

Astronomy ESFRI & Research Infrastructure Cluster ASTERICS - 653477



3rd ASTERICS-OBELICS International School

8-12 April 2019, Annecy, France.



H2020-Astronomy ESFRI and Research Infrastructure Cluster (Grant Agreement number: 653477).





Machine Learning Tutorial I - Introduction

3rd ASTERICS-OBELICS International School 8-12 April 2019, Annecy - France

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Summary

- I. Introduction to Machine Learning
- II. Introduction to Neural Networks by Alexandre

Boucaud

- III. Deep Learning by Alexandre Boucaud
- IV: Beyond textbook Machine Learning

Acknowledgments

Adam Miller

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David Kirby

Daniela Huppenkothen

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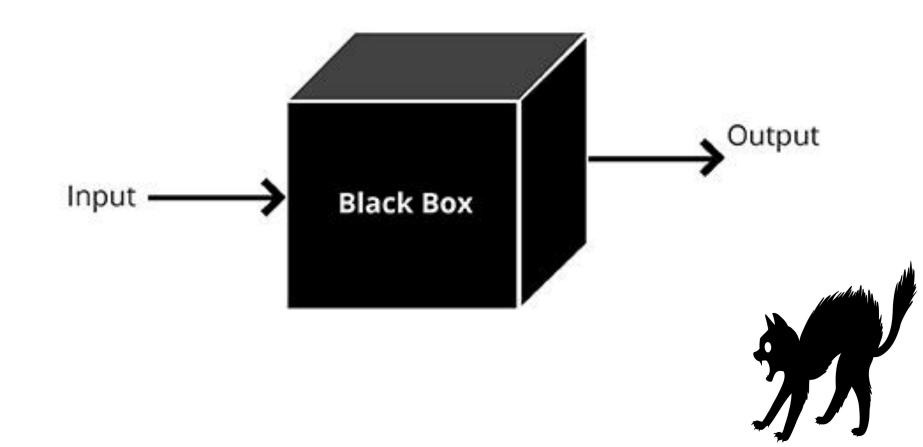
Joshua Bloom

Ricardo Vilalta

The Cosmostatistics Initiative

Disclaimer 1

Beware of Black Boxes!!!



Disclaimer 2



for now ...

What is learning ? (real question, google it!)

What is learning ?

"A relatively permanent change in behaviour due to past experiences."

D. Coon, Introduction to psychology: exploration and application (1983)

What is Machine Learning ?

(you know what to do)

Machine Learning: a definition

"A computer program L is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E."

Presented by R. A. Fisher (1936)

50 samples of each class

Petal length	Petal width	Sepal length	Sepal width	Class
5.1	3.5	1.4	0.2	Setosa
6.5	1.0	4.5	1.3	Versicolor
5.9	3.0	5.1	1.8	Virginica





Versicolor



Virginica

Setosa

Presented by R. A. Fisher (1936)

50 samples of each class

Petal length	Petal width	Sepal length	Sepal width	Class
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Setosa



Versicolor



Virginica

What can you hope to learn from this?

https://en.wikipedia.org/wiki/Iris_flower_data_set

Presented by R. A. Fisher (1936)

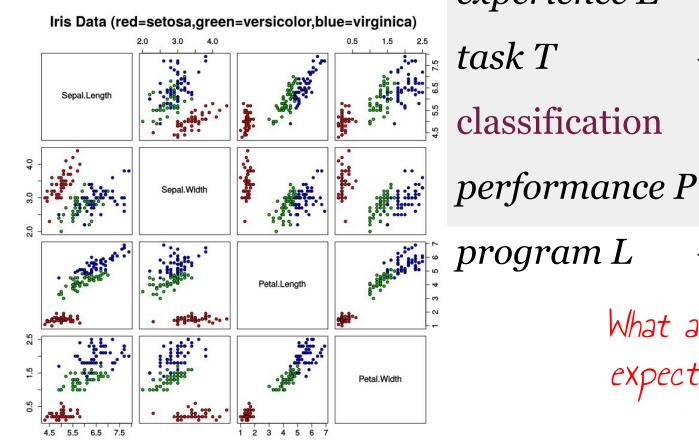
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5.9	3.0	5.1	1.8	Virginica

experience $E \rightarrow data$ task T classification performance $P \rightarrow \text{accuracy}$ $program L \rightarrow strategy$ What are your expectations?

