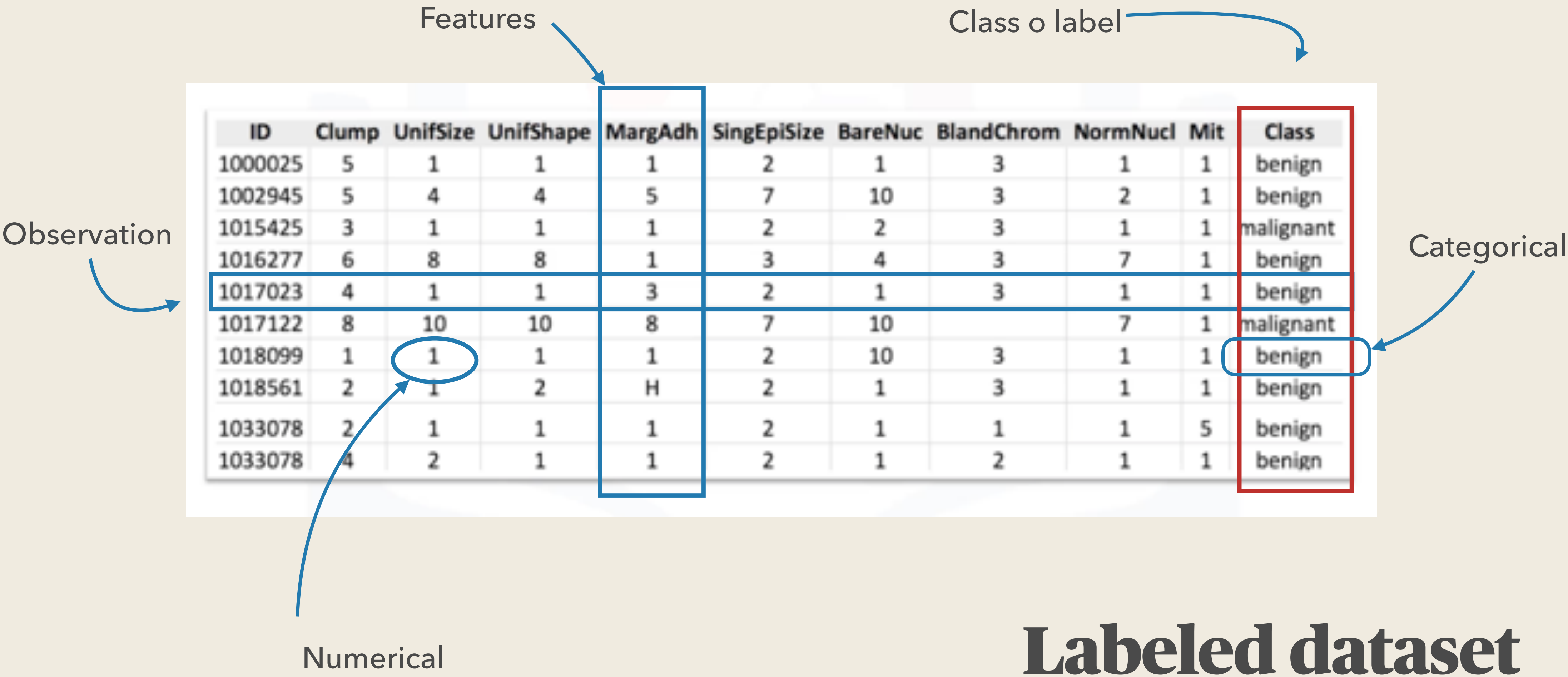
1017023	4	1	1	3	2	1	3	1	1	benign
1017122	8	10	10	8	7	10		7	1	malignant
1018099	1	1	1	1	2	10	3	1	1	benign
1018561	2	1	2	H	2	1	3	1	1	benign
1033078	2	1	1	1	2	1	1	1	5	benign
1033078	4	2	1	1	2	1	2	1	1	benien

Supervised model

In supervised models, we teach the model by training it with some data from labeled dataset



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1018561	2	1	2	H	2	1	3	1	1	benign
1033078	2	1	1	1	2	1	1	1	5	benign
1033078	4	2	1	1	2	1	2	1	1	benign

Labeled dataset

I am going to teach you

1 –> 2

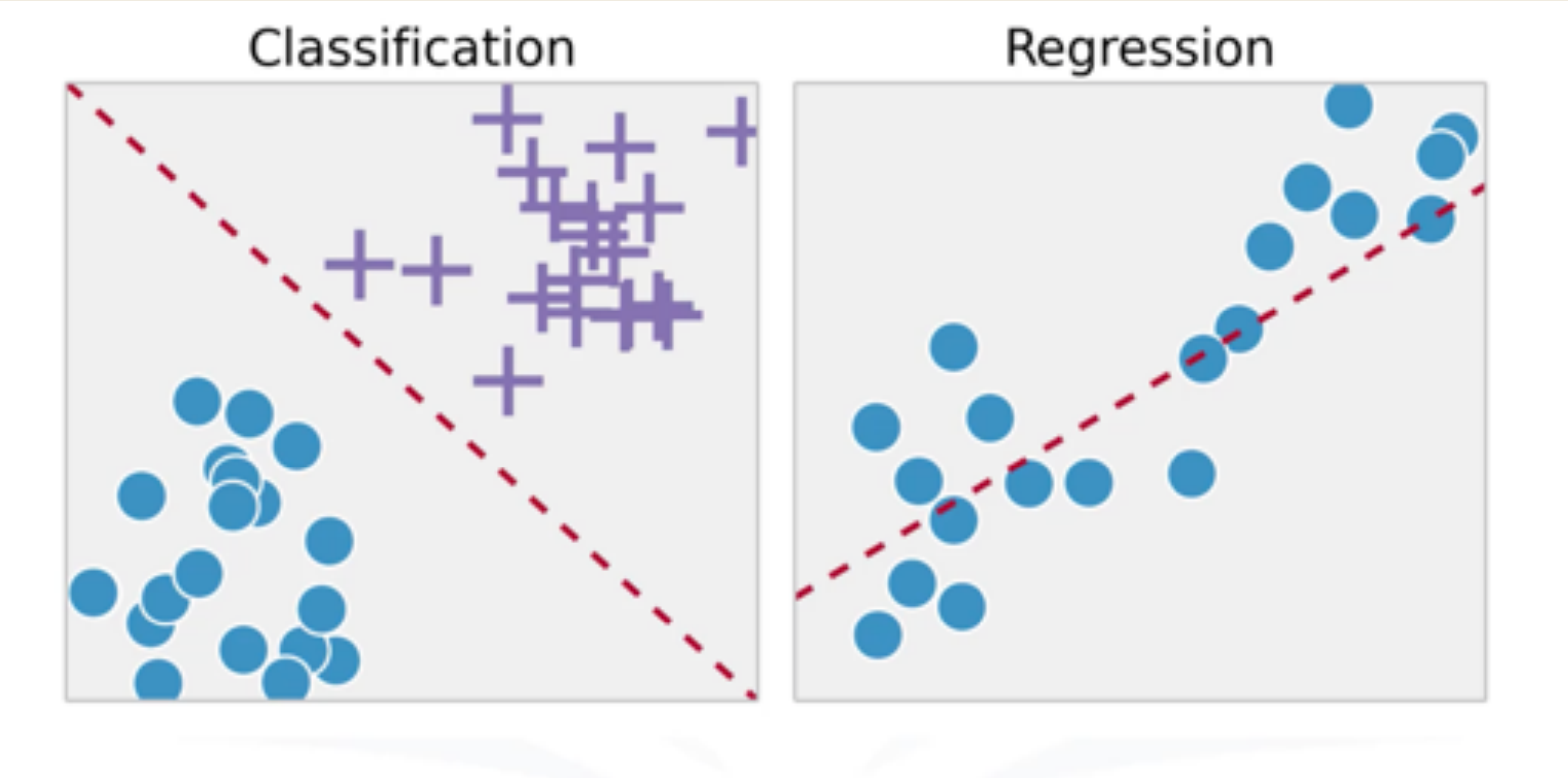
2 –> 4

5 –> 10

6 –> 12

10 –> ?

Types of supervised techniques

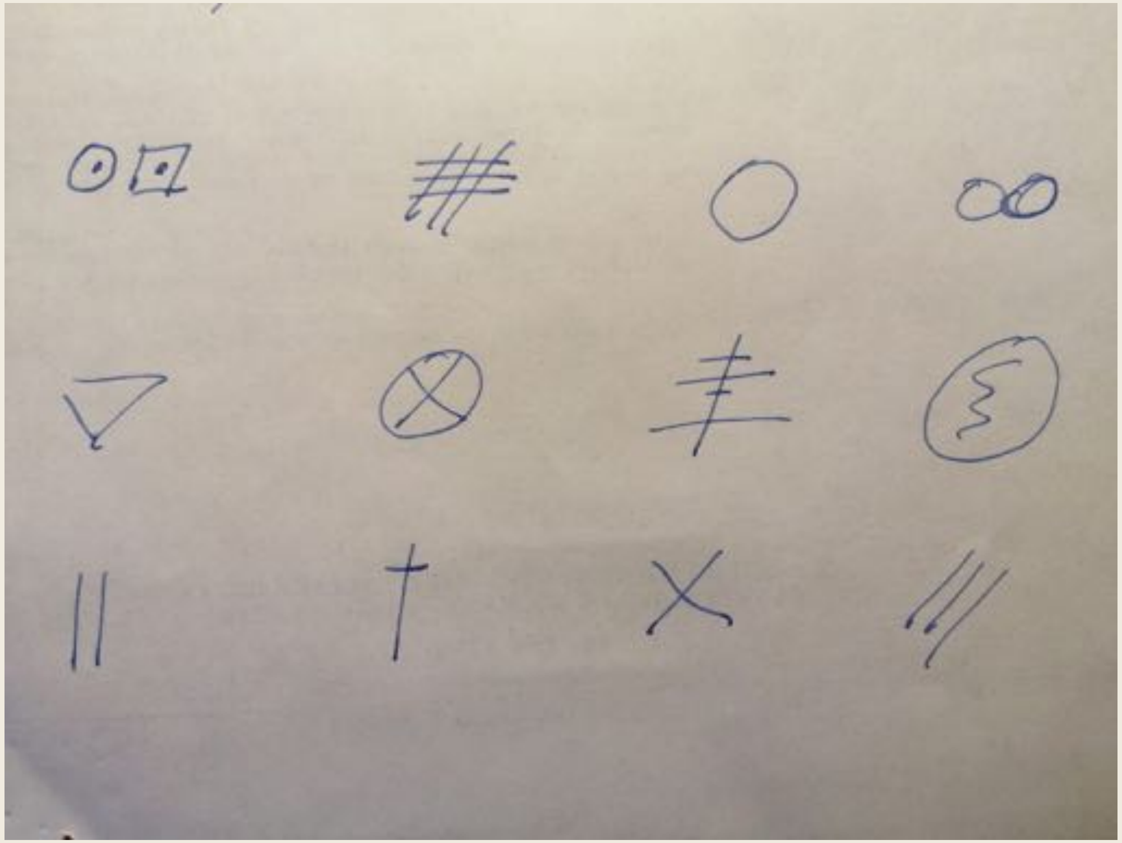


Customer Id	Age	Edu	Years Employed	Income	Card Debt	Other Debt	Address	DebtIncomeRatio
1	41	2	6	19	0.124	1.073	NBA001	6.3
2	47	1	26	100	4.582	8.218	NBA021	12.8
3	33	2	10	57	6.111	5.802	NBA013	20.9
4	29	2	4	19	0.681	0.516	NBA009	6.3
5	47	1	31	253	9.308	8.908	NBA008	7.2
6	40	1	23	81	0.998	7.831	NBA016	10.9
7	38	2	4	56	0.442	0.454	NBA013	1.6
8	42	3	0	64	0.279	3.945	NBA009	6.6
9	26	1	5	18	0.575	2.215	NBA006	15.5
10	47	3	23	115	0.653	3.947	NBA011	4
11	44	3	8	88	0.285	5.083	NBA010	6.1
12	34	2	9	40	0.374	0.266	NBA003	1.6

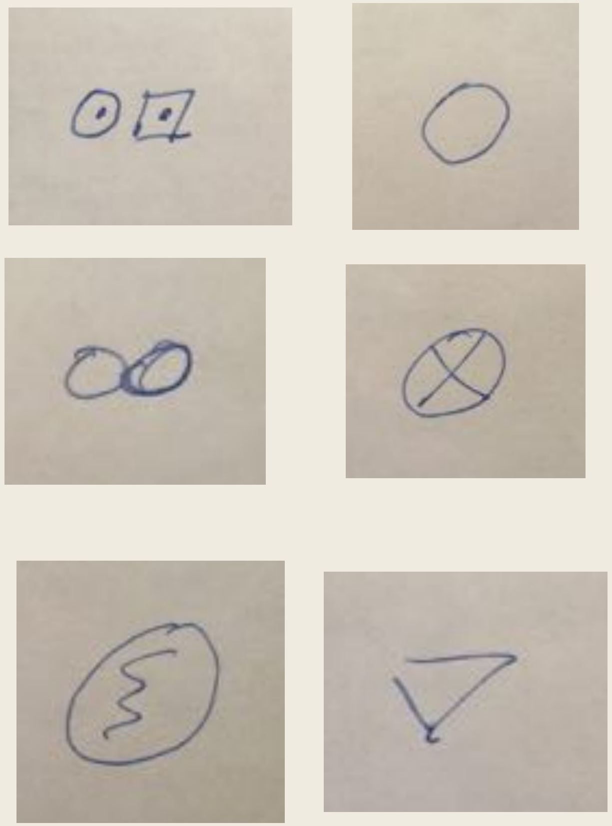
Unsupervised model

We do not supervise the model, but we let the model work on its own to discover information that may not be visible to the human eye.

