Machine Learning Tutorial
I - Introduction

ADA IX Summer School
20-22 May 2018, Valencia - Spain

Emille E. O. Ishida
Laboratoire de Physique de Clermont - Université Clermont-Auvergne
Clermont Ferrand, France

In collaboration with
Alexandre Boucaud
Paris-Saclay Center for Data Science

Emille E. O. Ishida

Researcher at the Laboratoire de Physique de Clermont

Clermont Ferrand, France

Type Ia Supernova + Machine Learning + Bayesian Statistics

Interdisciplinary science development

Co-chair of the Cosmostatistics Initiative (COIN)

CNRS - MOMENTUM Laureate

Clermont Ferrand, France

COIN
Cosmostatistics Initiative

UNIVERSITÉ Clermont Auvergne

Truffade

Large Synoptic Survey Telescope

ZTF

Puy-de-Dome

Summary

I. Introduction

II. Practical examples

III. From NN to CNN by *Alexandre Boucaud*

IV. Data Science Workflow by *Alexandre Boucaud*

V: Beyond textbook Machine Learning

Acknowledgments

Adam Miller

Andrew Ng

Fabian Gieseke

David Hogg

David Kirby

Daniela Huppenkothen

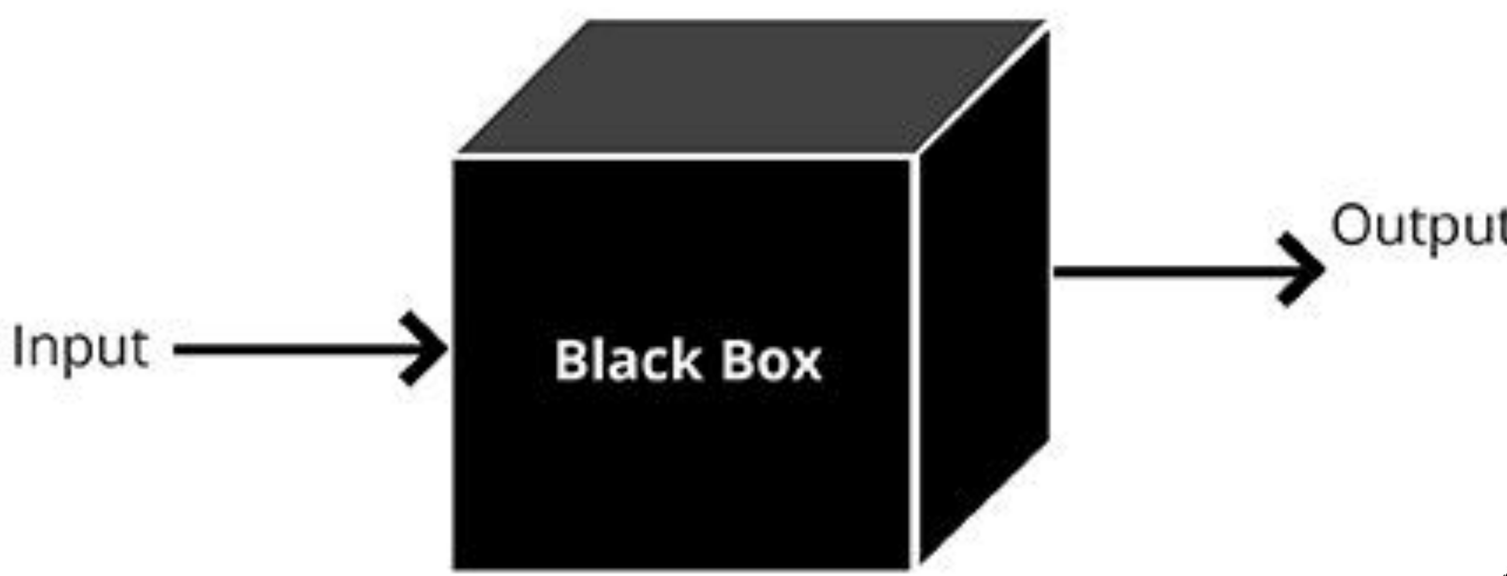
Jake VanderPlas

Ricardo Vilalta

The Cosmostatistics Initiative

Disclaimer 1

Beware of Black Boxes!!!



Disclaimer 2

for now ...

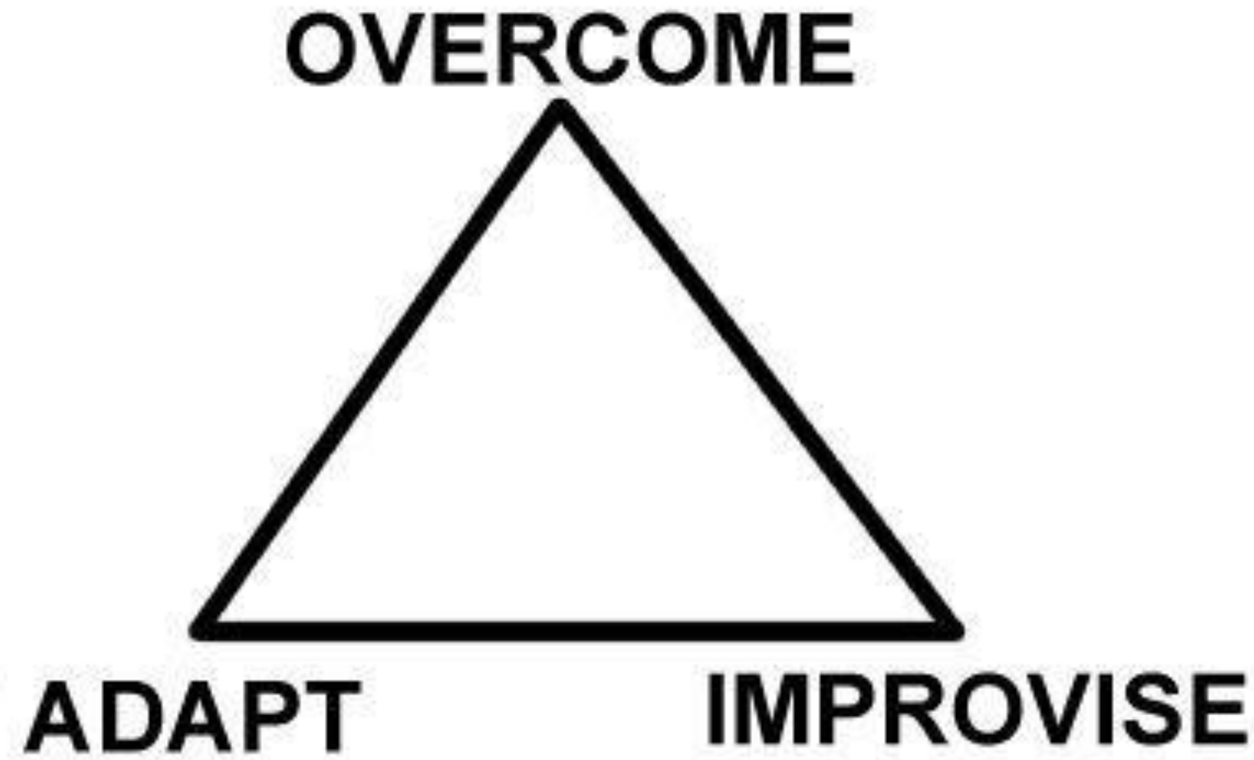
What is learning ?

What is learning ?

“A relatively permanent change in behaviour due to past experiences.”

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

Learning *or the Power to Adapt*



What is Machine Learning ?

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“ML is a field of computer science that gives computer systems the ability to learn with data, without being explicitly programmed.”

Samuel, Arthur (1959), *Some Studies in Machine Learning Using the Game of Checkers,* IBM JRD 3 (3)

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What is Machine Learning ?

WIKIPEDIA
The Free Encyclopedia

*ML is a field of computer science that gives computer systems the ability to "learn" **(i.e., progressively improve performance on a specific task)** with data, without being explicitly programmed.*

Samuel, Arthur (1959), *Some Studies in Machine Learning Using the Game of Checkers,* IBM JRD 3 (3)

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."

Mitchell, T. (1997). *Machine Learning*. McGraw Hill. p. 2

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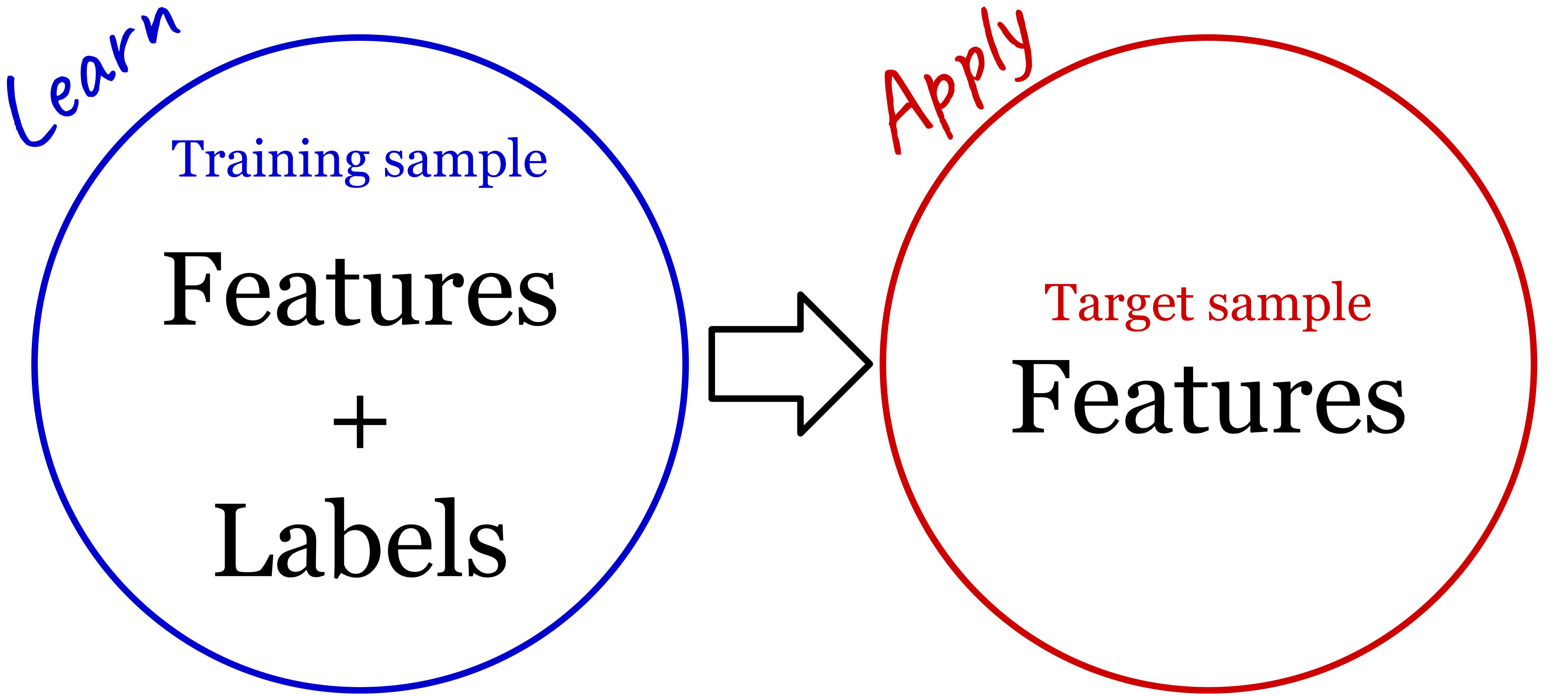
Categories of Machine Learning:

Supervised Learning

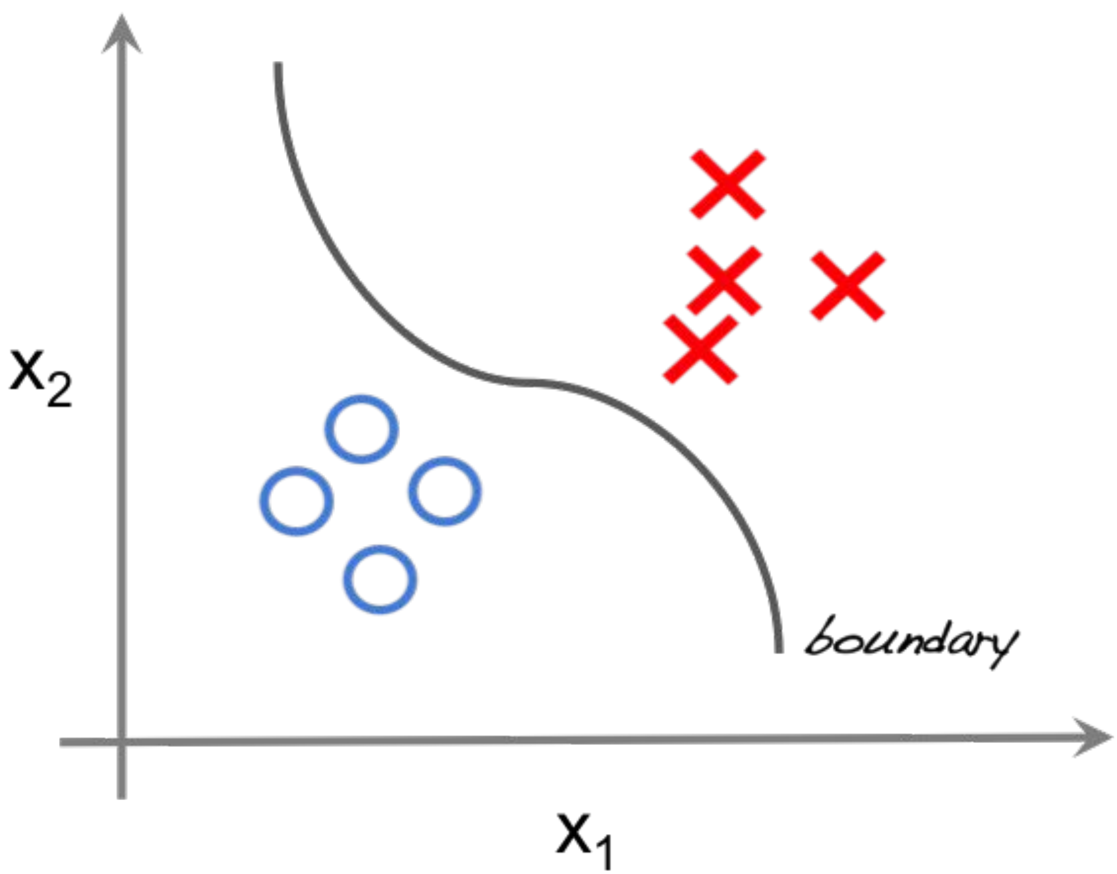
Learn by example



Categories of Machine Learning:

Supervised Learning

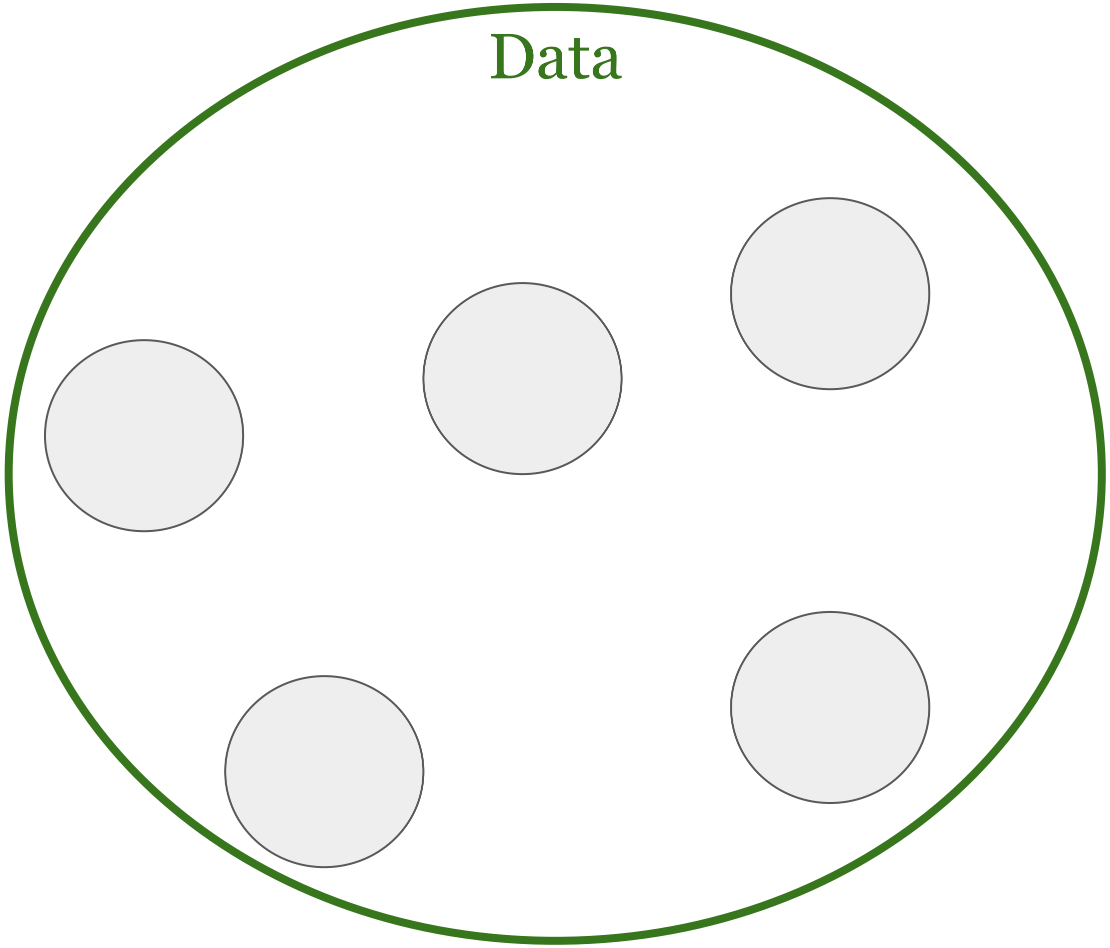
Learn by example



Categories of Machine Learning:

Unsupervised Learning

Search for data structures



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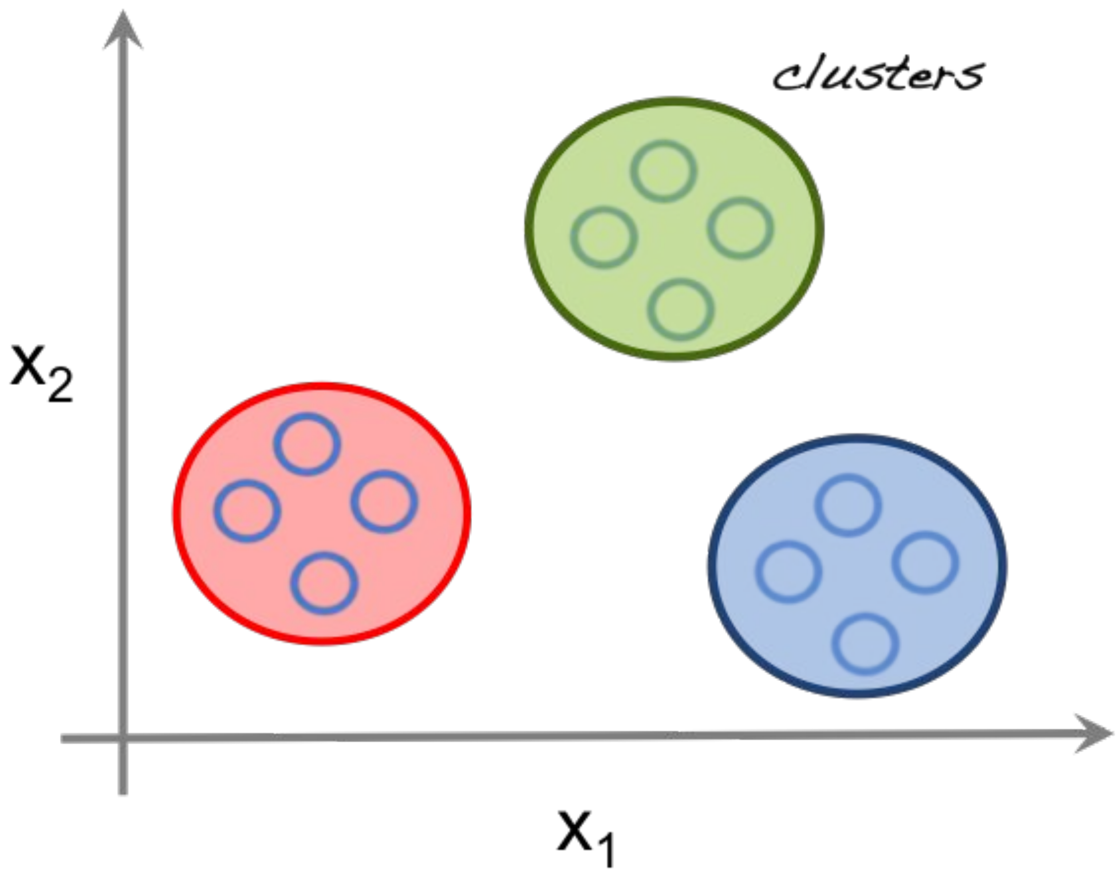
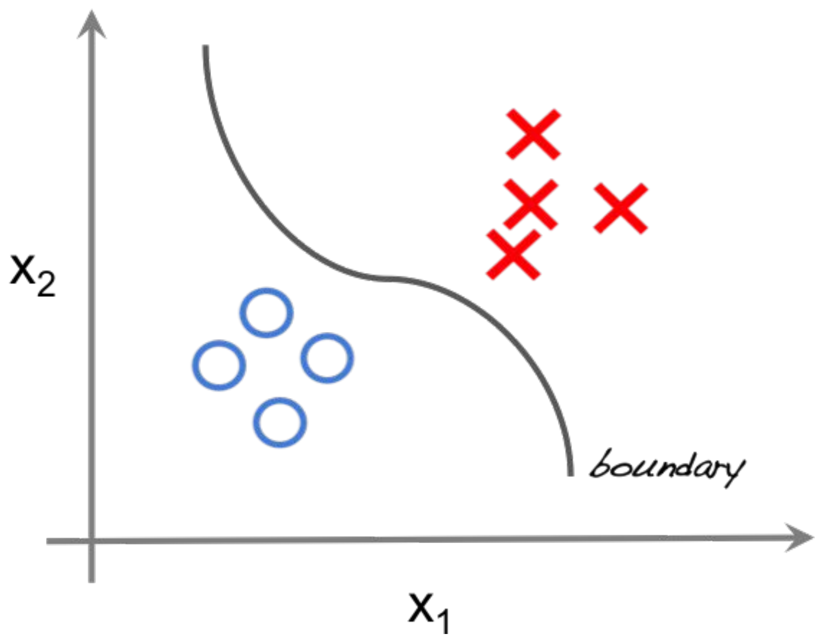