Presented by R. A. Fisher (1936)

50 samples of each class



experience $E \rightarrow data$ performance $P \rightarrow accuracy$ i program $L \rightarrow$ strategy What are your expectations?

https://en.wikipedia.org/wiki/Iris flower data set

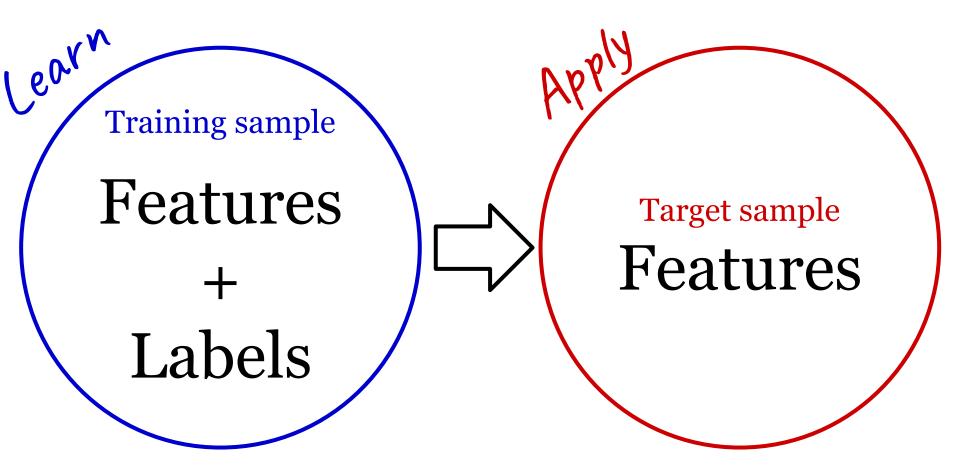
Example 2: SDSS

Notebook 1 EDA_SDSS.ipynb



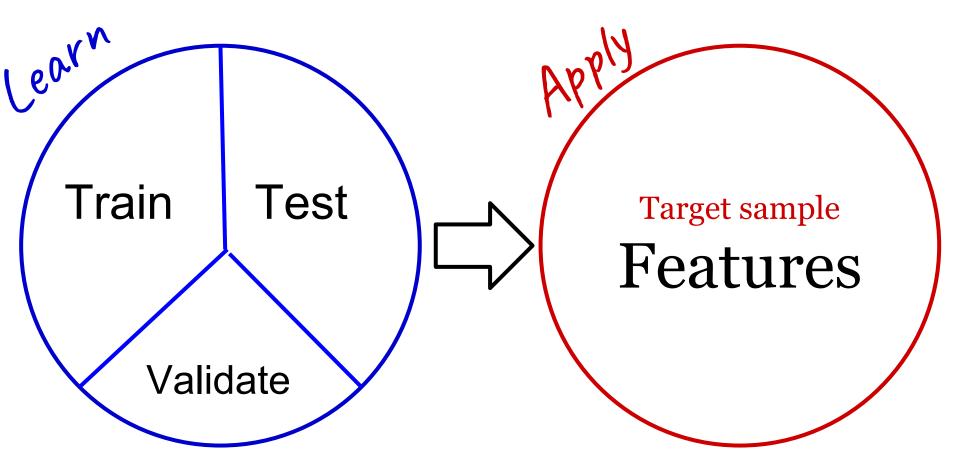
Supervised Learning

Supervised Learning Learn by example

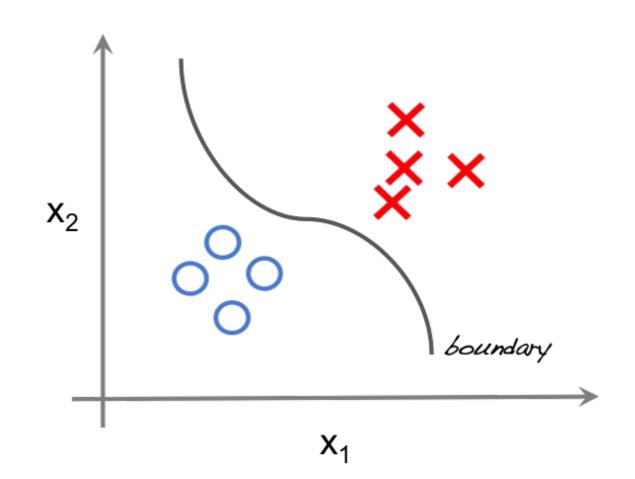


Supervised Learning

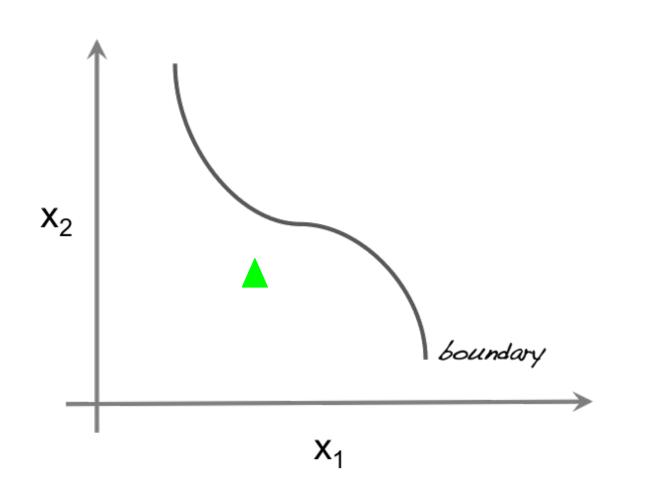
Learn by example