I am going to teach you as a unsupervised dataset

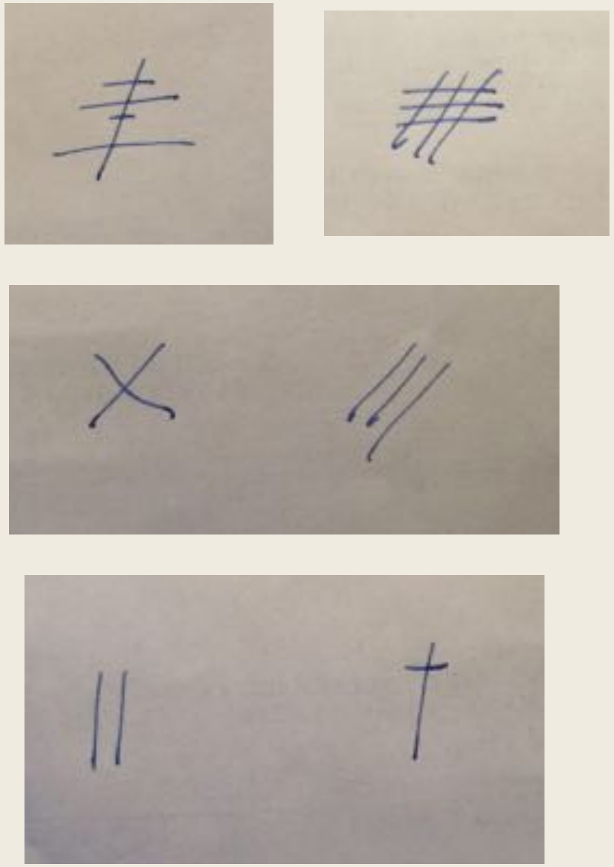


Polygonal language?

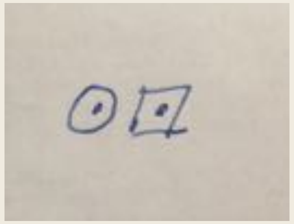
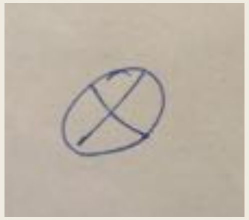


Two clusters

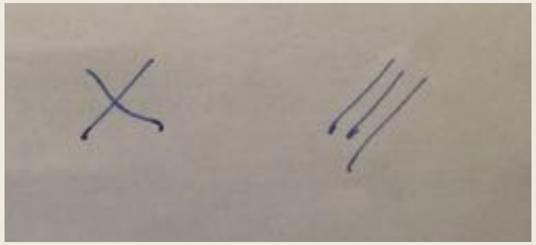
Linear language?



Fulled polygonal language?


Diagonal Linear language?

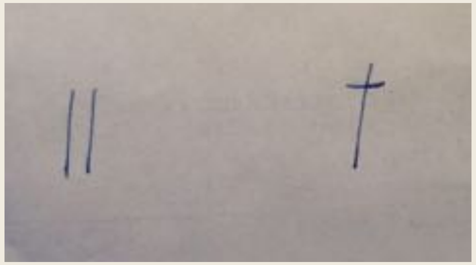



Four clusters?

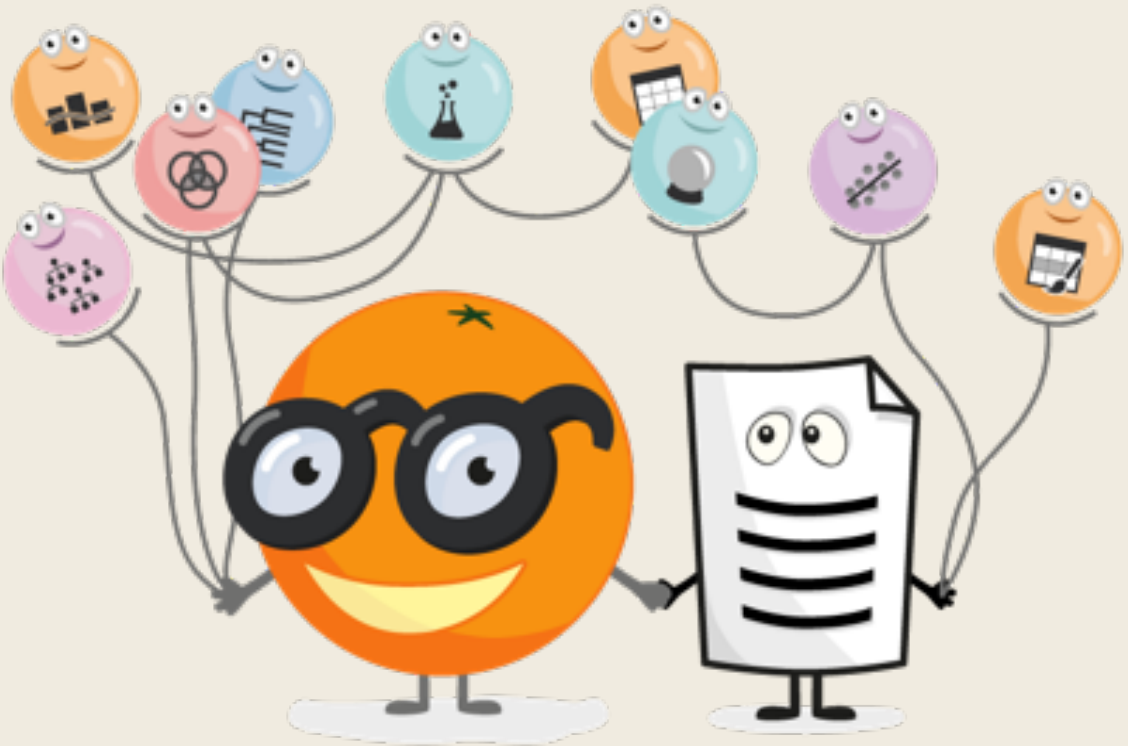
Empty polygonal language?



Straight Linear language?

First steps using Orange3



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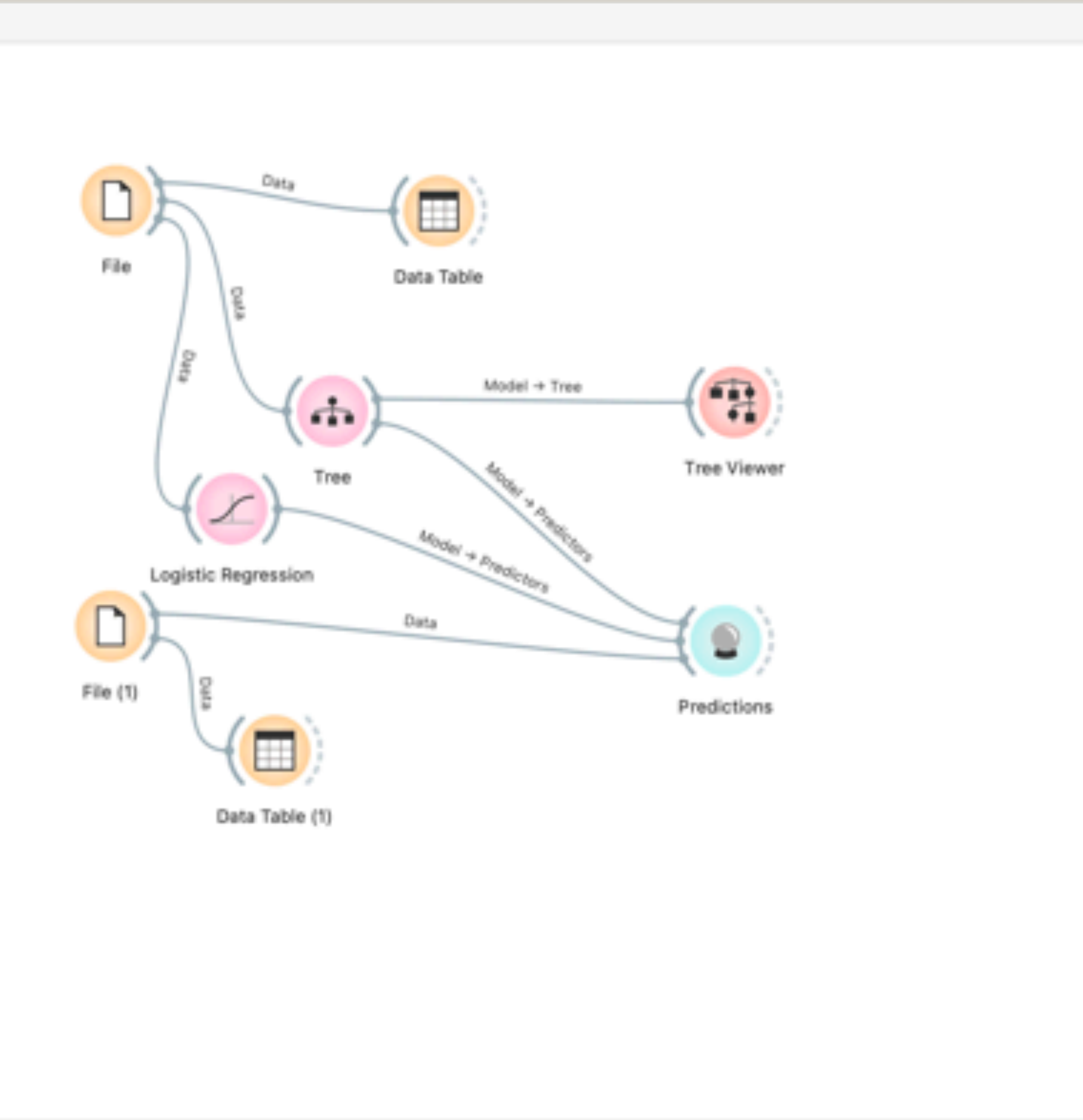
First program

- File –> Iris
- Data Table
- Scatter plot
- Selected data table



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First Predictions

- Download vegetables and fruits dataset
- Tree –> Tree viewer
- Test file
- Prediction
- Logistic Regression

Classification problem in ML

ID	Clump	UnifSize	UnifShape	MargAdh	SingEpiSize	BareNuc	BlandChrom	NormNucl	Mit	Class
1000025	5	1	1	1	2	1	3	1	1	benign
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1018099	1	1	1	1	2	10	3	1	1	benign
1018561	2	1	2	H	2	1	3	1	1	benign
1033078	2	1	1	1	2	1	1	1	5	benign
1033078	4	2	1	1	2	1	2	1	1	benign

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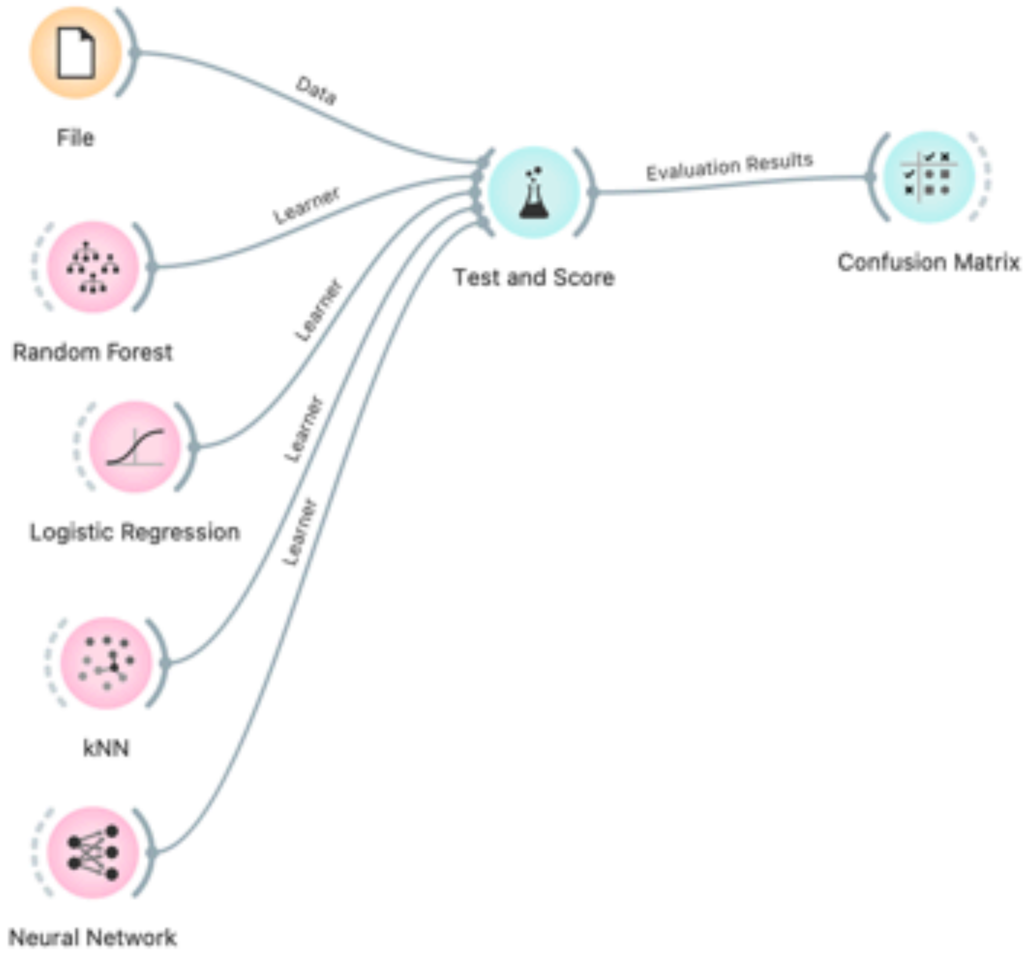
Classification

In classification, the goal is to predict a *class label*, which is a choice from a predefined list of possibilities.