Categories of Machine Learning:

Supervised x Unsupervised

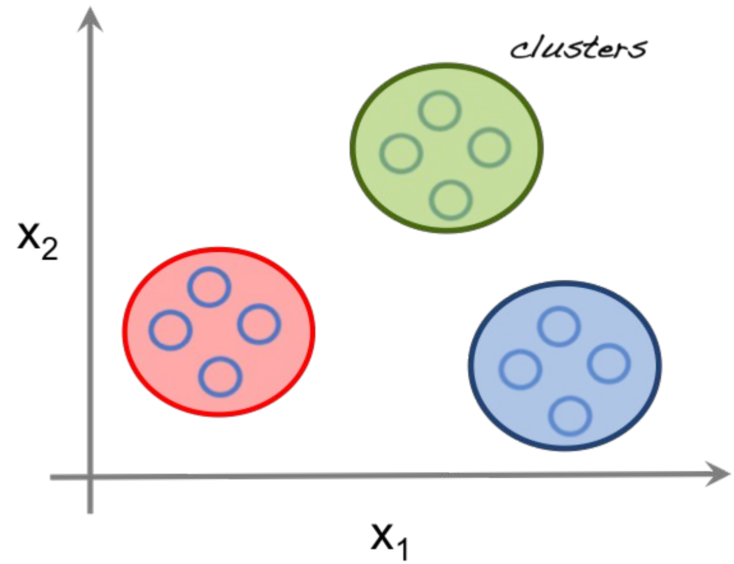


Tranining sample:

features + labels

Target sample:

features



Data sample:

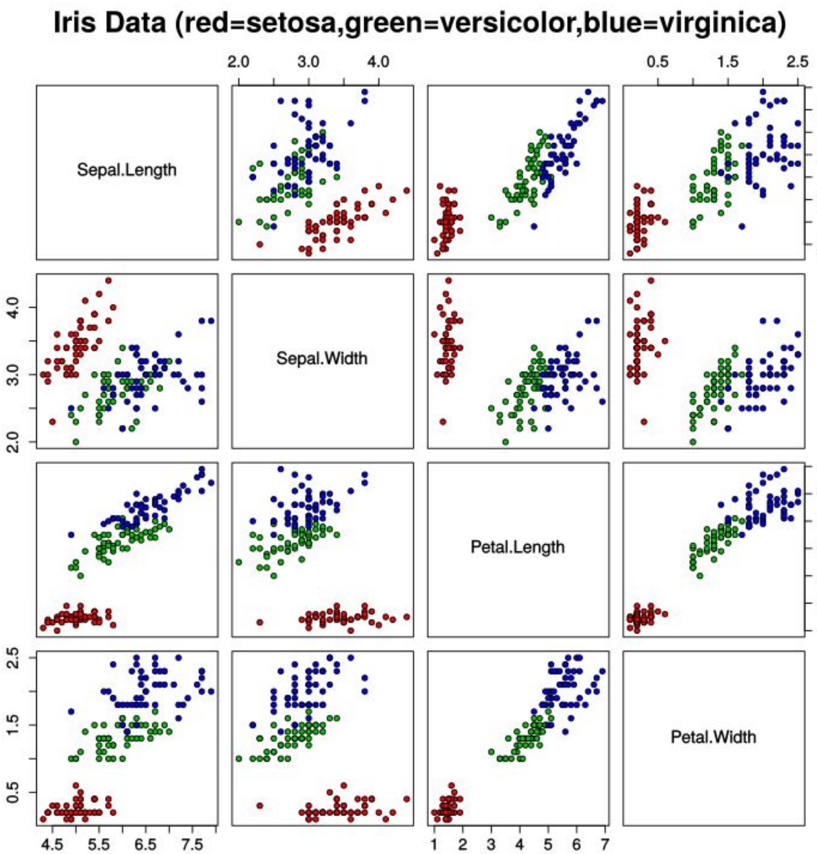
features

Supervised Learning

Example 1: the Iris dataset

Presented by R. A. Fisher (1936)

50 samples of each class



Setosa

Versicolor

Virginica

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

Example 1: the Iris dataset

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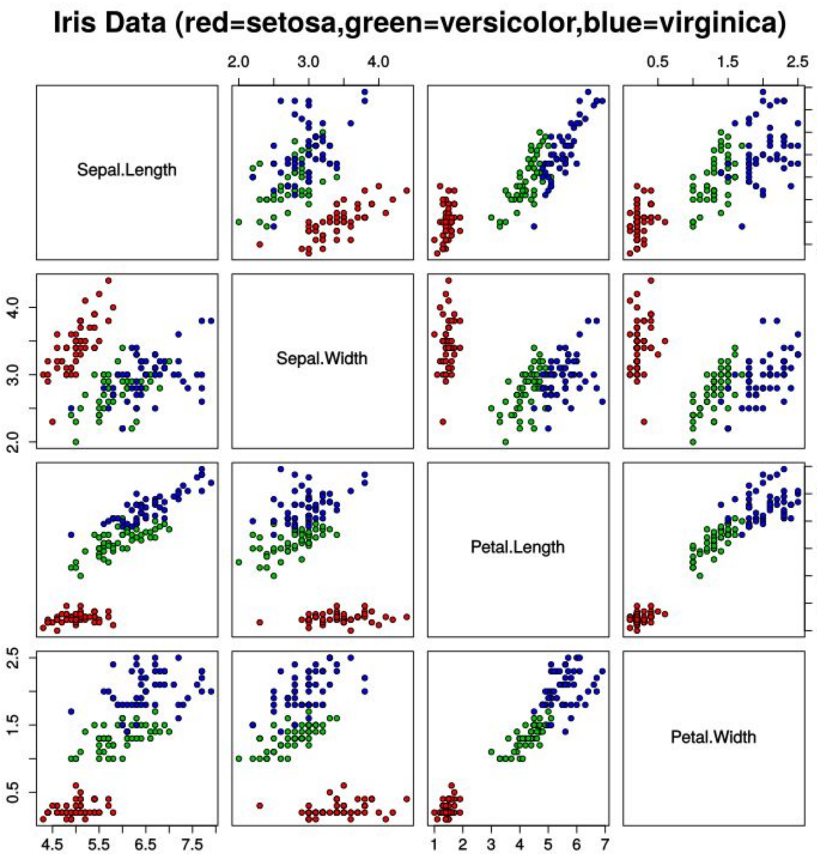

experience E	→	data
task T	→	problem
performance P	→	metric
program L	→	algorithm

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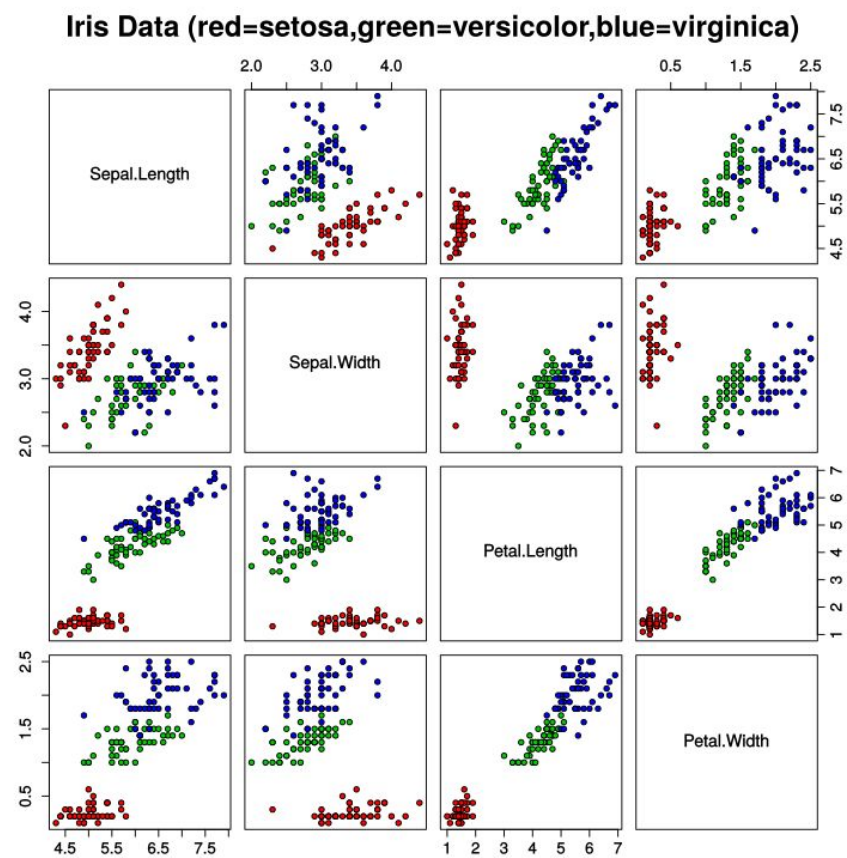


https://en.wikipedia.org/wiki/Iris_flower_data_set

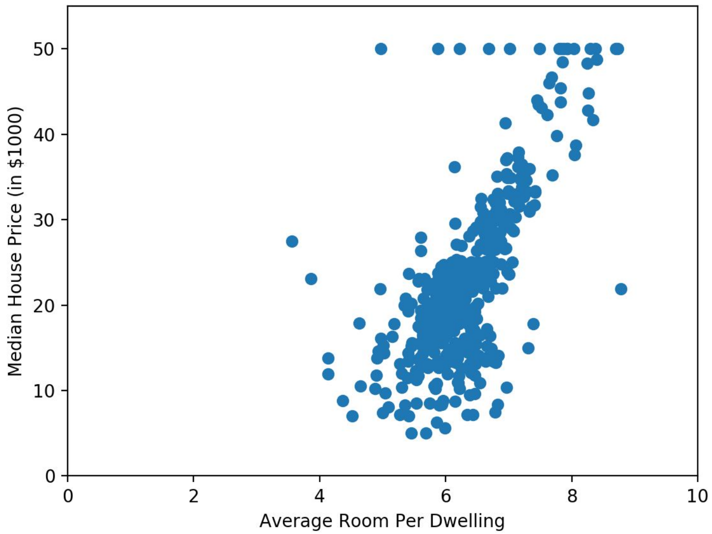
experience E	→	data
task T	→	class.
performance P	→	accuracy
program L	→	boundary

Does L learn?