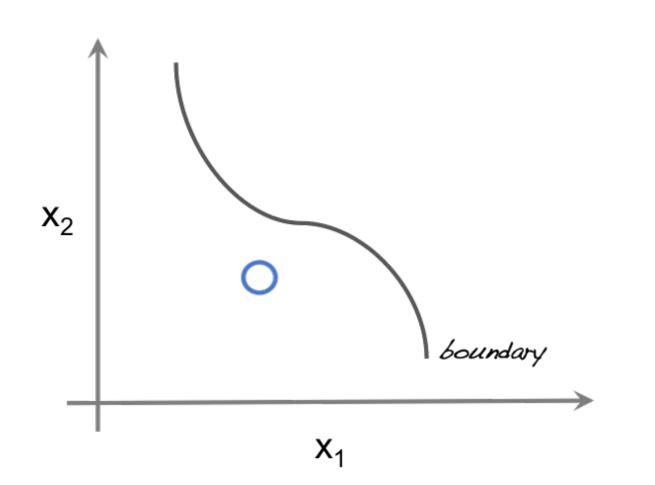
Supervised Learning Classification



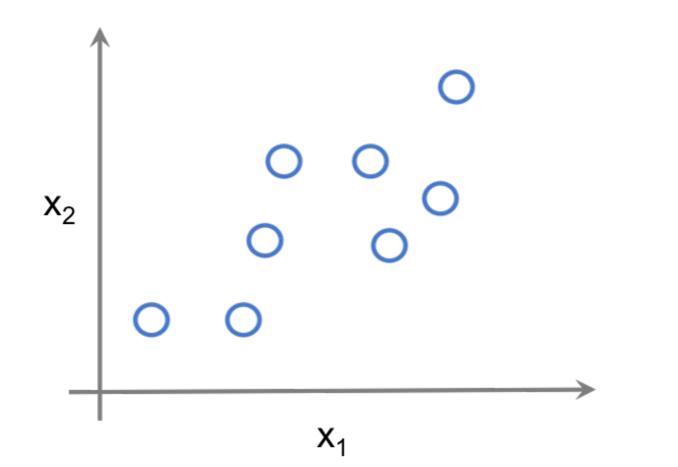
Supervised Learning Classification



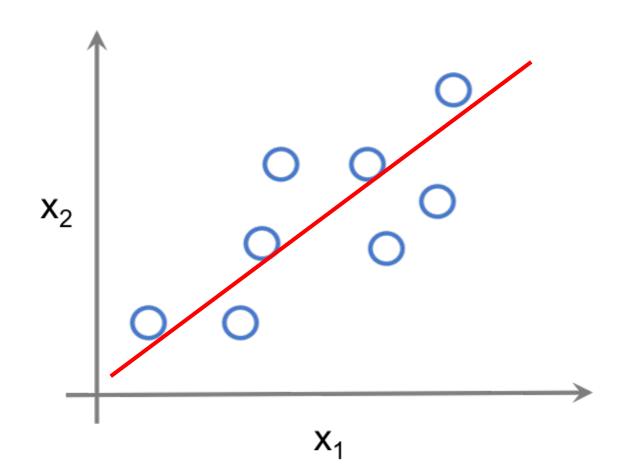
Supervised Learning Classification



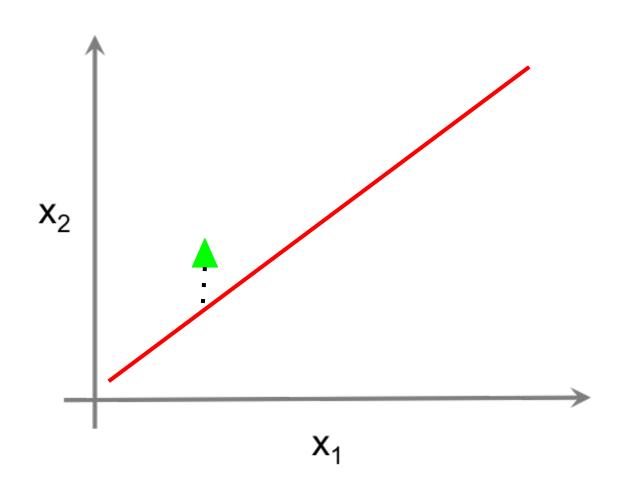
Supervised Learning Regression



Supervised Learning Regression



Supervised Learning Regression

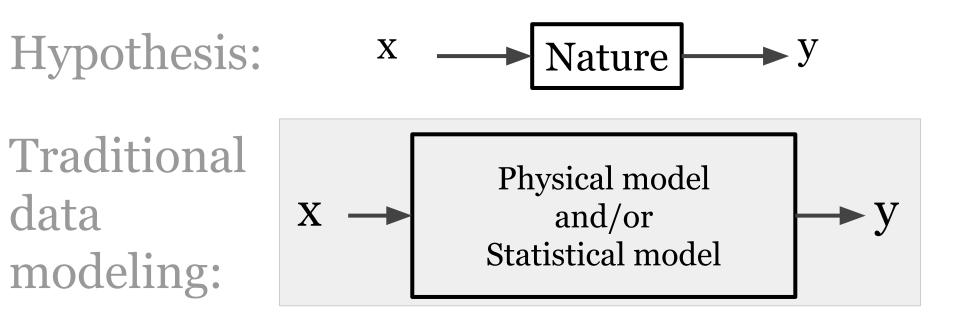


What is the difference between machine learning and a traditional data modelling?

Hypothesis:



Breiman, L., Statistical Modeling: The Two Cultures, Stat. SciVolume 16 (2001)



Breiman, L., Statistical Modeling: The Two Cultures, Stat. SciVolume 16 (2001)

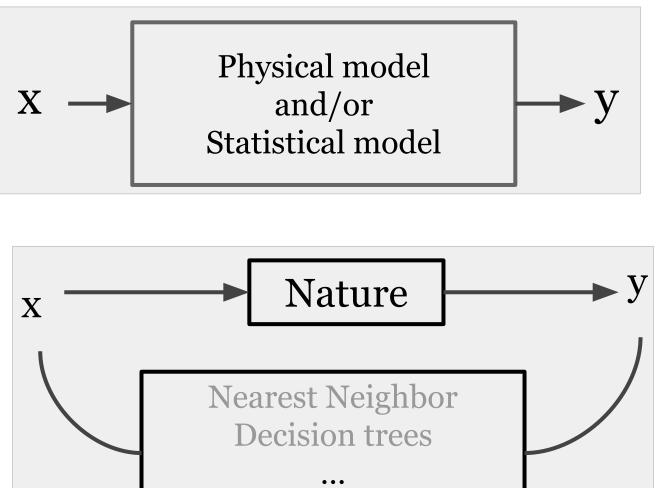
Hypothesis:



Traditiona

data modeling:

Algorithmic modeling:



Machine Learning model

Breiman, L., Statistical Modeling: The Two Cultures, Stat. Sci, Volume 16 (2001)

Supervised ML model

data training, target

χ set of all samples, xY set of possible labels, y

 $\begin{array}{ll} h_{train} & \text{learner: } y_{est;i} = h_{train}(x_i) \\ L & \text{loss function} \end{array}$