- Binary Classification
- Multiclass Classification



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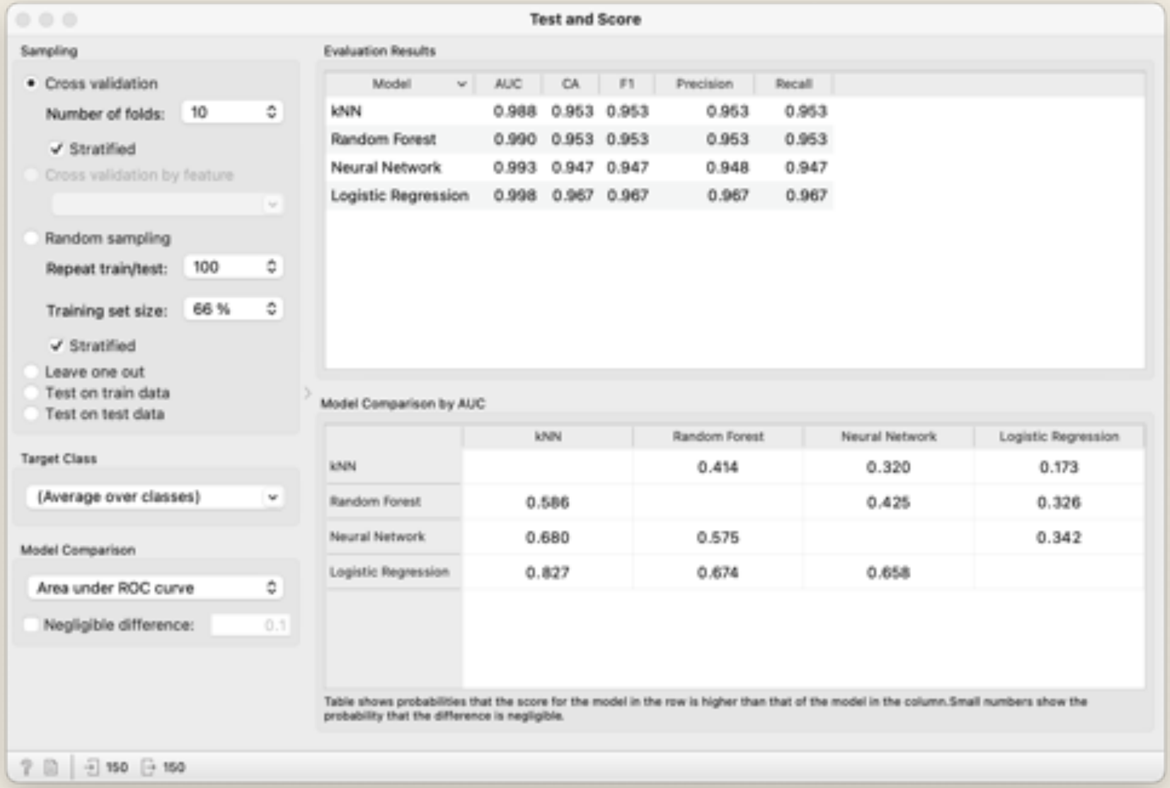
Scoring

- K-cross validation
- Test & Score
- Confusion Matrix



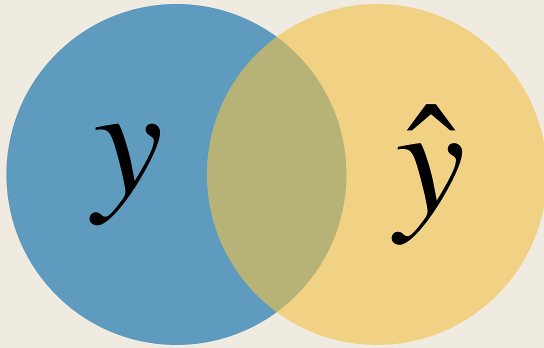
Evaluation metrics in classification

- We are talking about some metrics:
- Jaccard index,
- Confusion matrix

Jaccard index

y = True values (actual values)

$\hat{y}$ = Predicted values of our model



Jaccard index [0,1]

$$J(y, \hat{y}) = \frac{|y \cap \hat{y}|}{|y \cup \hat{y}|} = \frac{|y \cap \hat{y}|}{|y| + |\hat{y}| - |y \cap \hat{y}|}$$

Ejemplo

$$y = [0,0,0,0,0,0,1,1,1,1,1] \;\; \hat{y} = [1,1,0,0,0,0,1,1,1,1,1]$$

$$J(y, \hat{y}) = \frac{|y \cap \hat{y}|}{|y| + |\hat{y}| - |y \cap \hat{y}|} = \frac{8}{10 + 10 - 8} = 0.66$$

Confusion Matrix

TP = True Positives

FN = False Negatives

FP = False Positives

TN = True Negatives

$$\textbf{Precision} = \frac{TP}{TP + FP}$$

$$\textbf{Recall} = \frac{TP}{TP + FN}$$

$$\textbf{F1-score}\ [0,1] = \frac{2 * Precision * Recall}{Precision + Recall}$$

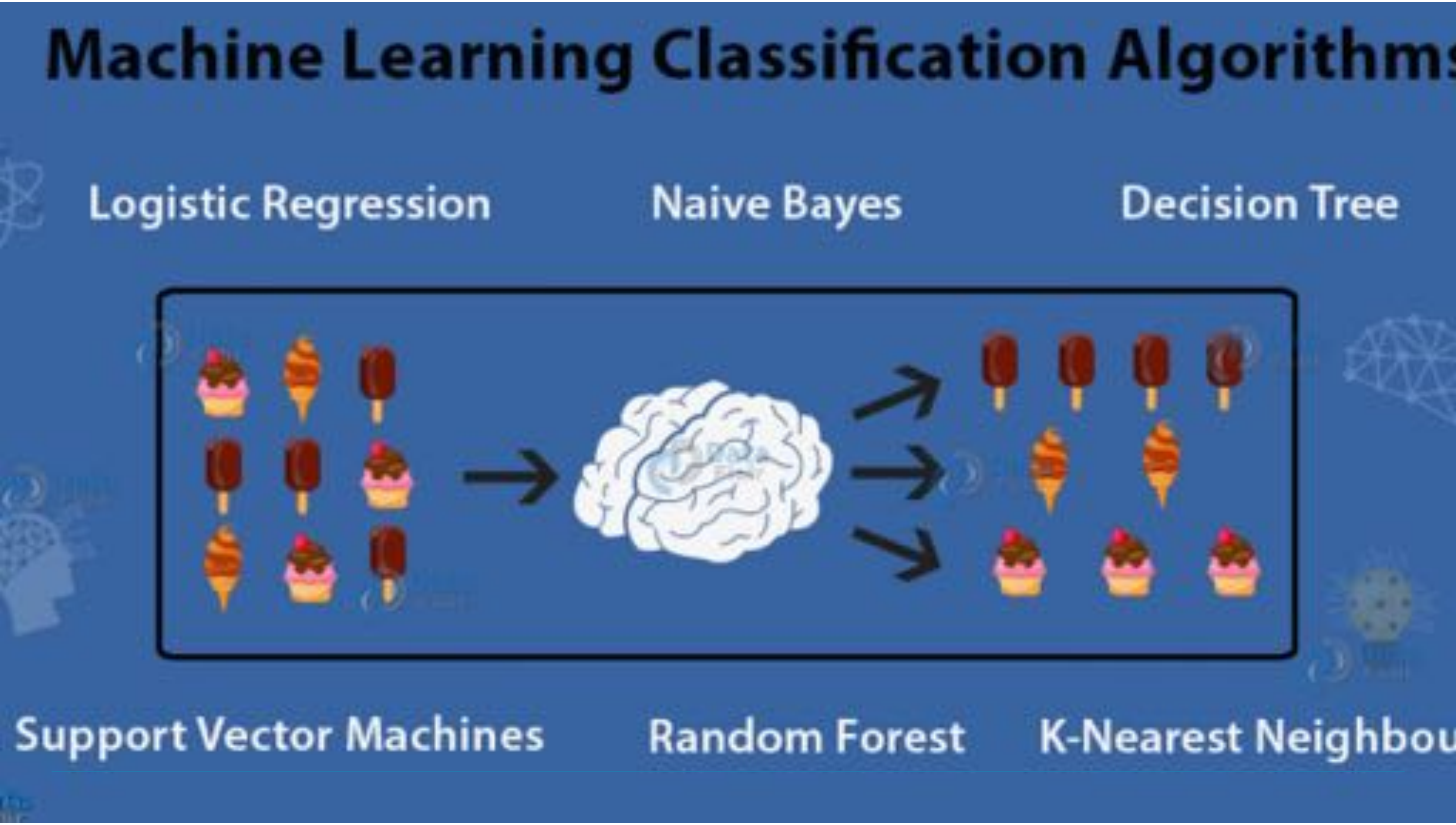
Confusion Matrix

Actual \ Predicted	Iris-setosa	Iris-versicolor	Iris-virginica	Σ
Iris-setosa	50	0	0	50
Iris-versicolor	0	47	3	50
Iris-virginica	0	2	48	50
Σ	50	49	51	150

Classification Accuracy is the proportion of correctly classified examples

$$CA = \frac{TP + TN}{Total}$$

Classification Algorithms



Machine Learning Classification Algorithms
Logistic Regression
Naive Bayes
Decision Tree
Support Vector Machines
Random Forest
K-Nearest Neighbou

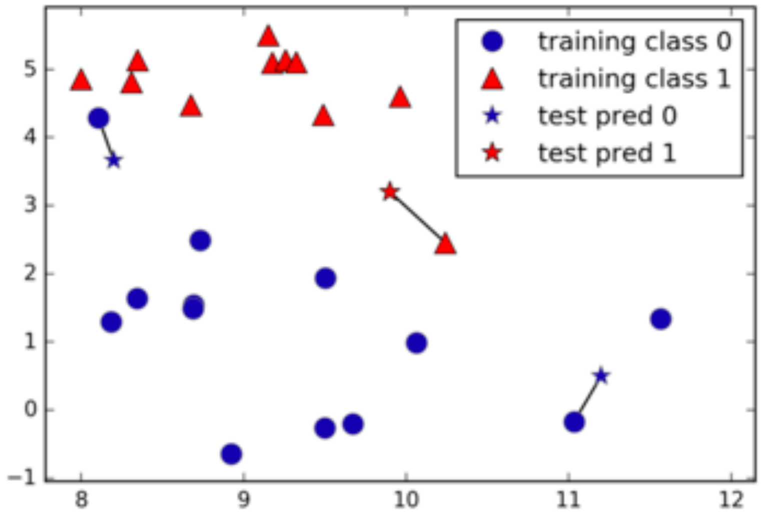


Figure 2-4. Predictions made by the one-nearest-neighbor model on the forge dataset

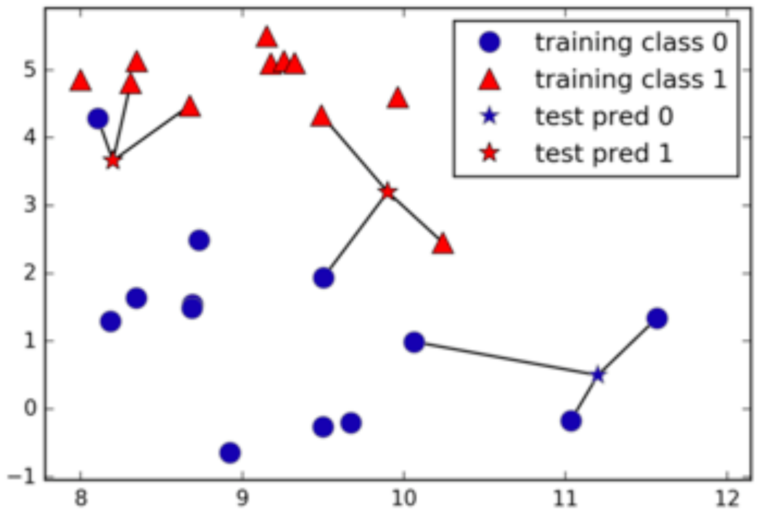


Figure 2-5. Predictions made by the three-nearest-neighbors model on the forge dataset

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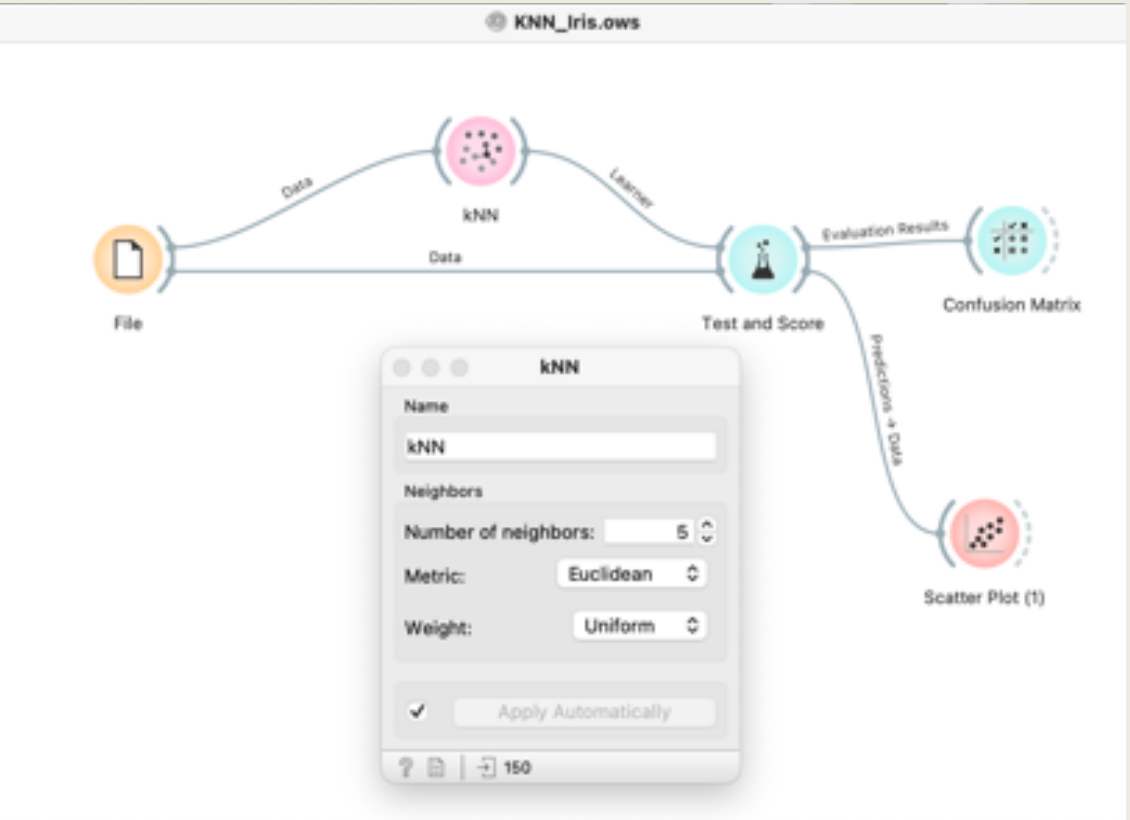
K-Nearest Neighbors

- Building the k-NN algorithm consists only of storing the training dataset.
- To make a prediction for a new data point, the algorithm finds the closest data points in the training dataset—its "nearest neighbors."