Example 2: the Boston dataset

Housing prices in Boston area

506 samples and 14 features



experience E	→	data
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Harrison, D. and Rubinfeld, D.L. *'Hedonic prices and the demand for clean air'*, JEE & M, vol.5, 81-102, 1978

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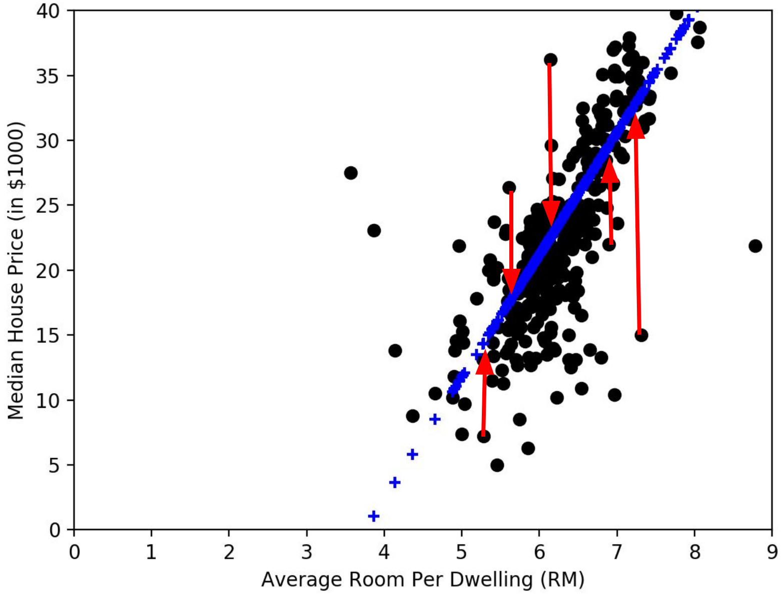

experience E	→	data
task T	→	reg.
performance P	→	RMS
program L	→	relation

y = ax + b

$$\{a, b\} \leftarrow \min \left[\sum_{i=1}^{N} (y_i - (ax_i + b))^2 \right]$$

Harrison, D. and Rubinfeld, D.L. *'Hedonic prices and the demand for clean air'*, JEE & M, vol.5, 81-102, 1978

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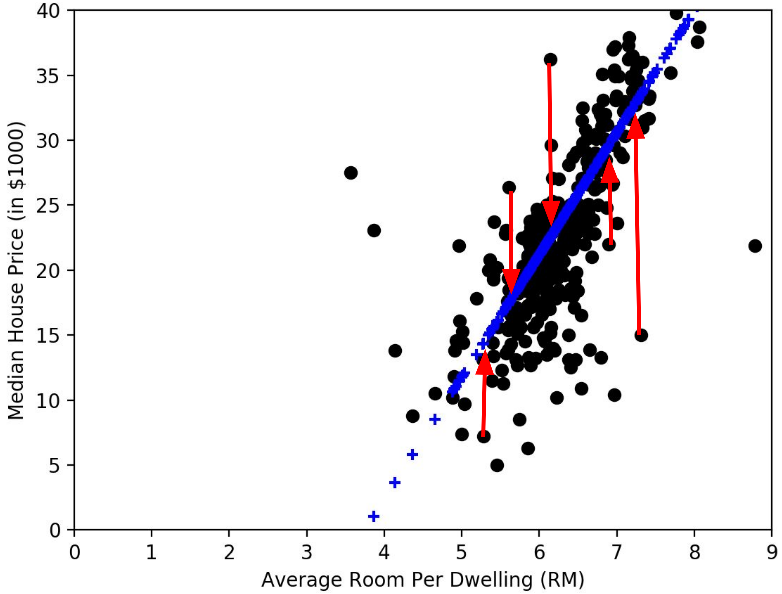


experience E	→	data
task T	→	reg.
performance P	→	res.^2
program L	→	relation

$$y = ax + b$$

$$\{a, b\} \leftarrow \min \left[\sum_{i=1}^{N} (y_i - (ax_i + b))^2 \right]$$

Does L learn?

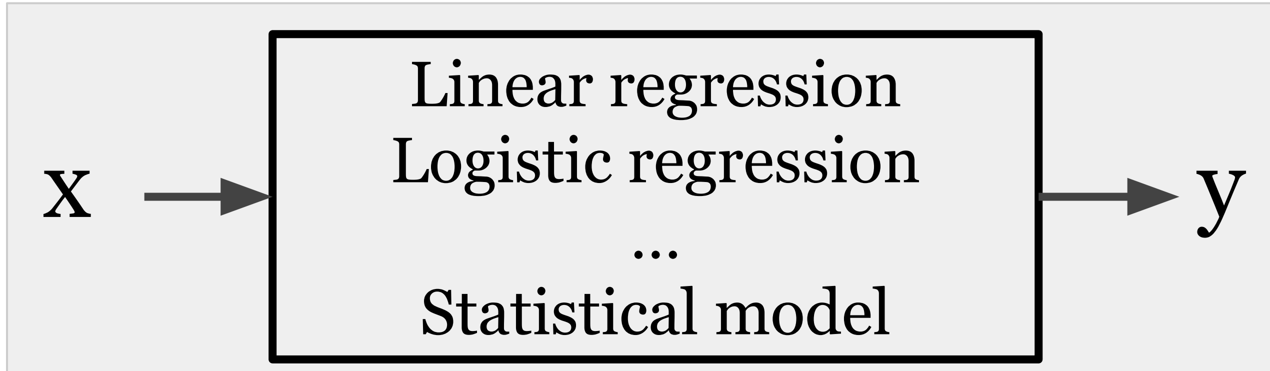
Harrison, D. and Rubinfeld, D.L. *'Hedonic prices and the demand for clean air'*, JEE & M, vol.5, 81-102, 1978

Hypothesis:

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

Hypothesis:

Data modeling:



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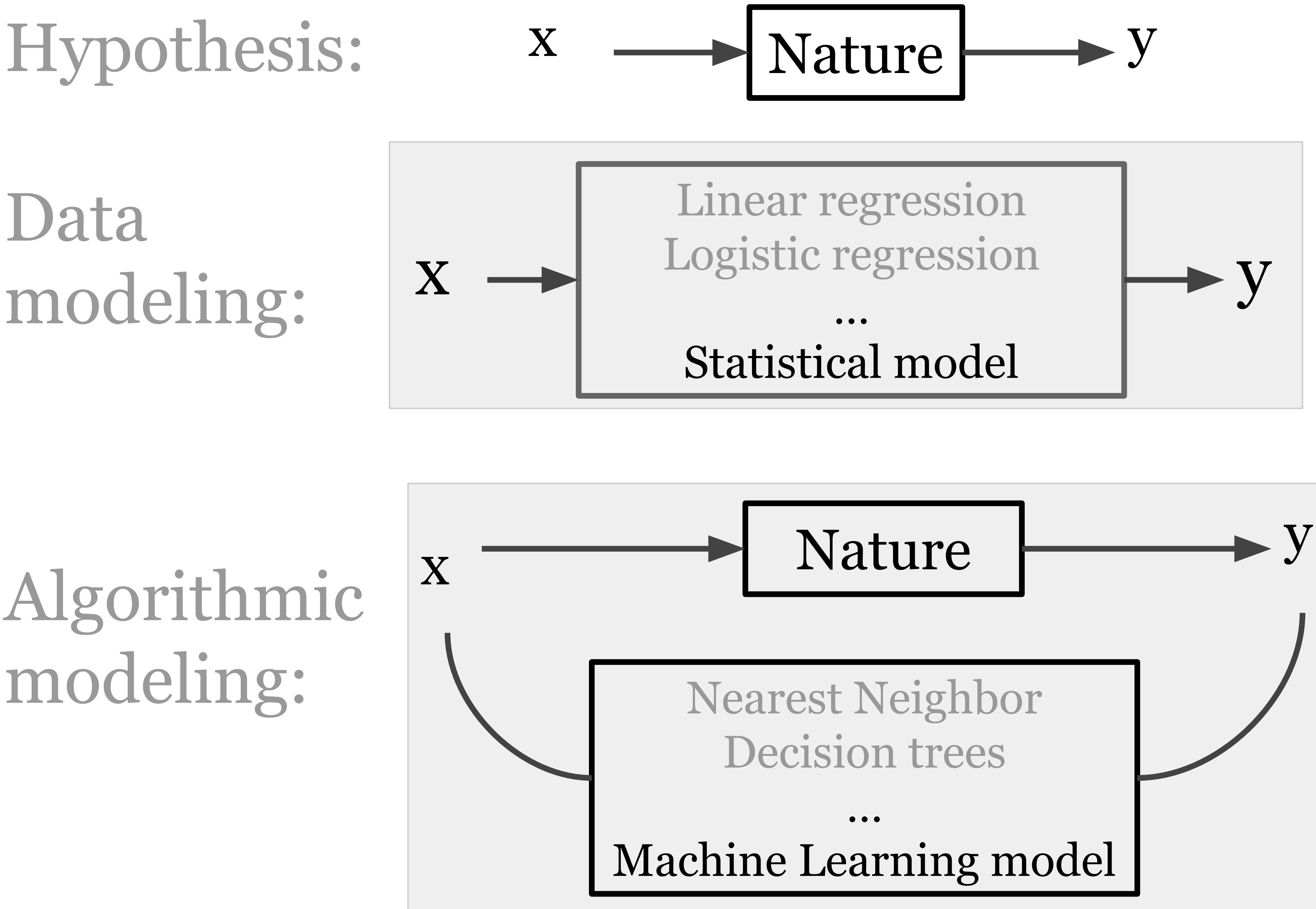

Breiman, L., *Statistical Modeling: The Two Cultures*, Stat. Sci, Volume 16 (2001)

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

Goal: *minimize L*

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

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Why should this work?