Goal: *minimize L*

Shai and Shai, Understanding ML: From Theory to Algorithms, 2014, CUP

Supervised ML model

data **training**, target

 $\begin{array}{ll} \chi & \text{set of all samples, } x \\ Y & \text{set of possible labels, } y \end{array}$

$$h_{train}$$
 learner: $y_{est;i} = h_{train}(x_i)$
L Loss function

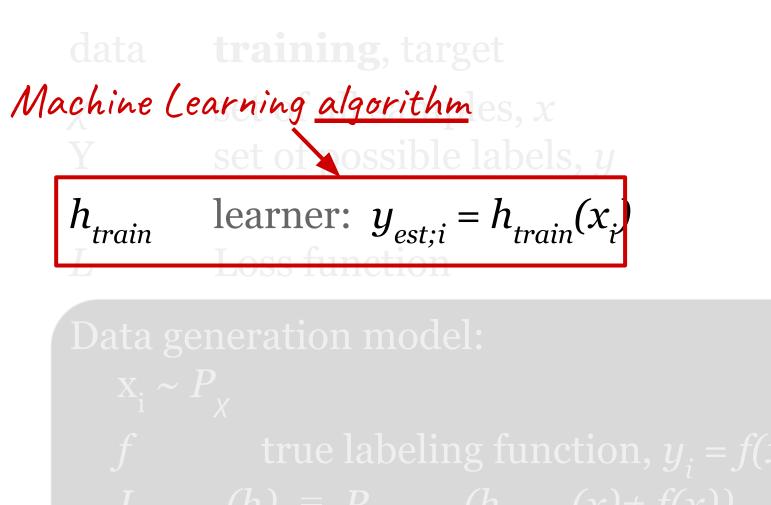
Data generation model:

$$x_i \sim P_{\chi}$$

 $f \rightarrow \text{ true labeling function, } y_i = f(x_i)$
 $L_{data,f}(h) \equiv P_{x \sim data}(h_{train}(x) \neq f(x))$

Shai and Shai, Understanding ML: From Theory to Algorithms, 2014, CUP

Supervised ML model



Shai and Shai, Understanding ML: From Theory to Algorithms, 2014, CUP

Machine Learning

algorithm

- 1. Linear Regression
- 2. Logistic Regression
- 3. Decision Tree
- 4. SVM
- 5. Naive Bayes
- 6. kNN
- 7. K-Means
- 8. Random Forest
- 9. Dimensionality Reduction Algorithms
- 10. Gradient Boosting algorithms
 - 1. GBM
 - 2. XGBoost
 - 3. LightGBM
 - 4. CatBoost

https://www.analyticsvidhya.com/blog/2017/09/common-machine-learning-algorithms/

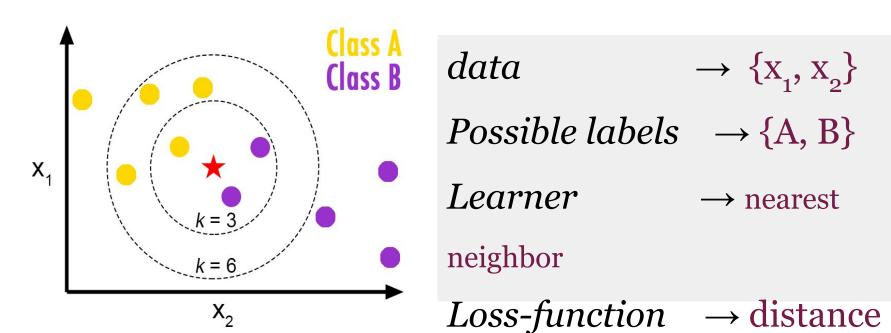
Example of supervised ML algorithm for classification

k-Nearest Neighbor (kNN)

Distance based

Hypothesis:

Objects from similar classes are clustered together



Notebook 2 Classification.ipynb

Example of supervised ML algorithm for classification

Support Vector Machines (SVM)