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K-nearest Neighbors

- Iris
- KNN –> Test Score –> Confusion Matrix
- Constant ->Test Score –> Confusion Matrix
- Scatter Plot (KNN)

Patient ID	Age	Sex	BP	Cholesterol	Drug
p1	Young	F	High	Normal	Drug A
p2	Young	F	High	High	Drug A
p3	Middle-age	F	Hiigh	Normal	Drug B
p4	Senior	F	Normal	Normal	Drug B
p5	Senior	M	Low	Normal	Drug B
p6	Senior	M	Low	High	Drug A
p7	Middle-age	M	Low	High	Drug B
p8	Young	F	Normal	Normal	Drug A
p9	Young	M	Low	Normal	Drug B
p10	Senior	M	Normal	Normal	Drug B
p11	Young	M	Normal	High	Drug B
p12	Middle-age	F	Normal	High	Drug B
p13	Middle-age	M	High	Normal	Drug B
p14	Senior	F	Normal	High	Drug A
p15	Middle-age	F	Low	Normal	?

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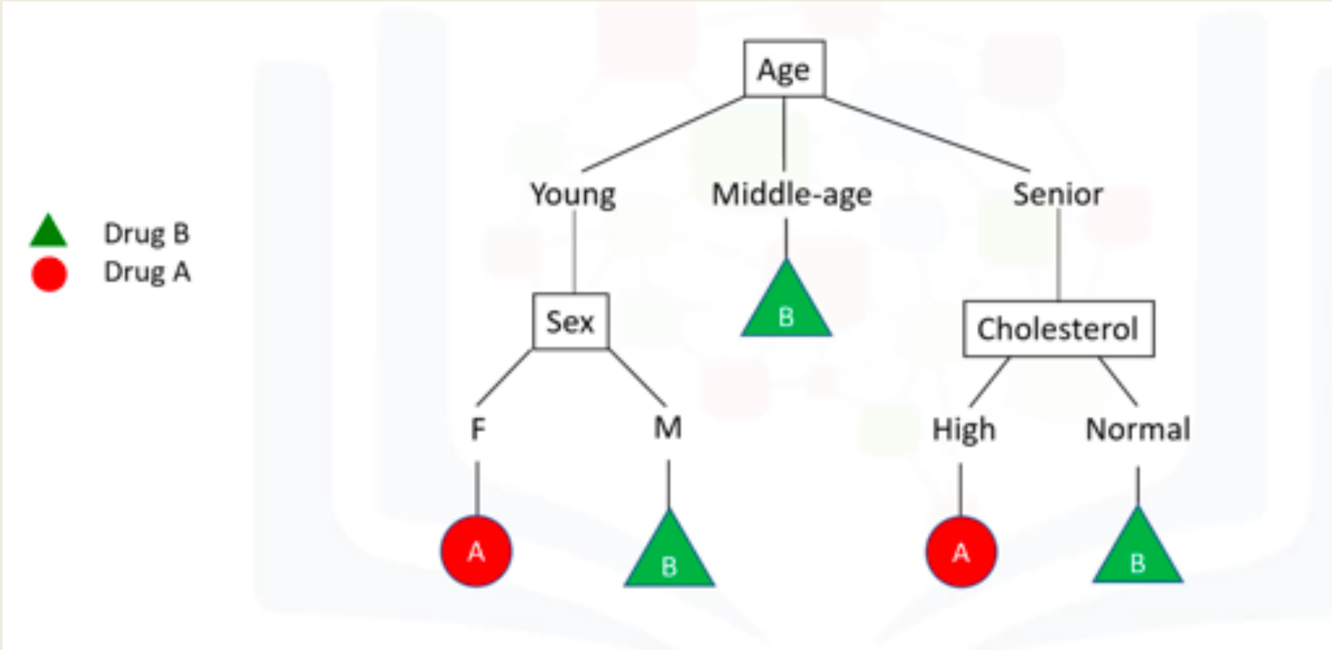
Decision Tree

- What exactly is a decision tree?

How to build a decision tree?

1. Choose an attribute from your dataset.
2. Calculate the significance of attribute in splitting of data.
3. Split data based on the value of the best attribute.
4. Go to step 1.



How to calculate the significance?

Information gain is the information that can increase the level of certainty after splitting.

Information Gain = (Entropy before split) – (weighted entropy after split)

In every step, we want to dismiss the impurity of the nodes. Impurity is calculated by Entropy of data in the node

$$E = -\sum_{i} p_i \log_2(p_i)$$

Entropy is the amount of information disorder. If the samples are completely homogeneous the entropy is zero.

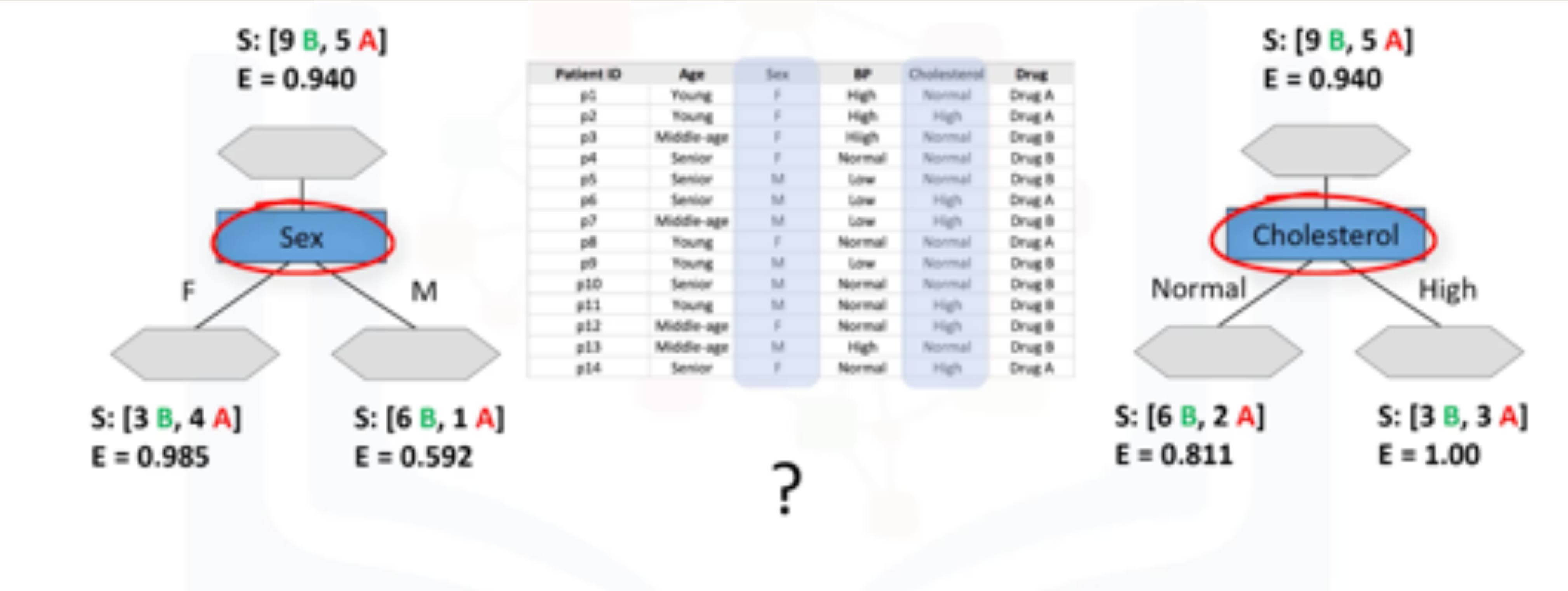
How to calculate the significance?

To compute Gini impurity for a set of items with J clases, suppose $i \in \{1,2,\ldots,J\}$, and let be the fraction of items labeled with class in the set.

$$\mathrm{I}_G(p) = \sum_{i=1}^{J}\left(p_i \sum_{k\neq i} p_k\right) = \sum_{i=1}^{J} p_i\left(1-p_i\right) = \sum_{i=1}^{J}\left(p_i - p_i^2\right) = \sum_{i=1}^{J} p_i - \sum_{i=1}^{J} p_i^2 = 1 - \sum_{i=1}^{J} p_i^2$$

This is the other way to measure the significance

Which attributes is the best?



Patient ID	Age	Sex	BP	Cholesterol	Drug
p1	Young	F	High	Normal	Drug A
p2	Young	F	High	High	Drug A
p3	Middle-age	F	High	Normal	Drug B
p4	Senior	F	Normal	Normal	Drug B
p5	Senior	M	Low	Normal	Drug B
p6	Senior	M	Low	High	Drug A
p7	Middle-age	M	Low	High	Drug B
p8	Young	F	Normal	Normal	Drug A
p9	Young	M	Low	Normal	Drug B
p10	Senior	M	Normal	Normal	Drug B
p11	Young	M	Normal	High	Drug B
p12	Middle-age	F	Normal	High	Drug B
p13	Middle-age	M	High	Normal	Drug B
p14	Senior	F	Normal	High	Drug A

$$E = -\sum_i p_i \log(p_i)$$

Gain (s, Sex)
= 0.940 – [(7/14)0.985 + (7/14)0.592]
=0.151

Patient ID	Age	Sex	BP	Cholesterol	Drug
p1	Young	F	High	Normal	Drug A
p2	Young	F	High	High	Drug A
p3	Middle-age	F	High	Normal	Drug B
p4	Senior	F	Normal	Normal	Drug B
p5	Senior	M	Low	Normal	Drug B
p6	Senior	M	Low	High	Drug A
p7	Middle-age	M	Low	High	Drug B
p8	Young	F	Normal	Normal	Drug A
p9	Young	M	Low	Normal	Drug B
p10	Senior	M	Normal	Normal	Drug B
p11	Young	M	Normal	High	Drug B
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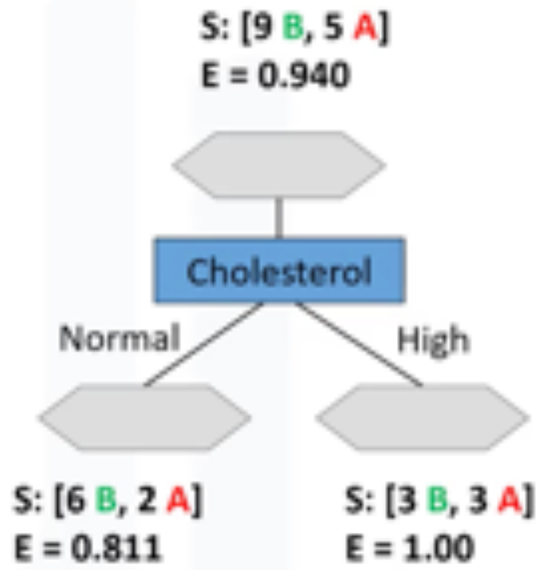
p14	Senior	F	Normal	High	Drug A

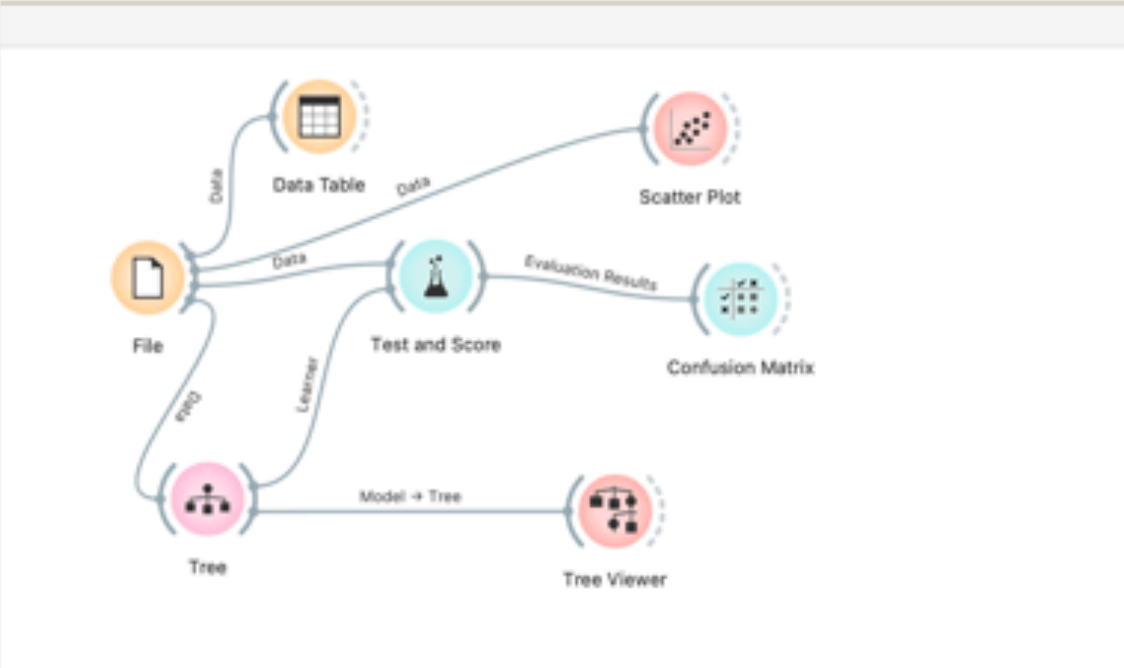
?