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Hypothesis

Data generation model:

$\mathrm{x}_\mathrm{i} \sim P_\chi$

f true labeling function, $y_i = f(x_i)$

$L_{data,f}(h) \equiv P_{x\sim data}(h_{train}(x) \neq f(x))$

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Supervised ML model

We will never have access to P and f

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Data generation model:

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

$\cancel{f}$ true labeling function, $y_i = f(\cancel{x_i})$

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Supervised ML model

We will never have access to P and f

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 $\leftarrow$ good approximation

Goal: *minimize L*

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

Supervised ML **model**

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Supervised ML **model**

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X	set of all examples, x
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Machine Learning algorithm

Hypothesis: Data dependent

Data generation model:

$x_i \sim P_X$

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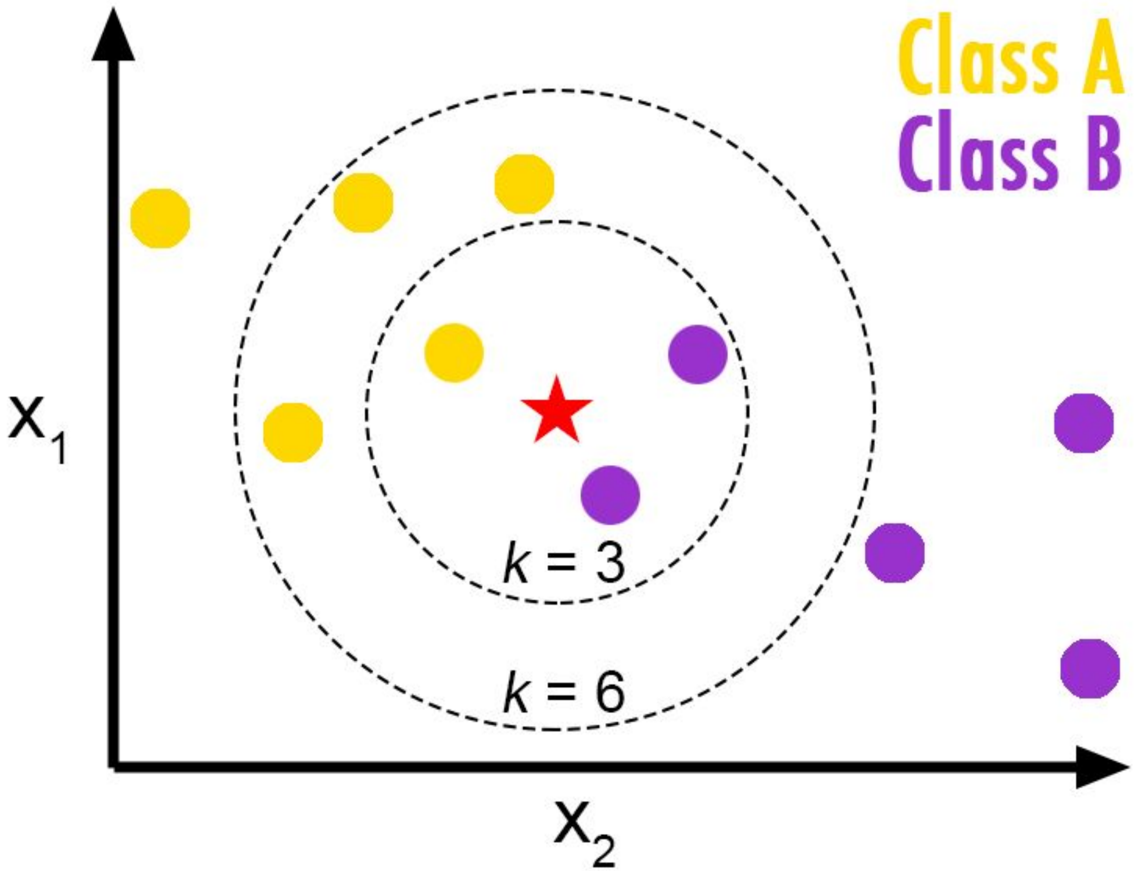
Example of supervised ML algorithm for classification

k-Nearest Neighbor (kNN)

Distance based

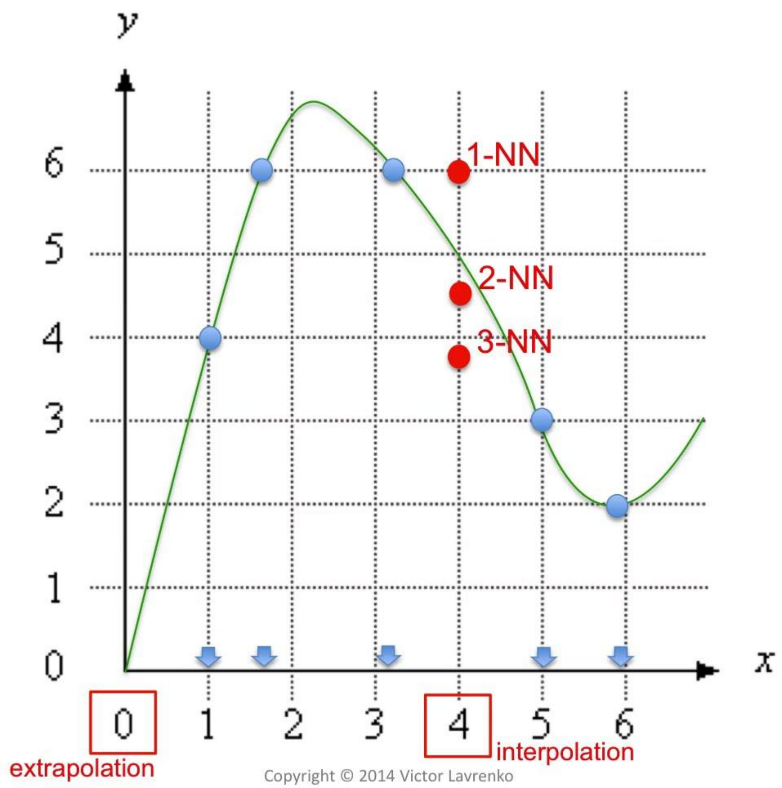


Example of supervised ML algorithm for regression

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

Support Vector Machines (SVM)

Search for hyperplanes

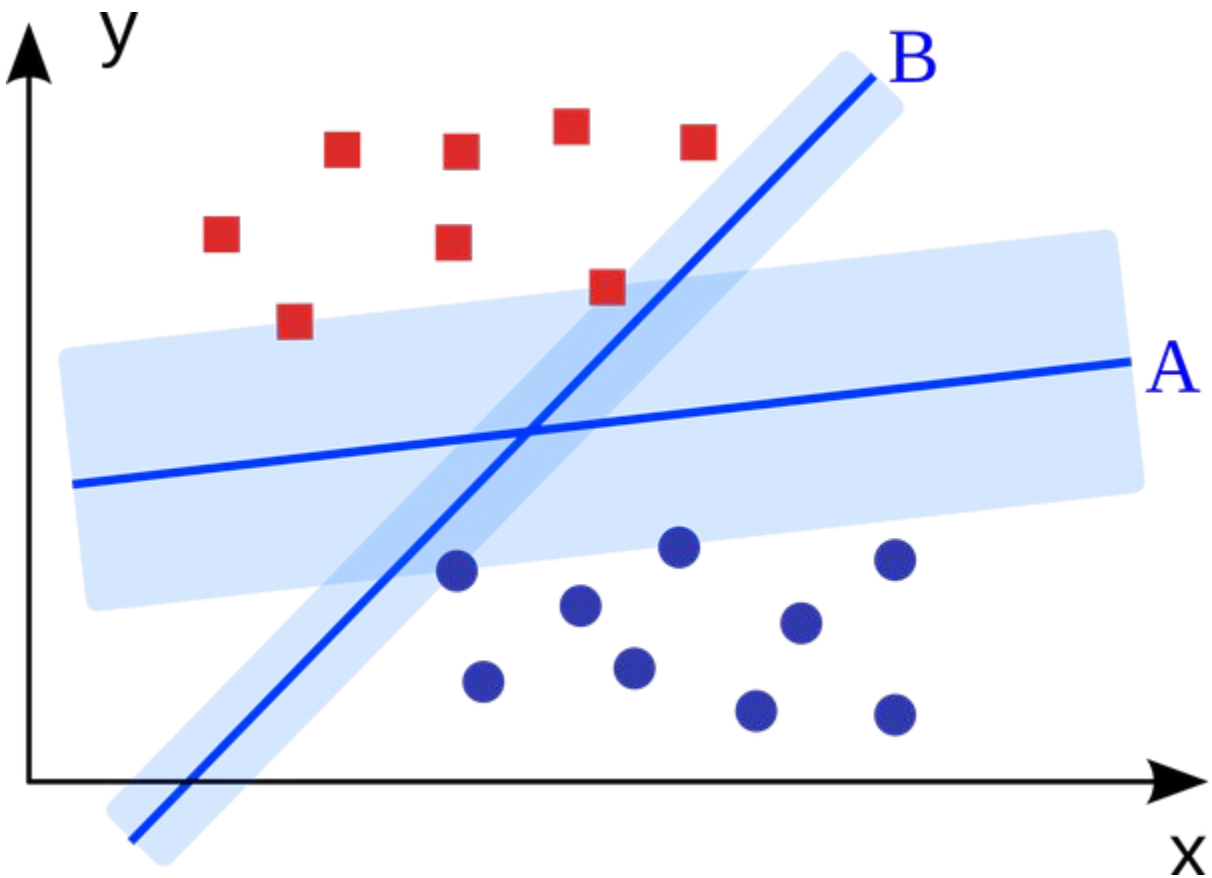
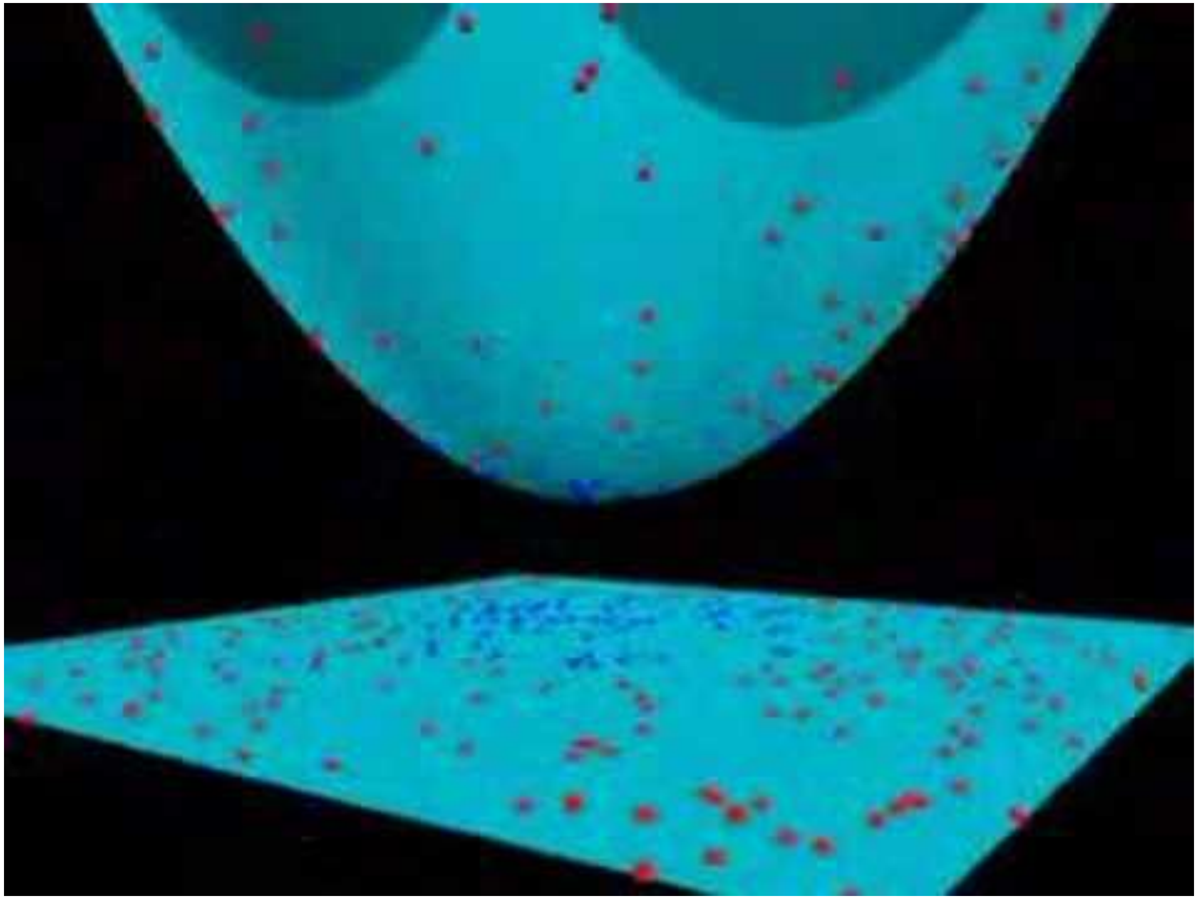