Search for hyperplanes

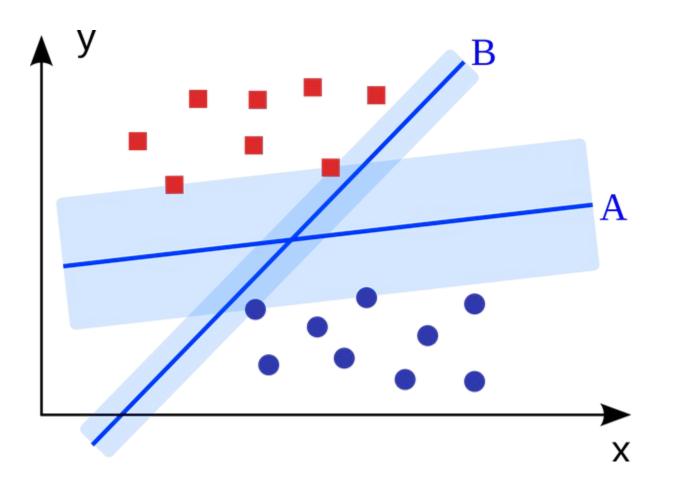
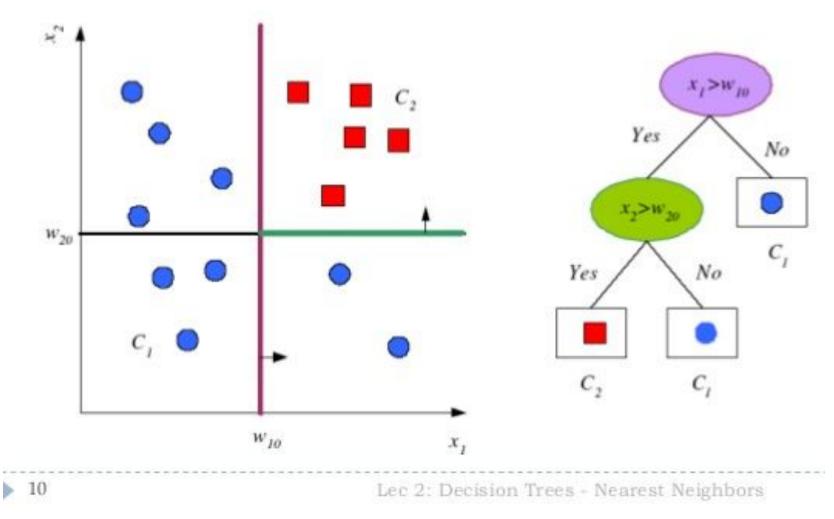


Image from: https://www.quora.com/What-is-a-Support-Vector-Machine

Example of supervised ML algorithm

Decision Trees

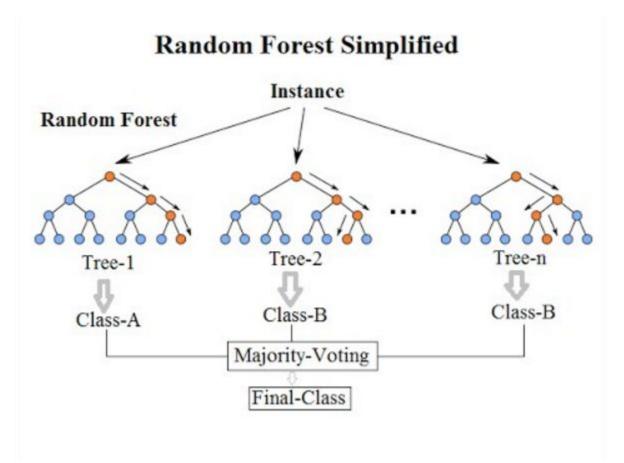


http://www.lewisgavin.co.uk/Machine-Learning-Decision-Tree/

Example of supervised ML algorithm

Random Forests

Ensemble method

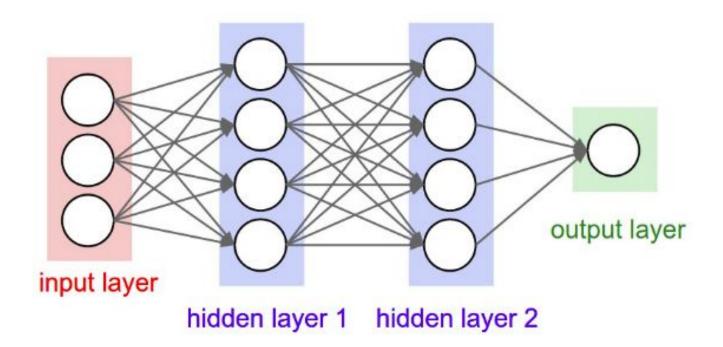


https://medium.com/@williamkoehrsen/random-forest-simple-explanation-377895a60d2d

Example of supervised ML algorithm:

(Deep) Neural Network

All layers internal to the network (not input or output layer) are considered hidden layers. See Alex's tutorial tomorrow



Slide by Alexandre Boucaud, ADA IX, 2018

Supervised ML model

data **training**, target

- χ set of all samples, x
- Y set of possible labels, *y*

$$h_{train}$$
 learner: $y_{est;i} = h_{train}(x_i)$
L Loss function

Data generation model:

$$x_i \sim P_{\chi}$$

 $f \rightarrow \text{ true labeling function, } y_i = f(x_i)$
 $L_{data,f}(h) \equiv P_{x \sim data}(h_{train}(x) \neq f(x))$