Gain (s, Cholesterol)
= 0.940 – [(8/14).811 + (6/14)1.0]
=0.048

Information gain is the information that can increase the level of certainty after splitting.

Information Gain = (Entropy before split) – (weighted entropy after split)



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Decision Tree

- Iris dataset
- Test and Score –> confusion Matrix
- Tree –> Tree Viewer

Linear Models
For classification

- Linear models are a class of models that is widely used in practice.
- Linear models make a prediction using a linear function of the input features

Linear Binary classification

In this case, the prediction is made using the formula:

$$\hat{y} = w[0] * x[0] + w[1]*x[1] + \ldots + w[p]*x[p] + b > 0$$

Where:

X [0,..p] are the features (columns)

W[0,..,p] and b are the parameters of the model

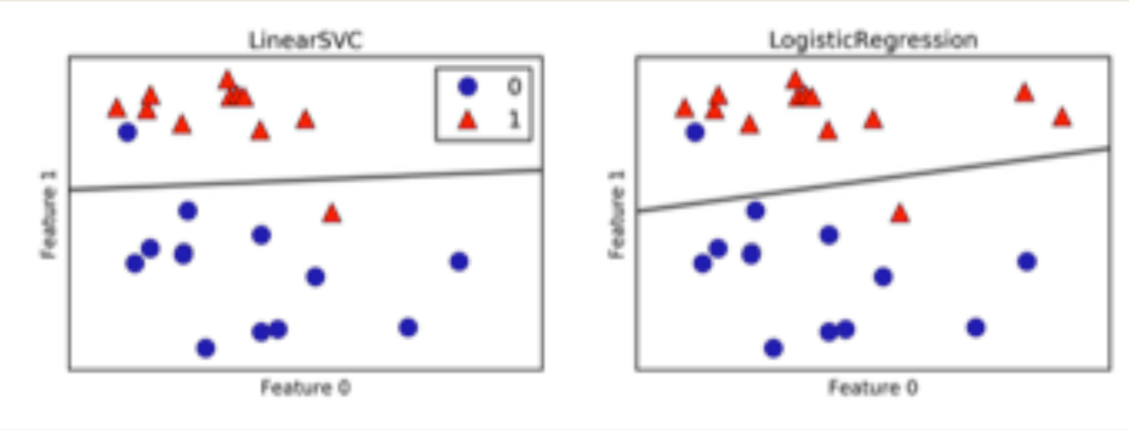
Y is the prediction of the model

Linear Models
For classification

A linear classifier is a classifier that separates two classes using a line, a plane or a hyperplane

The most common models:

- Logistic Regression
- Support Vector Machine



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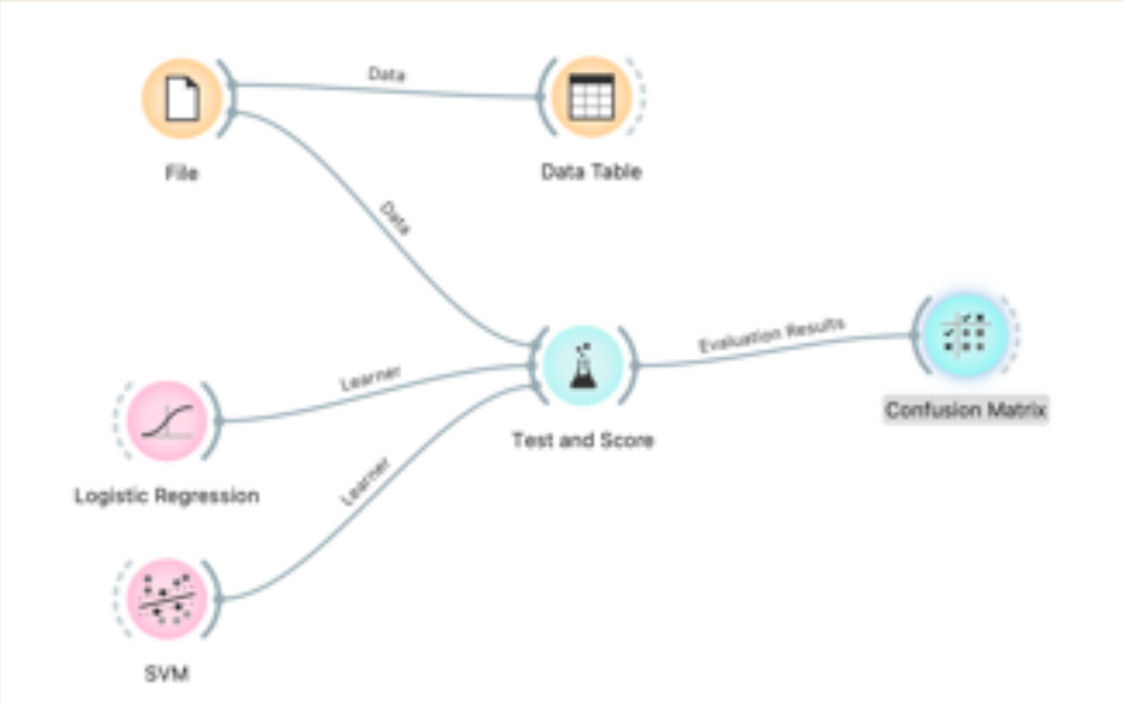
Linear models

- Linear SVC
- Logistic Regression.



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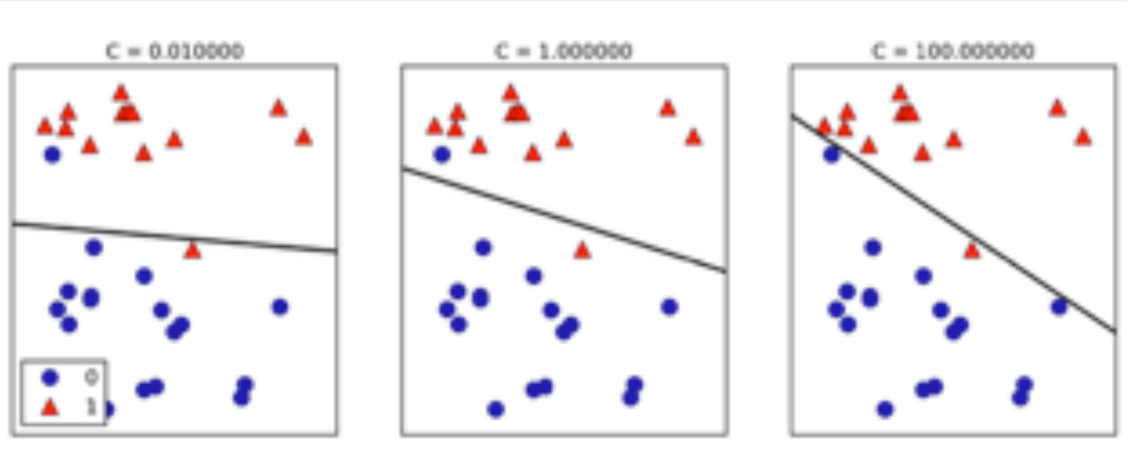
Linear Models

- Iris dataset
- SVM -> Test and Score -> Confusion M.
- LR -> Test and Score -> Confusion M.
- C values
- Regularization type: L1, L2



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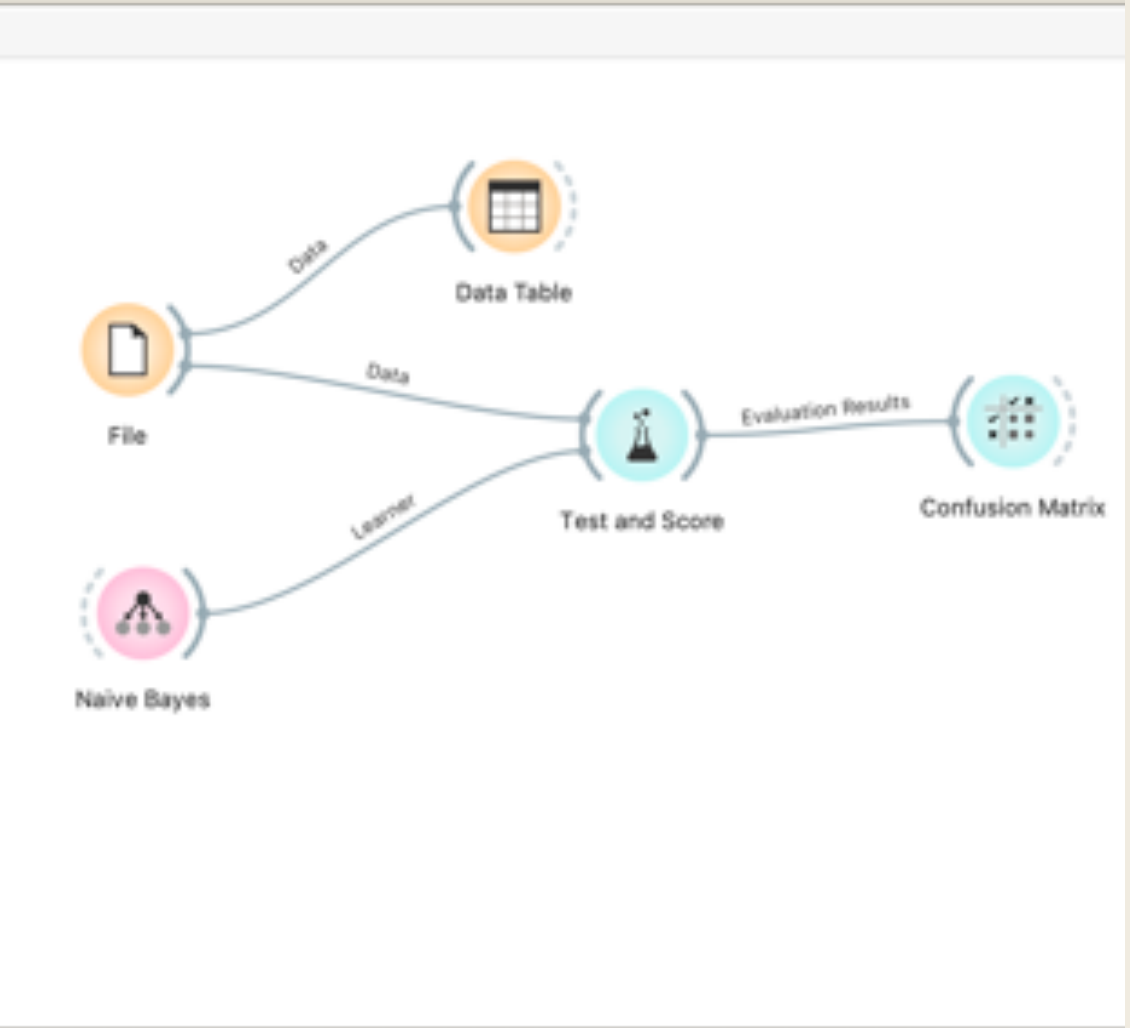
Linear models

- Studying different C values
- Studying different regularizations.



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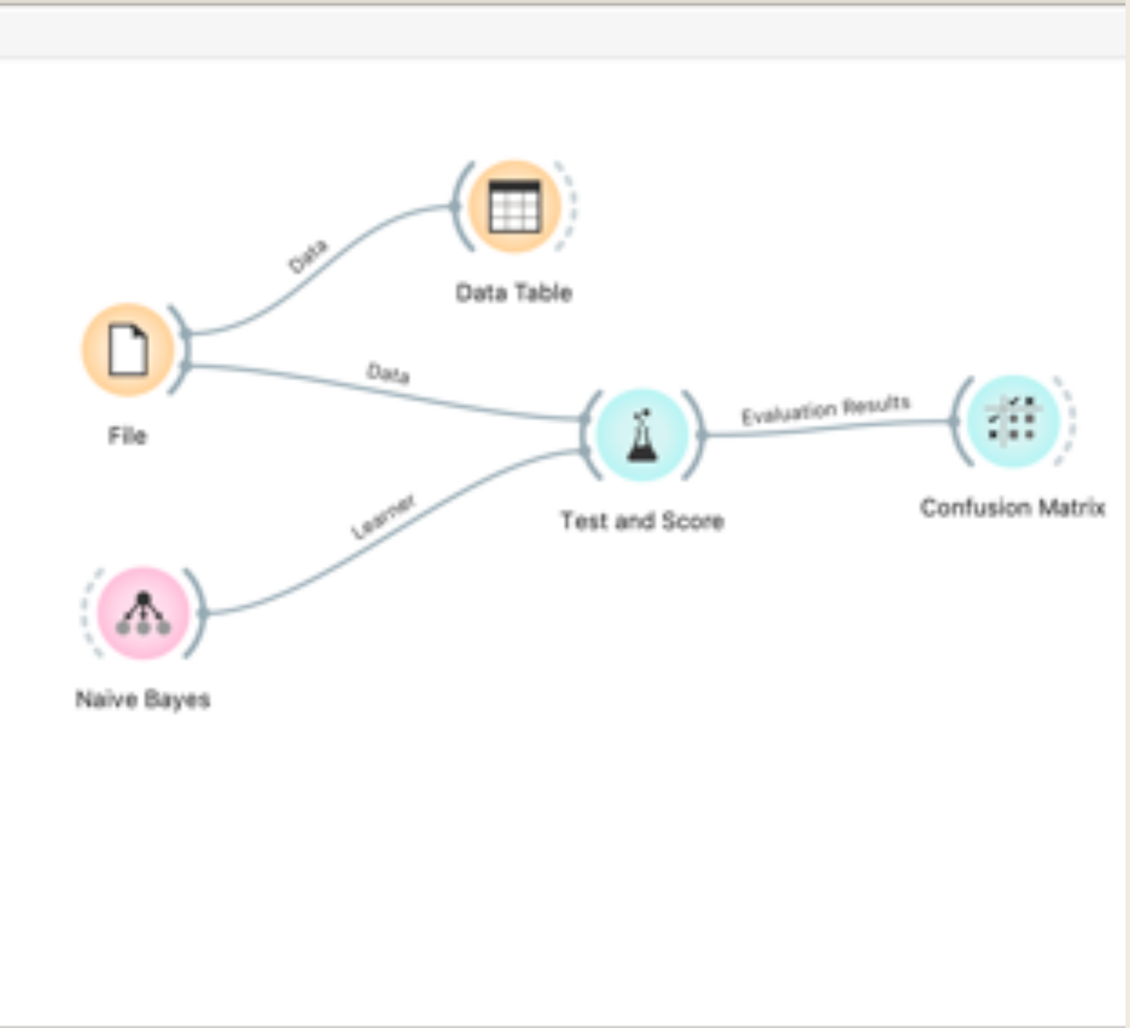
Naive Bayes models