Image from: https://www.quora.com/What-is-a-Support-Vector-Machine

Example of supervised ML algorithm for classification

Support Vector Machines (SVM)

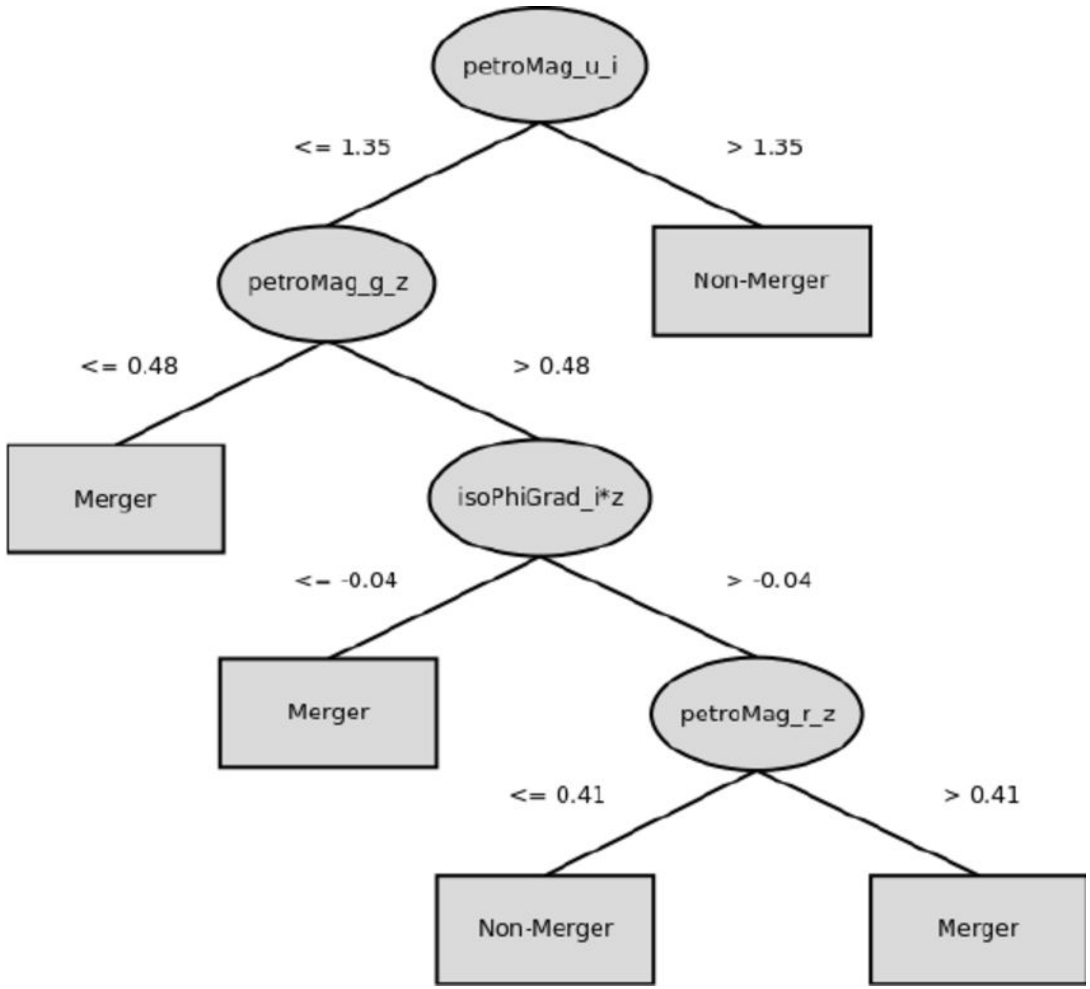
Search for hyperplanes - kernel trick



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

Example of supervised ML algorithm for classification

Decision Trees

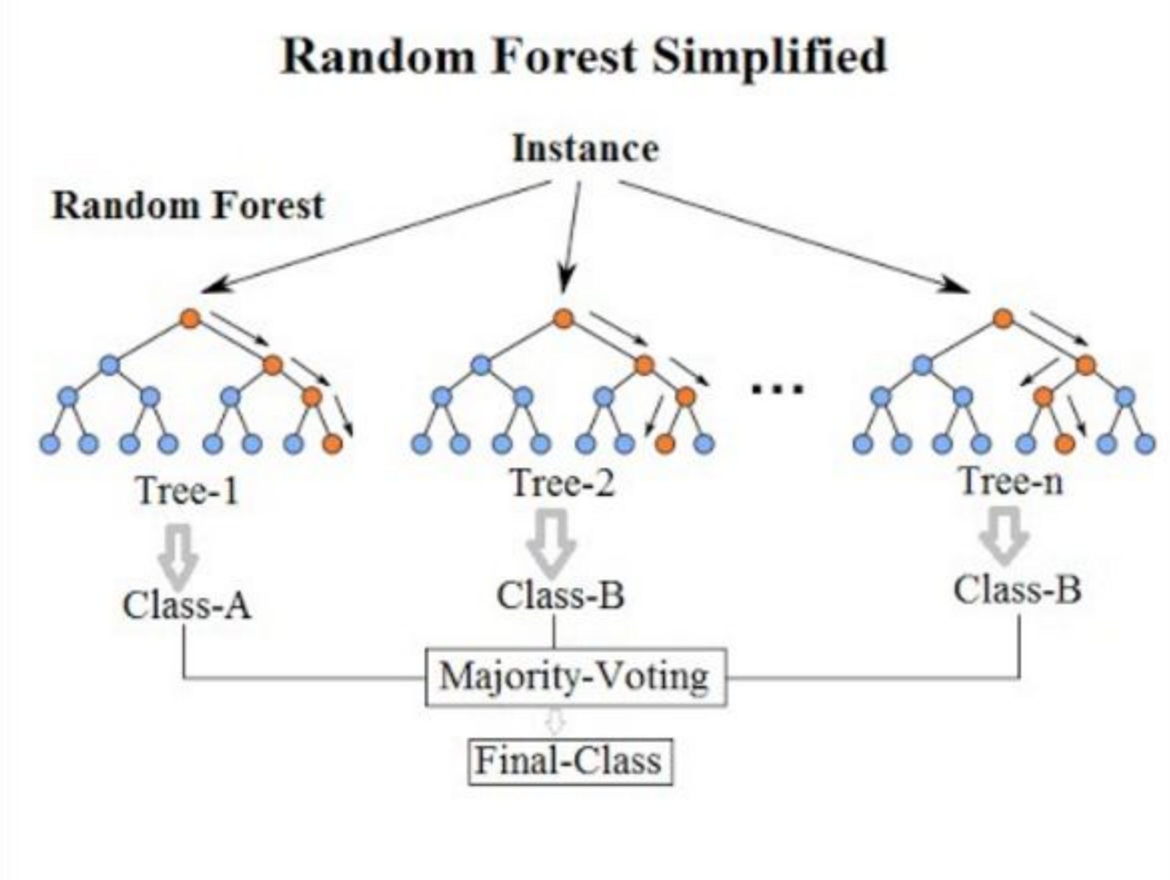


https://www.researchgate.net/figure/Visualization-of-decision-tree-built-using-the-weakest-mergers_fig4_221601336

Example of supervised ML algorithm for classification

Random Forests

Ensemble method

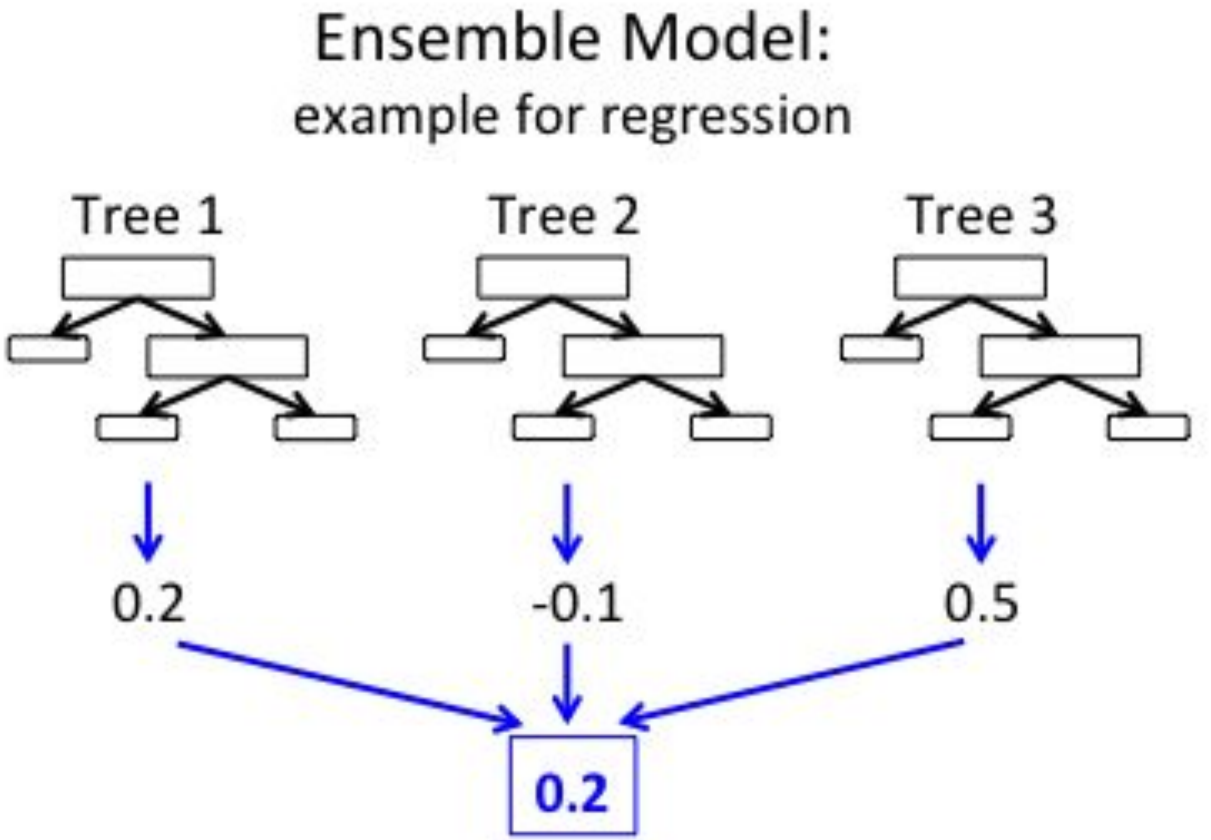


https://medium.com/@williamkoehrsen/random-forest-simple-explanation-377895a60d2d