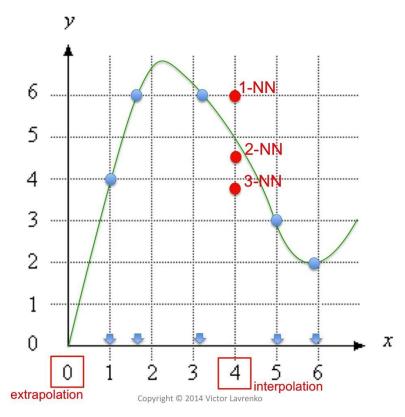
Shai and Shai, Understanding ML: From Theory to Algorithms, 2014, CUP

It also works for regression...

Example of supervised ML algorithm for regression

k-Nearest Neighbor (kNN) Distance based

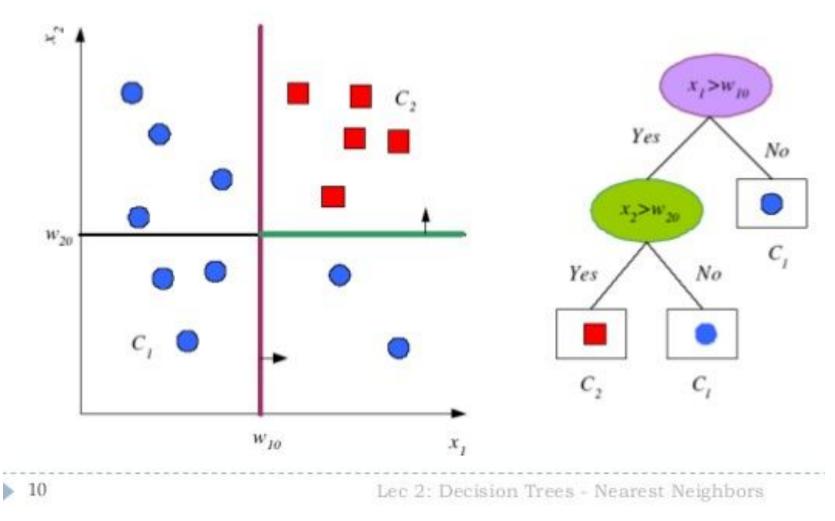
Example: kNN regression in 1-d



https://www.youtube.com/watch?v=3lp5CmSwrHI

Example of supervised ML algorithm for classification

Decision Trees

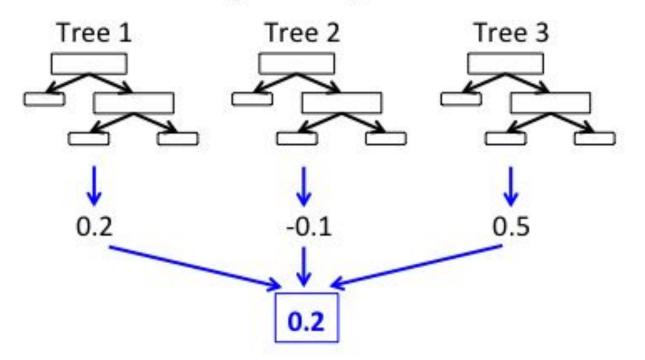


Example of supervised ML algorithm for regression

Random Forests

Ensemble method

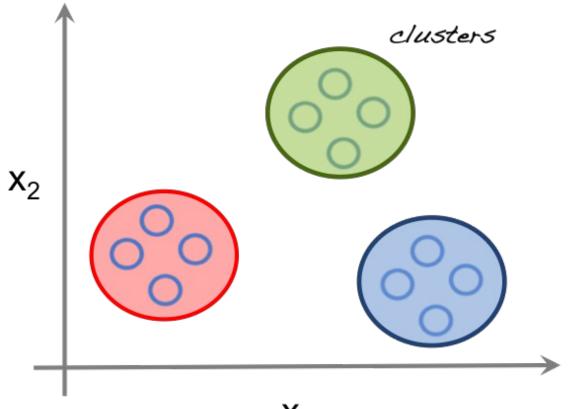
Ensemble Model: example for regression

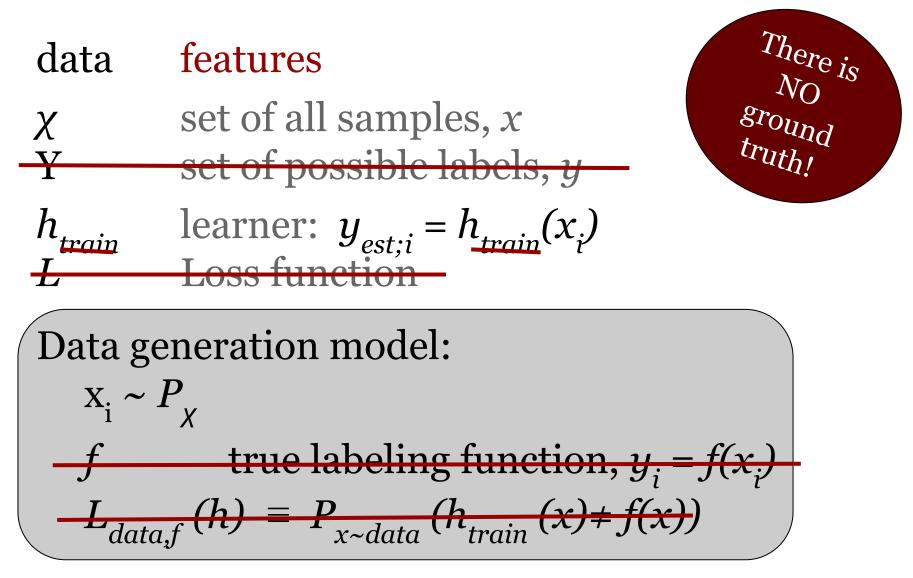


https://databricks.com/blog/2015/01/21/random-forests-and-boosting-in-mllib.html

Notebook 3 Regression.ipynb

Search for data structures





data features

 χ set of all samples, x

h learner:
$$y_{est;i} = h(x_i)$$

 $P(\chi)$ joint probability density

Goal: *characterize P*

Example of unsupervised ML algorithm

k-Means