- Naive Bayes classifiers are a family of classifiers that are quite similar to the linear models.
- However, they tend to be even faster in training.
- The price paid for this efficiency is that naive Bayes models often provide generalization performance that is slightly worse than that of linear classifiers



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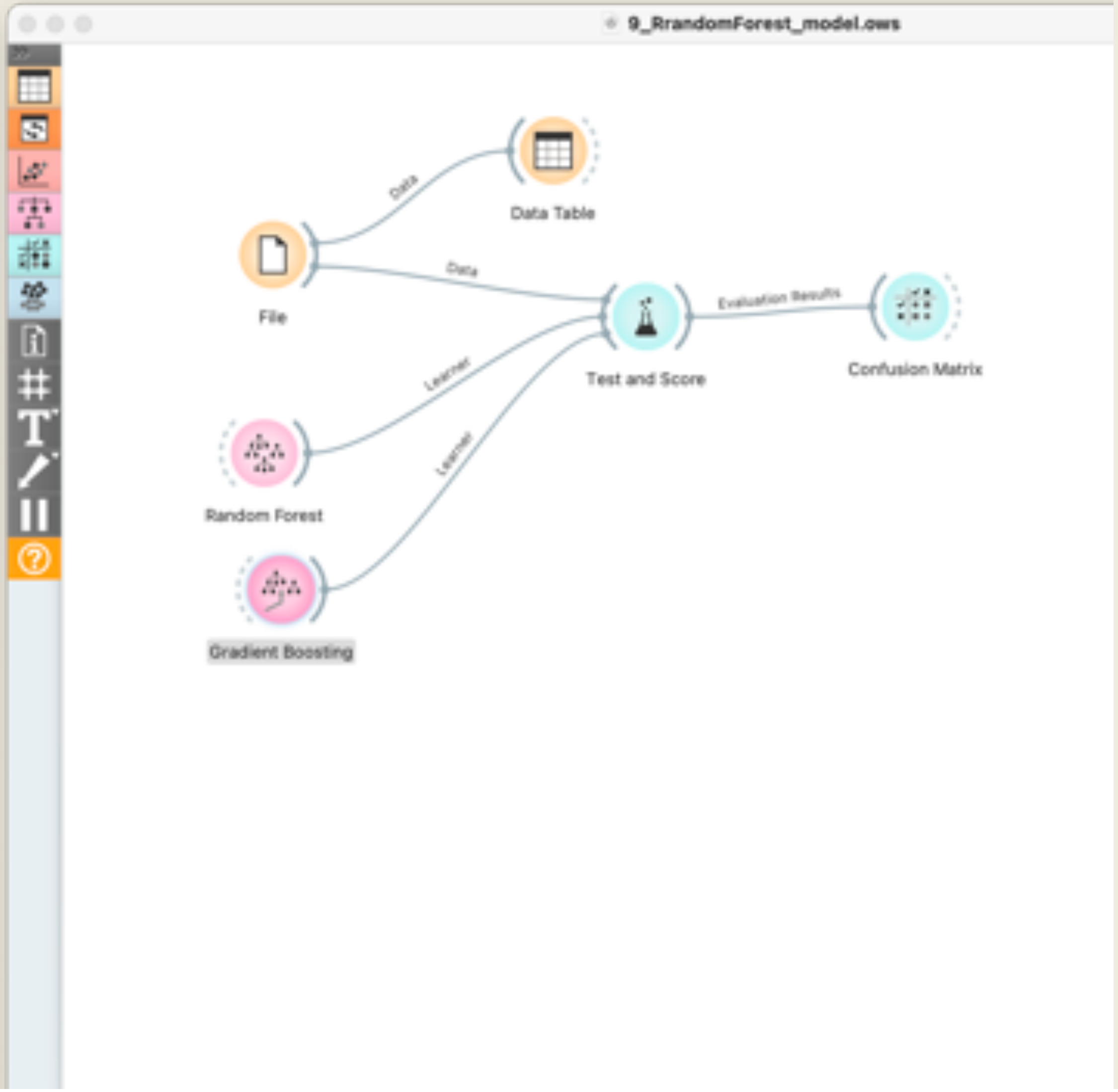
Naive Bayes models

- There are three kinds of naive Bayes classifiers: **GaussianNB, BernoulliNB,** and **MultinomialNB**.
- GaussianNB can be applied to any continuous data, while BernoulliNB assumes binary data and MultinomialNB assumes count data
- Naive Bayes models are great baseline models and are often used on very large datasets, where training even a linear model might take too long.



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Ensembles of Decision Trees

- Ensembles are methods that combine multiple machine learning models to create more powerful models.
- There are two ensemble models that have proven to be effective, both of which use decision trees as their building blocks: **random forests** and **gradient boosted decision trees.**

Random Forest

- The main drawback of decision trees is that they **tend to overfit** the training data. Random forests are one way to address this problem.
- A RF is essentially **a collection of decision trees**, where each tree is slightly different from the others. The idea behind random forests is that each tree might do a relatively good job of predicting, but will likely overfit on part of the data. If we build many trees, all of which work well and overfit in different ways, **we can reduce the amount of overfitting by averaging their results.**

Regression problems in ML

Customer Id	Age	Edu	Years Employed	Income	Card Debt	Other Debt	Address	DebtIncomeRatio
1	41	2	6	19	0.124	1.073	NBA001	6.3
2	47	1	26	100	4.582	8.218	NBA021	12.8
3	33	2	10	57	6.111	5.802	NBA013	20.9
4	29	2	4	19	0.681	0.516	NBA009	6.3
5	47	1	31	253	9.308	8.908	NBA008	7.2
6	40	1	23	81	0.998	7.831	NBA016	10.9
7	38	2	4	56	0.442	0.454	NBA013	1.6
8	42	3	0	64	0.279	3.945	NBA009	6.6
9	26	1	5	18	0.575	2.215	NBA006	15.5
10	47	3	23	115	0.653	3.947	NBA011	4
11	44	3	8	88	0.285	5.083	NBA010	6.1
12	34	2	9	40	0.374	0.266	NBA003	1.6

Regression

In Regression, the goal is to predict a *continuos value*

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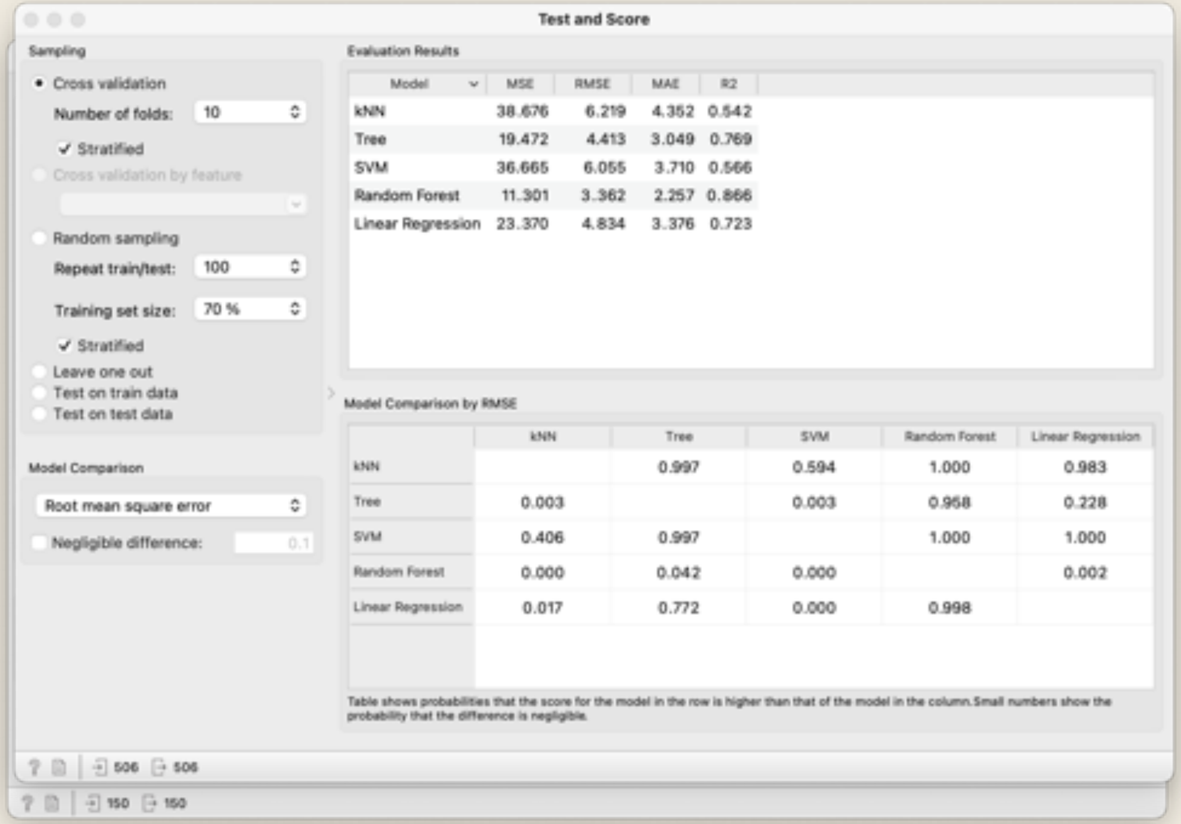
Scoring

- Abalone data (numeric Target)
- Test & Score



Evaluation metrics in classification

- We are talking about some metrics:
  - MSE: Mean Squared Error
  - RMSE: Root Mean Squared Error
  - MAE: Mean Absolute Error
  - R^2

Error coefficients

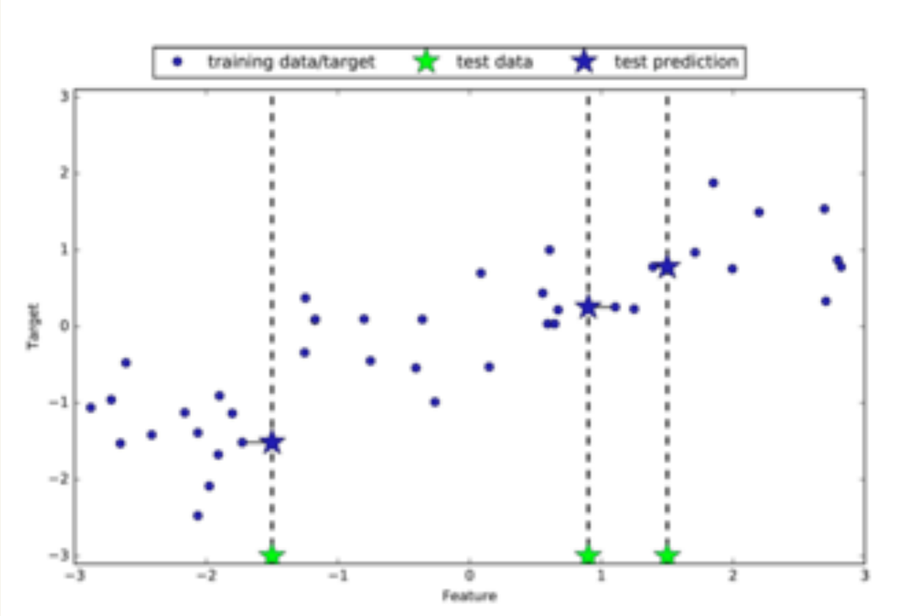
$$\text{MSE} = \frac{1}{n}\sum_{i-1}^{n}\left(Y_i - \hat{Y}_i\right)^2$$

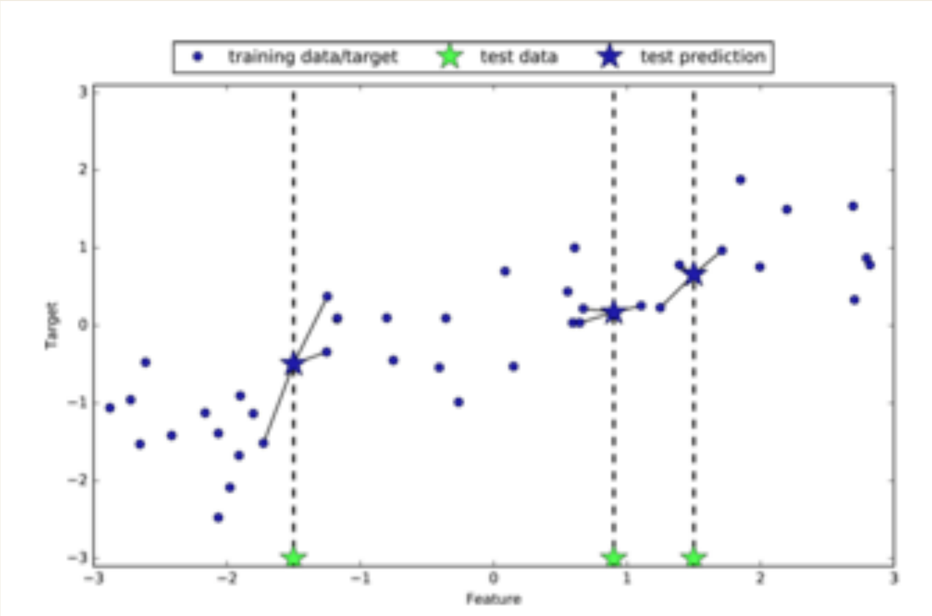
$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i-1}^{n}\left(Y_i - \hat{Y}_i\right)^2}$$

$$\text{MAE} = \frac{\sum_{i=1}^{n}\left|y_i - x_i\right|}{n} = \frac{\sum_{i=1}^{n}\left|e_i\right|}{n}$$

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}} = 1 - \frac{\sum_i \left(y_i - \hat{y}_i\right)^2}{\sum_i \left(y_i - \bar{y}\right)^2}$$

Regression Algorithms





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K-Nearest Neighbors

- Building the k-NN algorithm consists only of storing the training dataset.
- To make a prediction for a new data point, the algorithm finds the closest data points in the training dataset—its "nearest neighbors."