Example of supervised ML algorithm for regression

Random Forests

Ensemble method

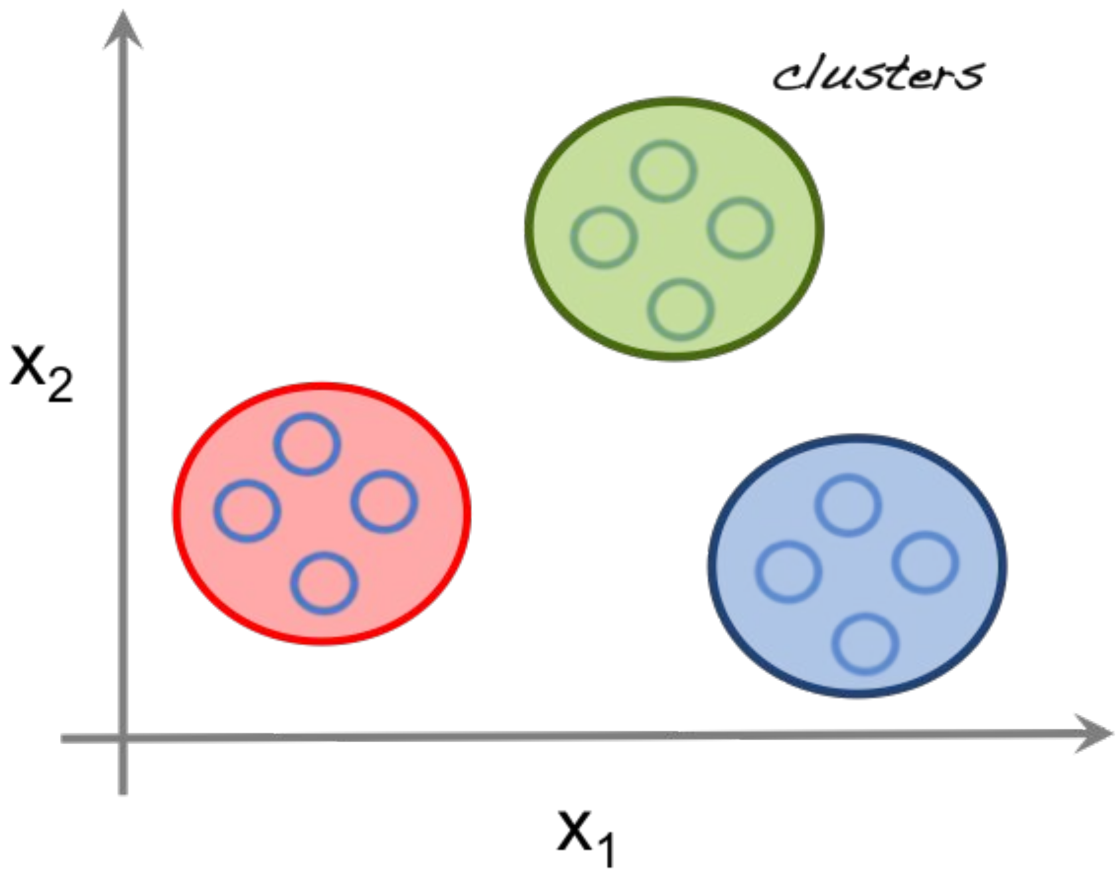


https://databricks.com/blog/2015/01/21/random-forests-and-boosting-in-mllib.html

Unsupervised Learning

Unsupervised Learning

Search for data structures



Unsupervised Learning

There is NO ground truth!

data	features
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~~Y~~	~~set of possible labels, y~~
$h_{\cancel{train}}$	learner: $y_{est;i} = h_{\cancel{train}}(x_i)$
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~~$L_{data,f}(h) = P_{x\sim data}(h_{train}(x) \neq f(x))$~~

Unsupervised Learning

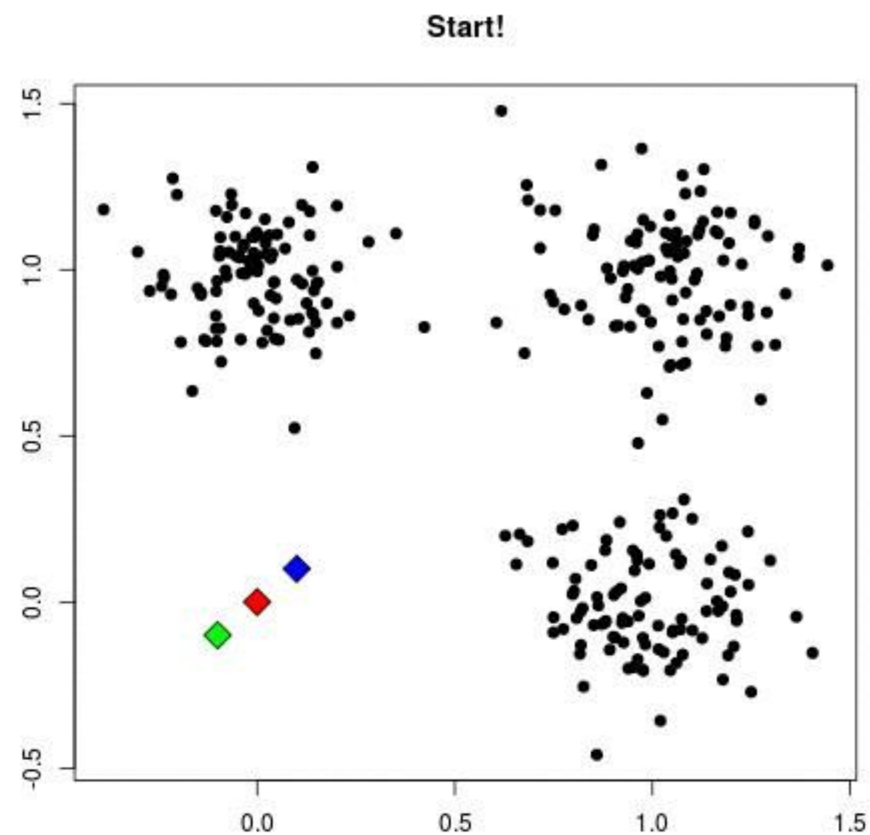
data	features
χ	set of all samples, x
h	learner: $y_{est;i} = h(x_i)$
$P(\chi)$	joint probability density

Goal: *characterize P*

Example of unsupervised ML algorithm

k-Means

Clustering



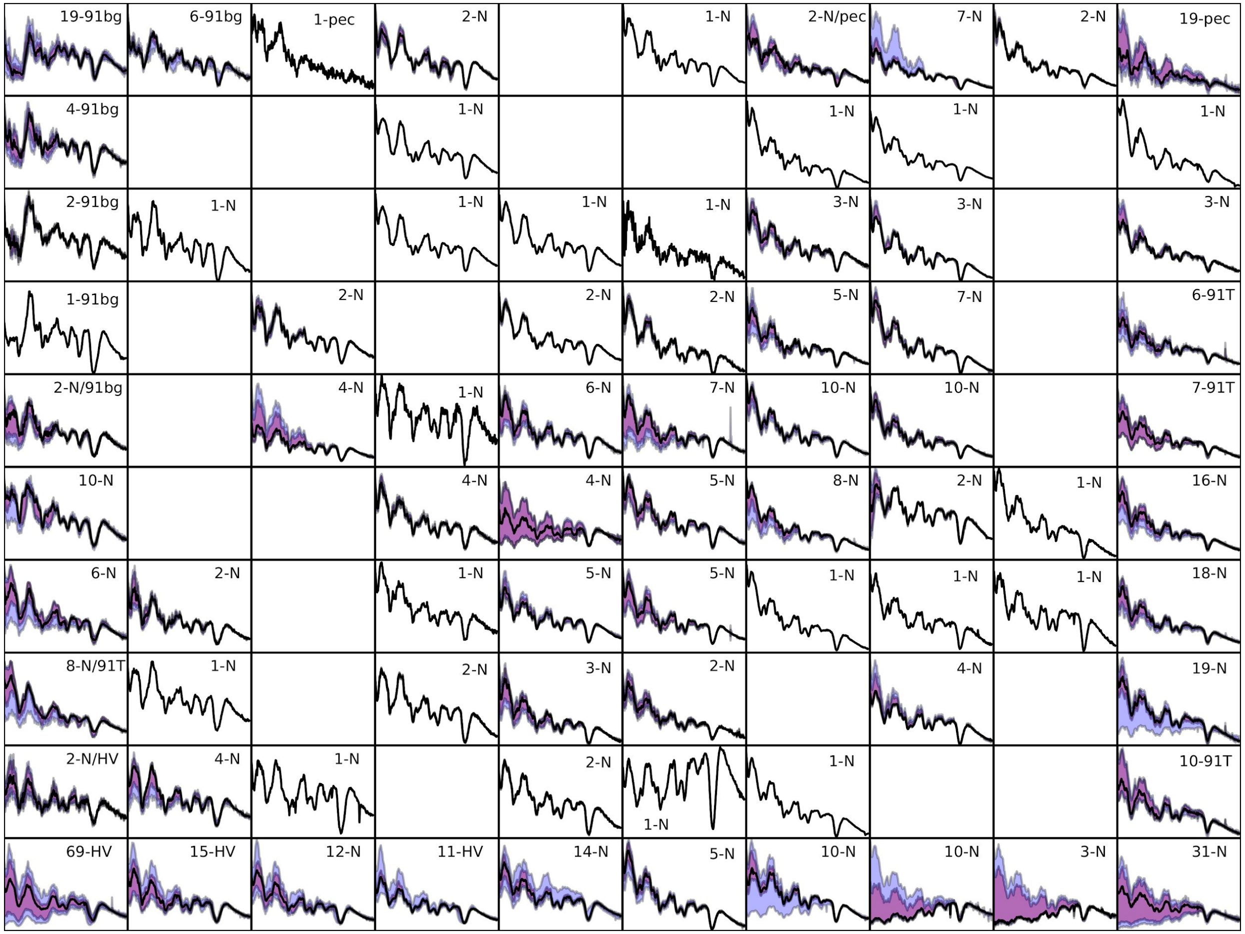
https://mubaris.com/2017/10/01/kmeans-clustering-in-python/

Example of unsupervised ML algorithm

Self-Organized Maps (SOM)

Clustering

Similar objects end up closer to each other



*Sasdelli, **Ishida** et al, 2016, MNRAS, 461, Issue 2, p.2044 - from CRP #2*

Example of unsupervised ML algorithm

Self-Organized Maps (SOM)