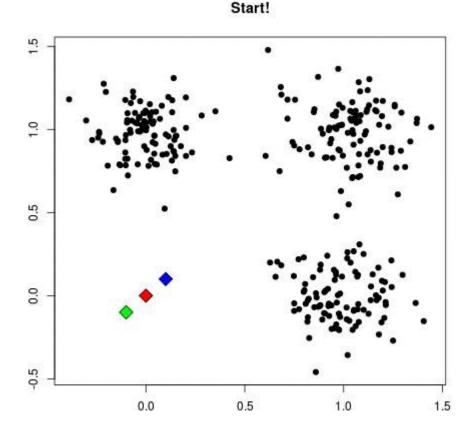
Clustering

1: assign centroids

2: each data point is attributed to the closest centroid

3: the centroid is moved to the center of the data points attributed to it

Repeat 2 and 3 until convergence

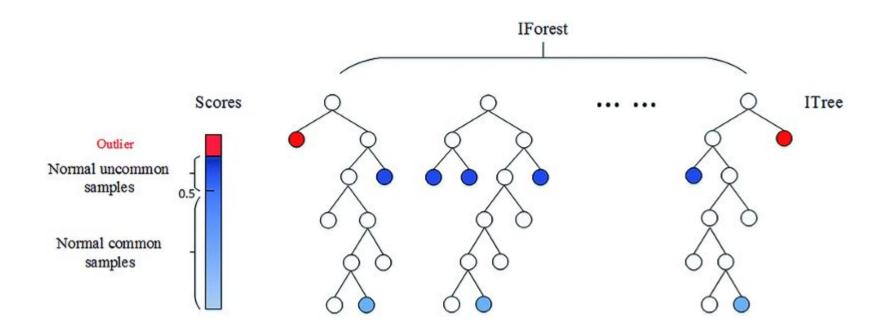


https://mubaris.com/2017/10/01/kmeans-clustering-in-python/

Example of unsupervised ML algorithm

Isolation Forests

Outlier detection



https://towardsdatascience.com/a-brief-overview-of-outlier-detection-techniques-1e0b2c19e561

Summary

What you should remember from this session

1. The definition of learning is different for machines

2. Supervised Machine Learning
 ↓
 Minimize loss function

3. The Machine Learning <u>algorithm</u>, or learner, is only 1 element in a larger Machine Learning <u>model</u> ⇒ you should pay attention to the other elements as well!





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Acknowledgement

• H2020-Astronomy ESFRI and Research Infrastructure Cluster (Grant Agreement number: 653477).