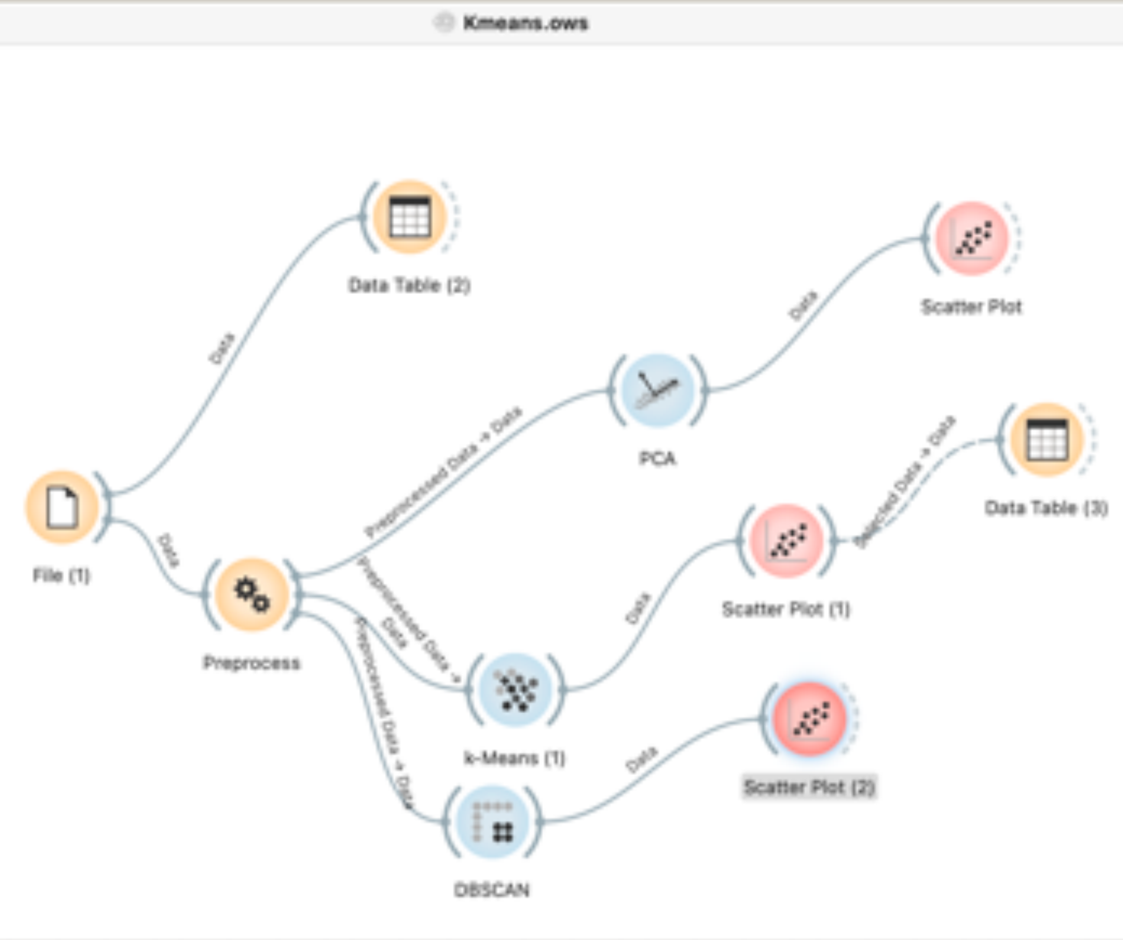
Unsupervised Learning

Challenges in Unsupervised Learning

A major challenge in unsupervised learning is evaluating whether the algorithm learned something useful. Unsupervised learning algorithms are usually applied to data that does not contain any label information, so we don't know what the right output should be. Therefore, **it is very hard to say whether a model "did well."**

Type of unsupervised learning

- **Unsupervised transformations** of a dataset are algorithms that create a new representation of the data which might be easier for humans or other machine learning algorithms to understand compared to the original representation of the data (dimensionality reduction)
- **Clustering**, on the other hand, partition data into distinct groups of similar items
-



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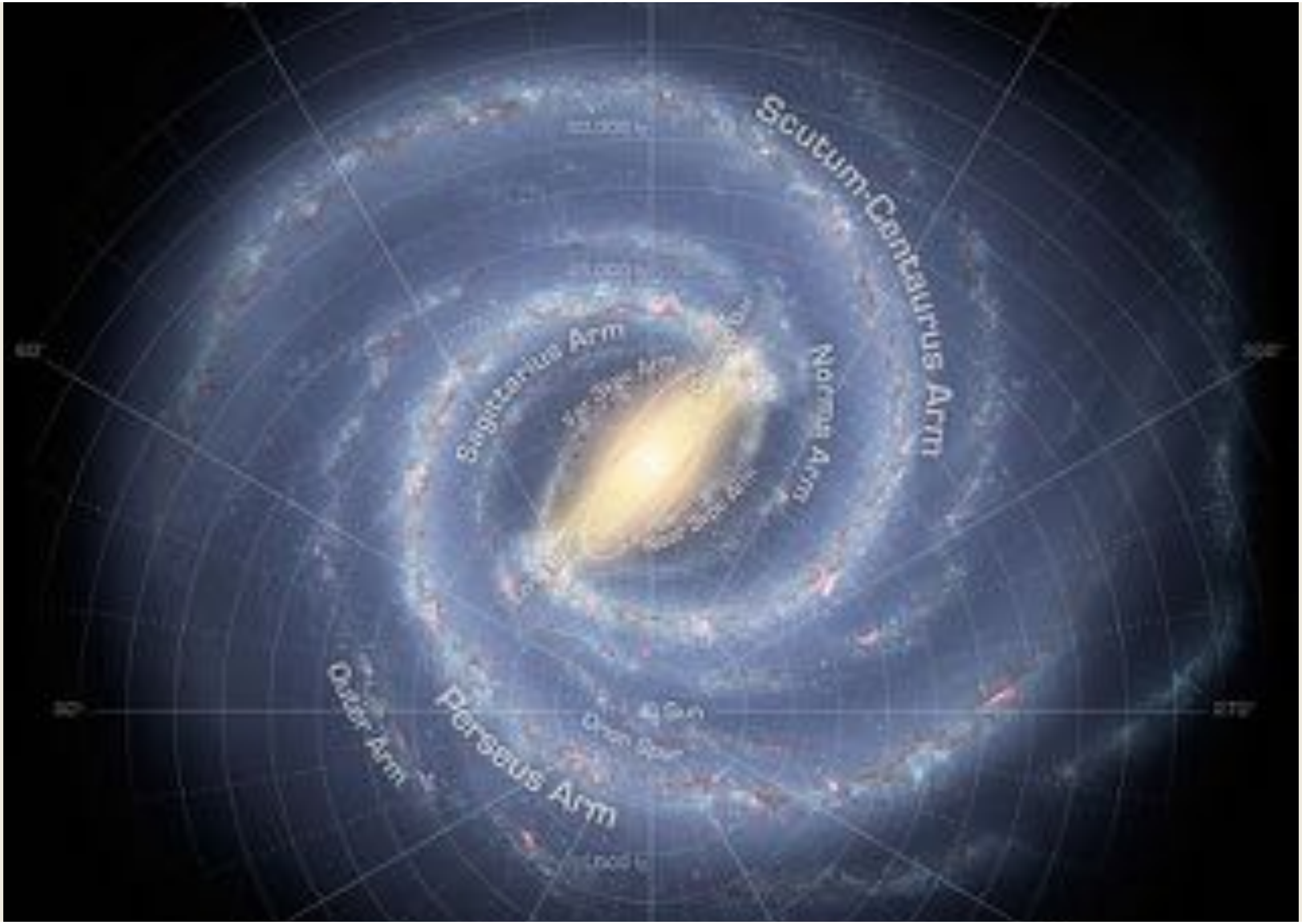
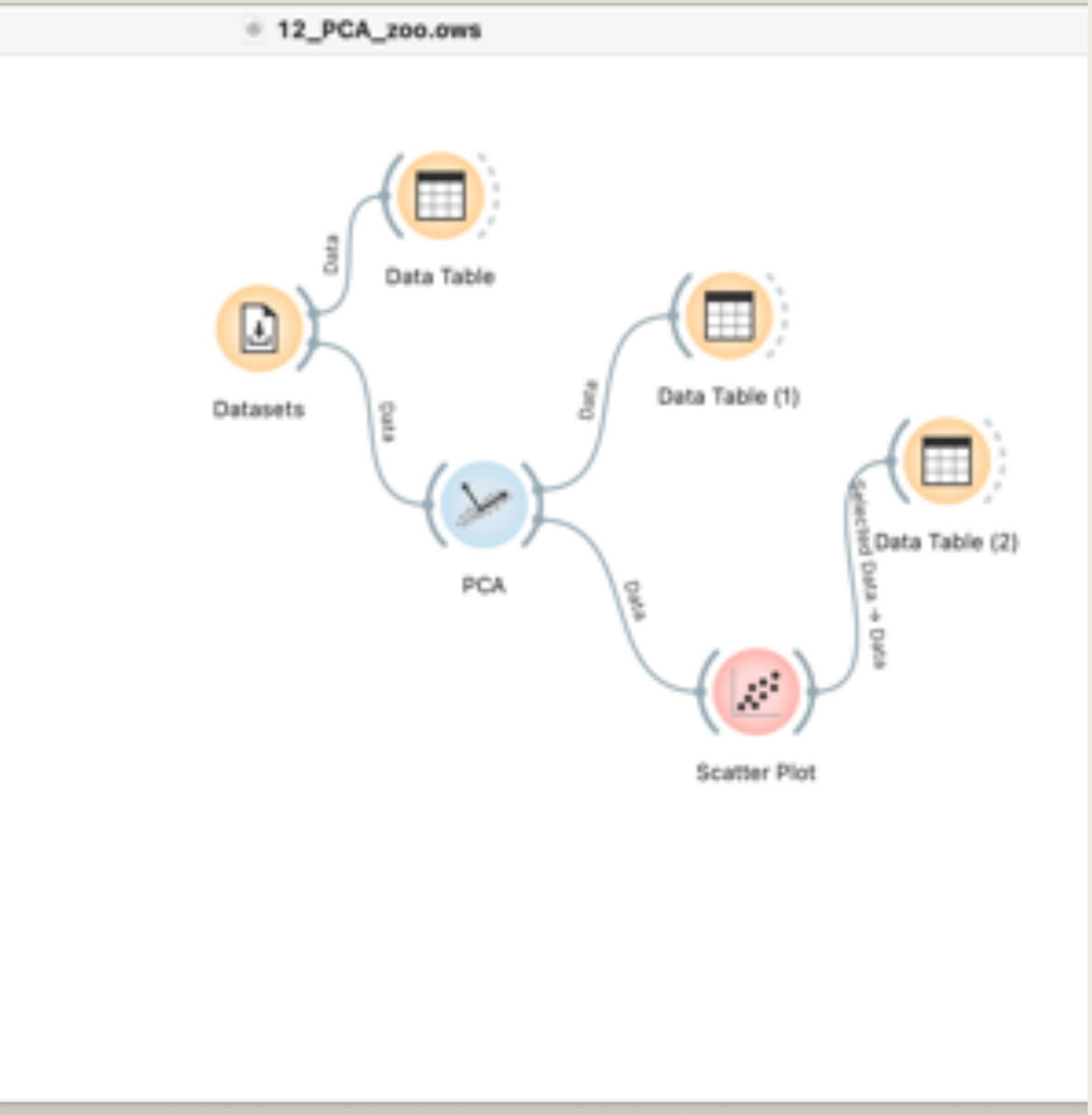
Preprocessing and Scaling

- StandardScaler
- RobustScaler
- MinMaxScaler


Let’s talk about stars


Scutum-Centaurus Arm
Sagittarius Arm
Norma Arm
Perseus Arm
Outer Arm
Orion Spur
Sun