Clustering

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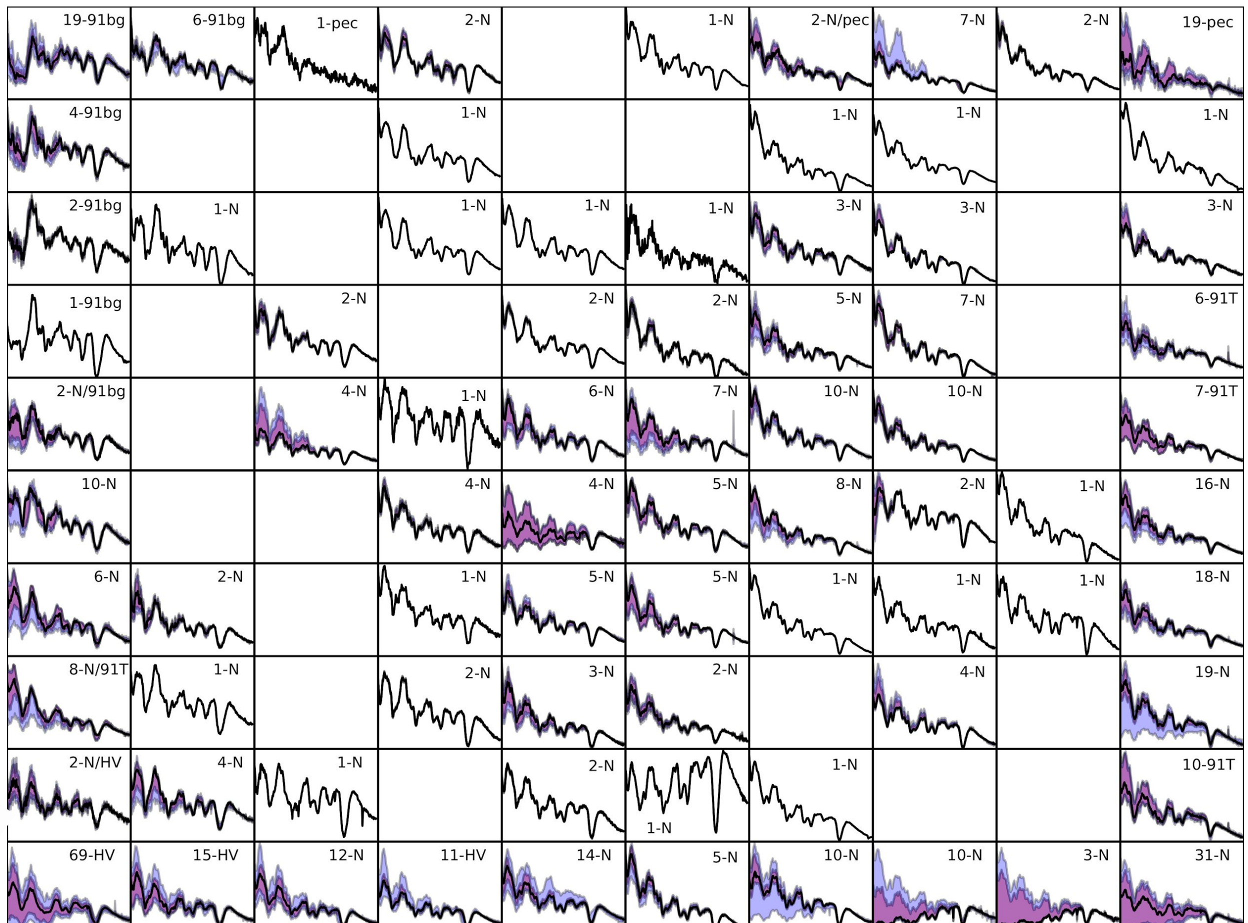


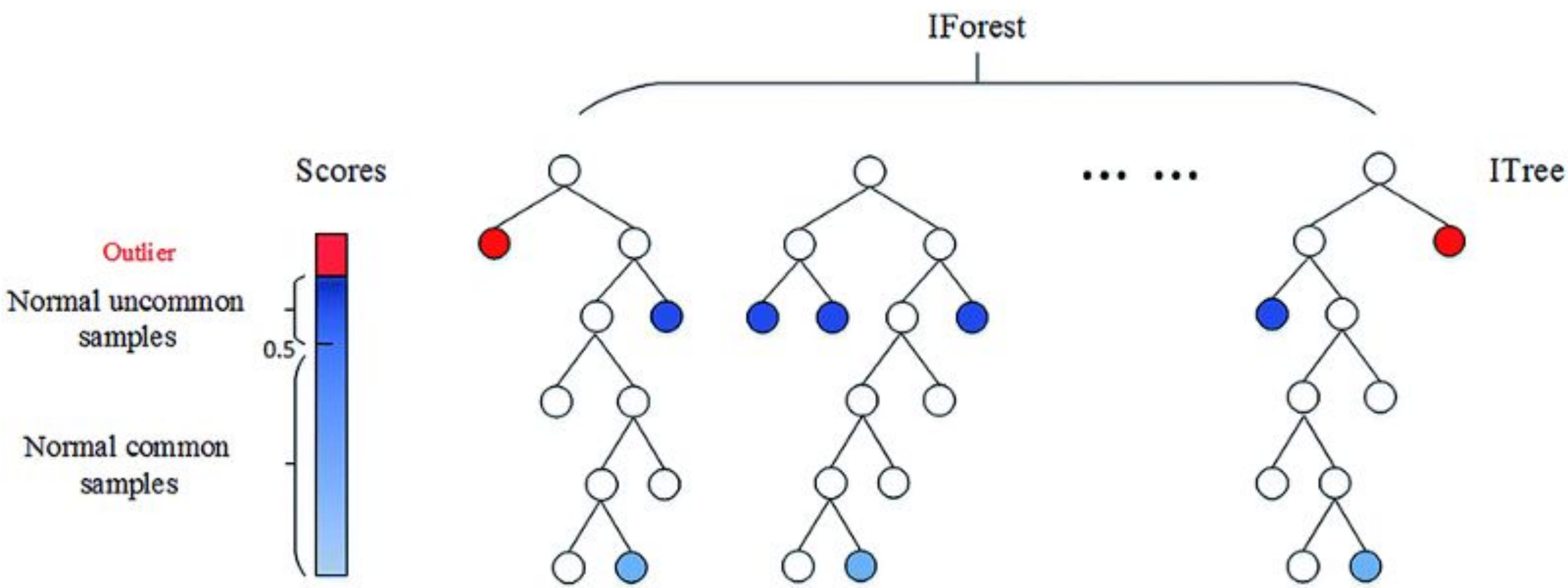
Are dimensionality reduction methods unsupervised learning?

Sasdelli, **Ishida** et al, 2016, MNRAS, 461, Issue 2, p.2044 - from CRP #2

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

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2. Supervised Machine Learning $\Longrightarrow$ Minimize loss function

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1. The definition of learning is different for machines

2. Supervised Machine Learning $\Longrightarrow$ Minimize loss function

3. Minimize loss function

$\Downarrow$

learn about the data generative model

Summary

What you should remember from this session

1. The definition of learning is different for machines

2. Supervised Machine Learning $\Longrightarrow$ Minimize loss function

3. Minimize loss function

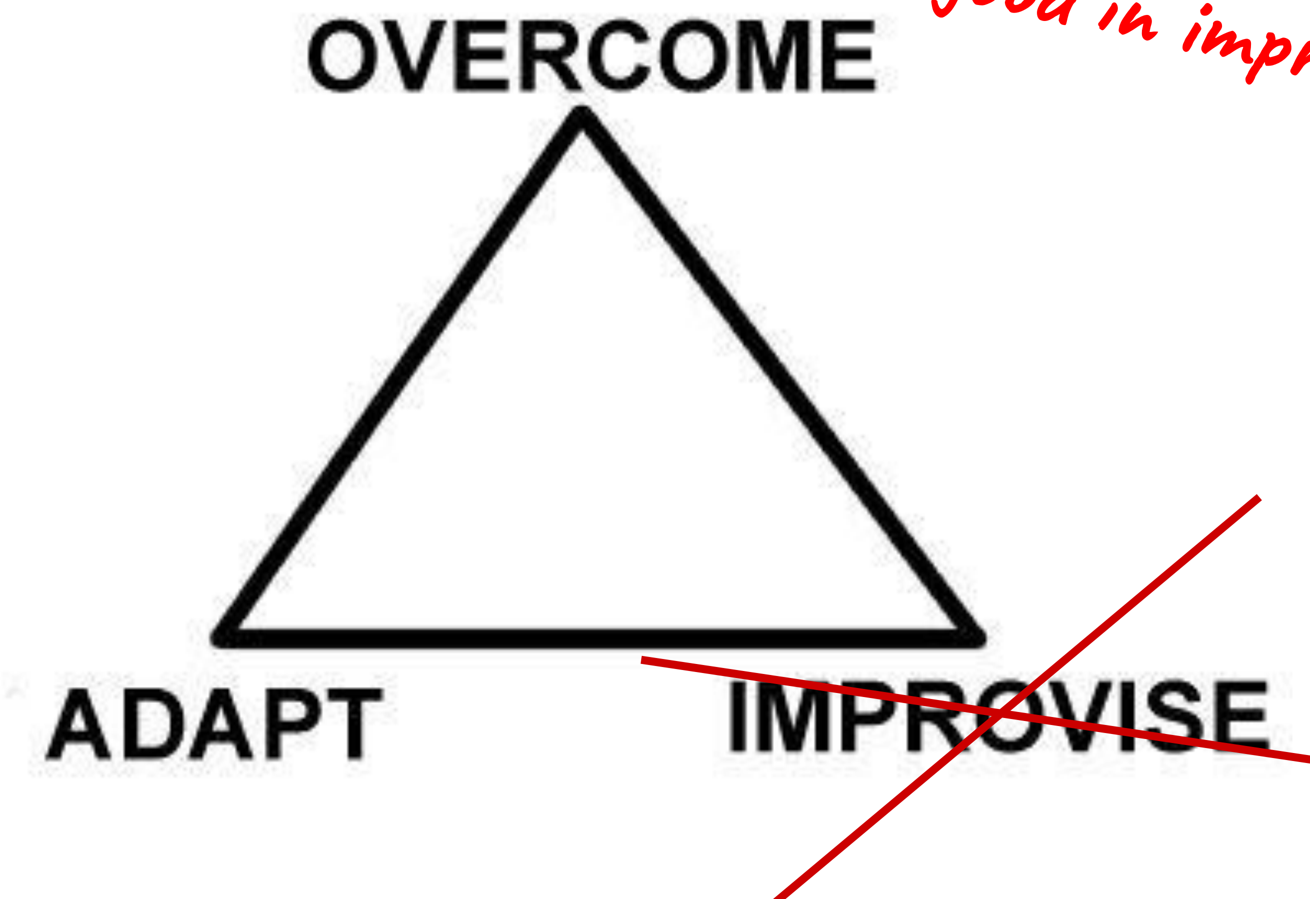
⇩

learn about the data generative model

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

Learning *or the Power to Adapt*

Machines are not good in improvising!




Thank
You