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PCA

- Datasets->Zoo
- PCA
- Scatter Plot

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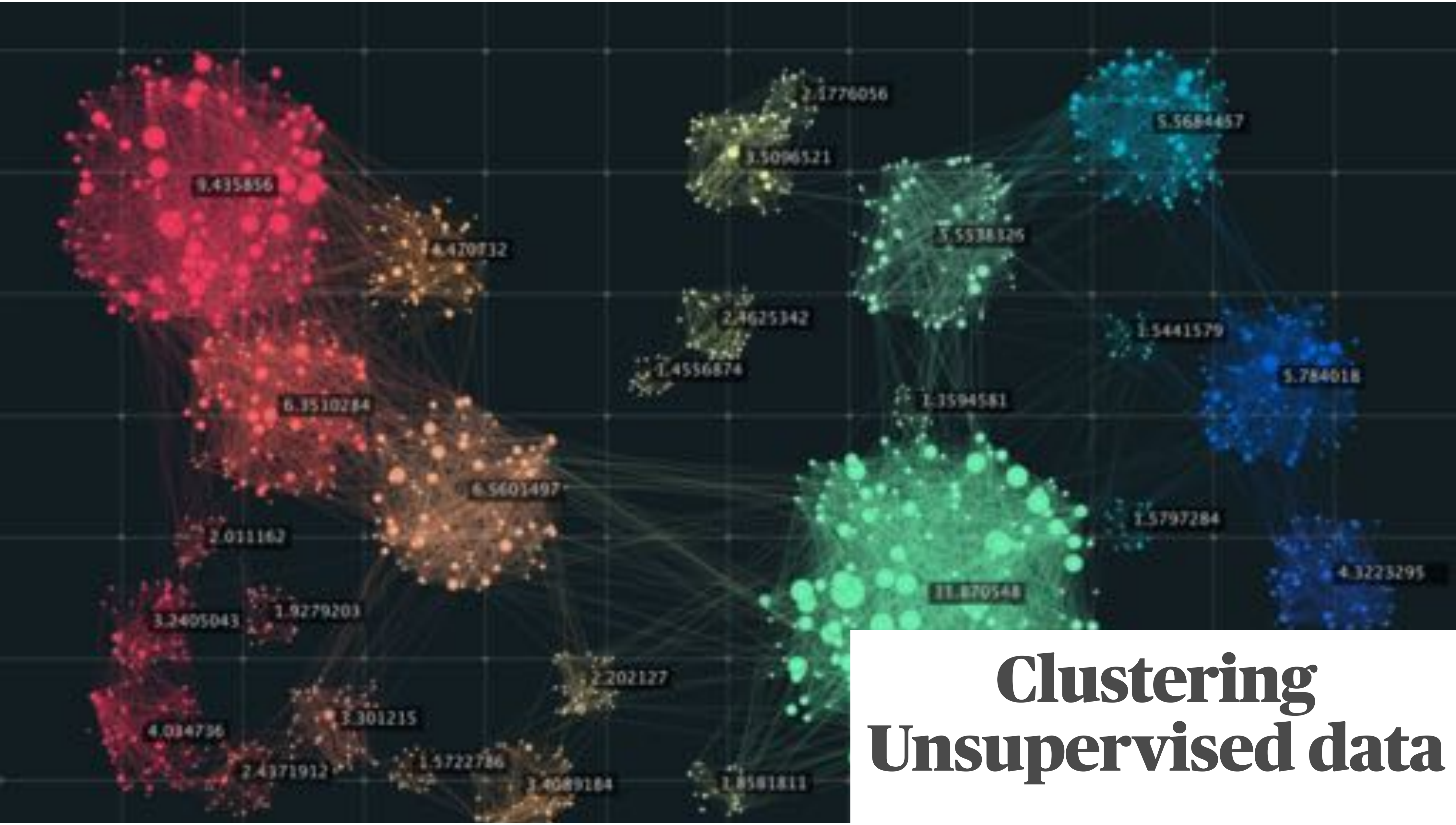
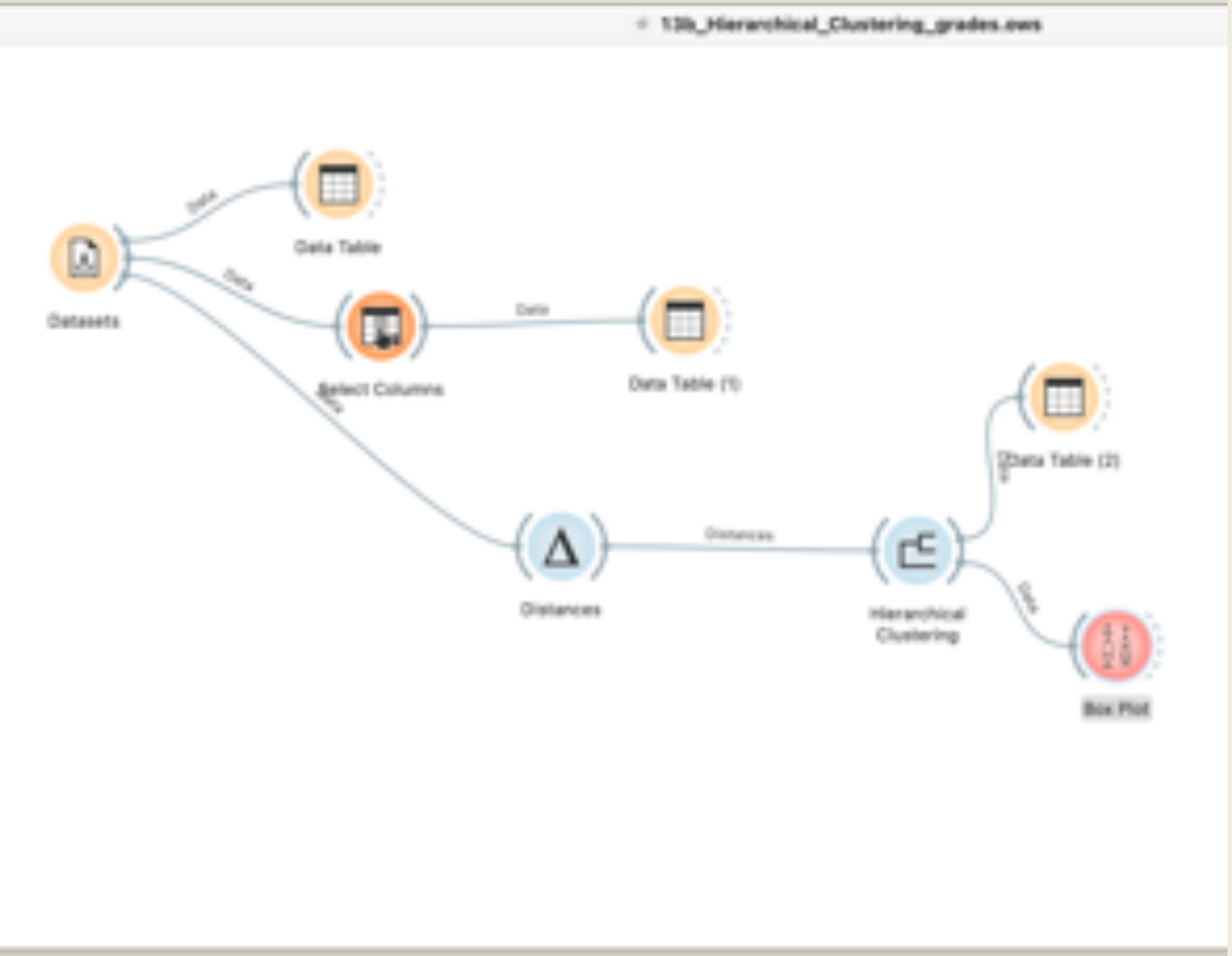
MDS and t-SNE

- Datasets->Zoo
- Distances
- MDS and t-SNE



Clustering Unsupervised data



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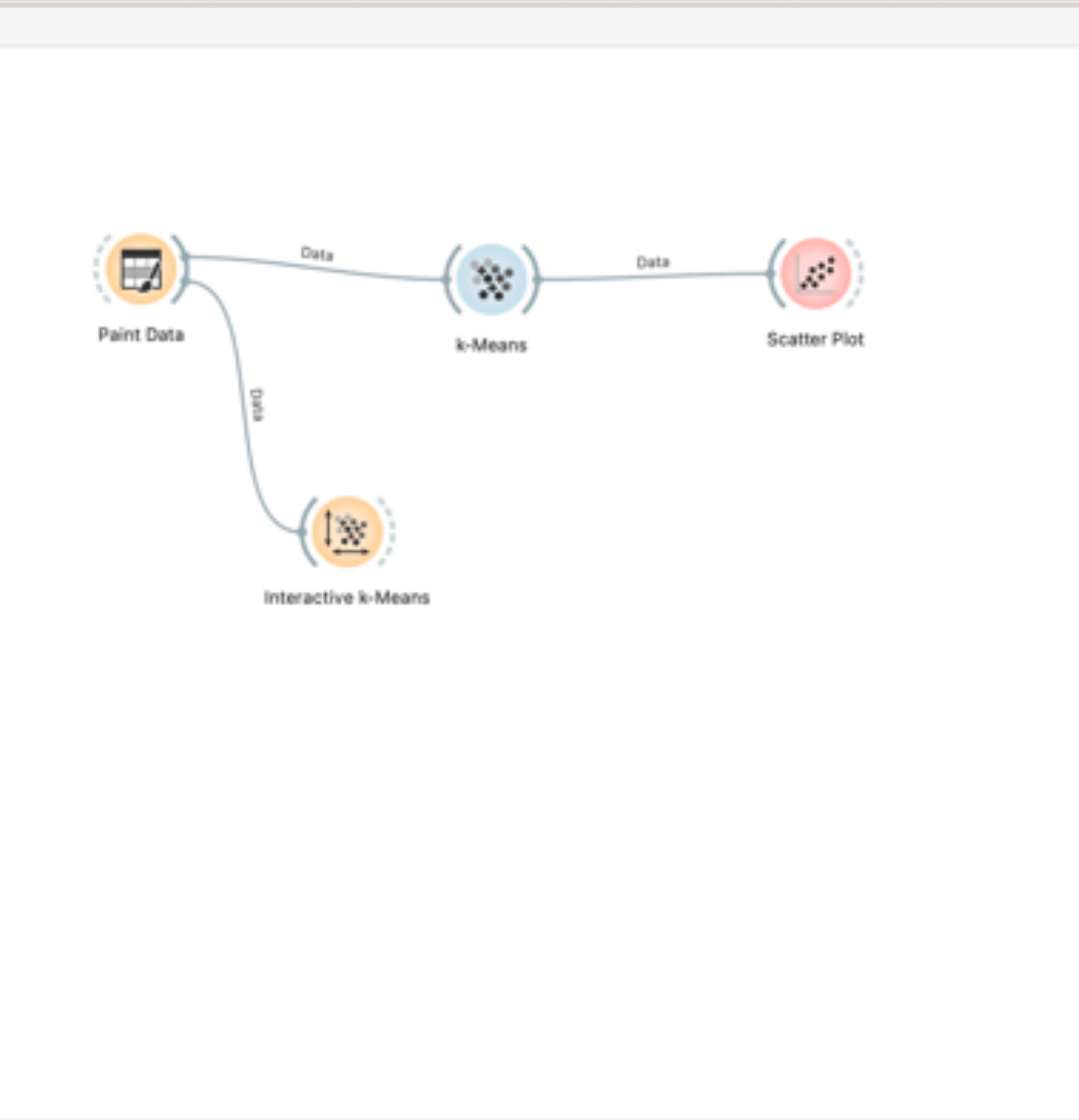
Hierarchical clustering

- Grades –> Data Table
- Distances –> hierarchical clustering
- Scatter plot
- Box plot



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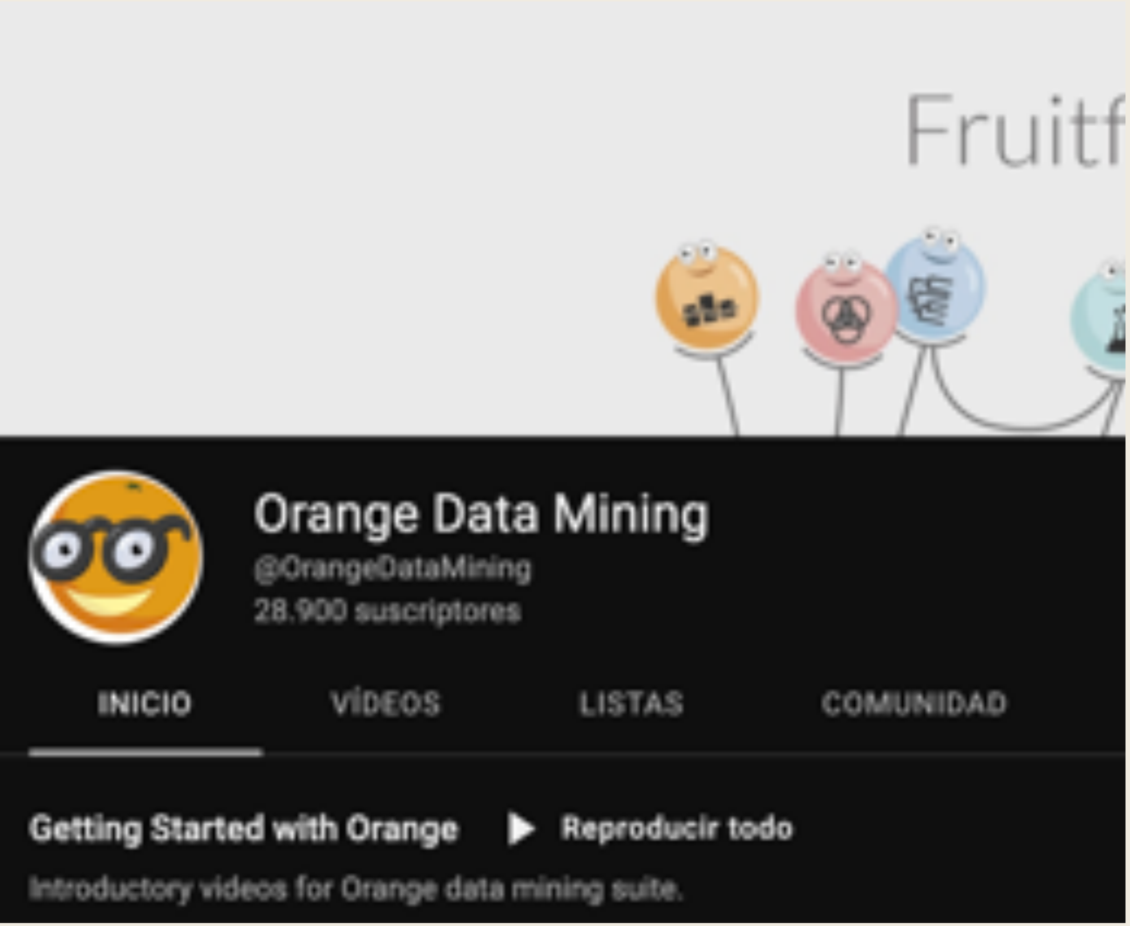
K-means

- Paint Data
- K-means –> Scatter plot
- Interactive K-Means
- 2 example:
- Iris Data



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