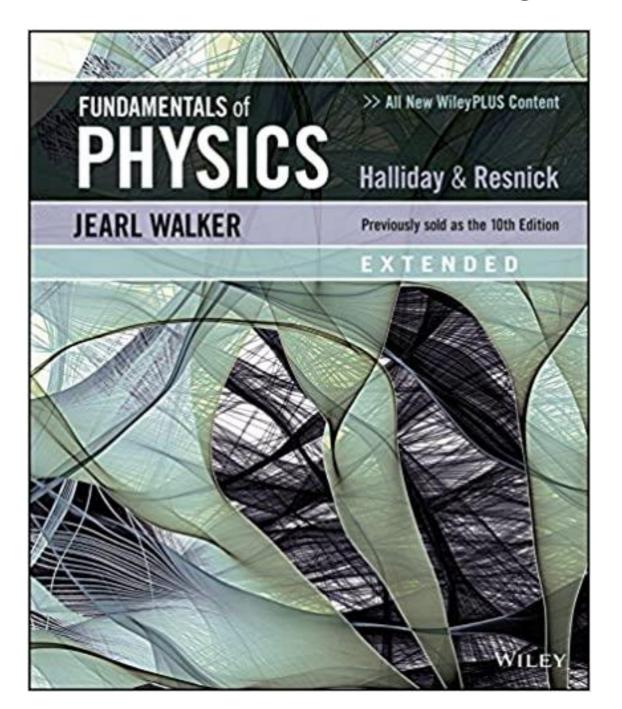
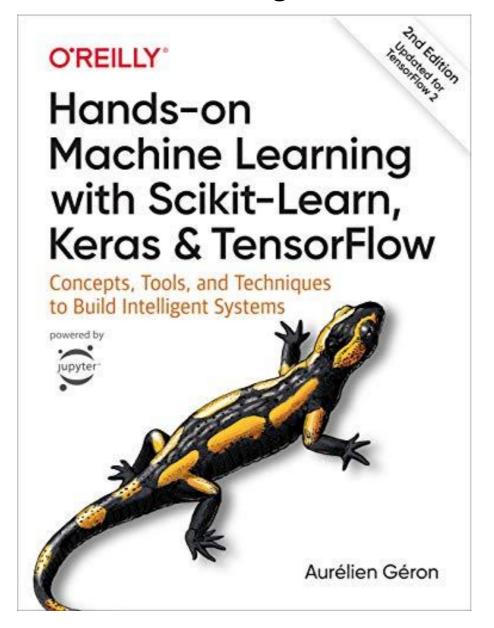
# Supervised Learning

**Unsupervised Learning** 

### Supervised learning



### Reading the book with the goal: Learning ML



Supervised learning

### Paying attention with the goal: Learning to paint





Paying attention with the goal: Producing gold

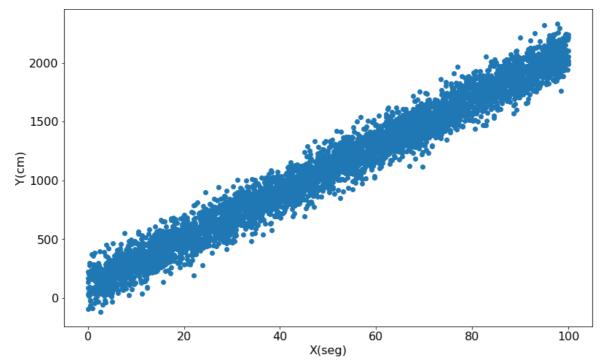
Supervised learning

# Supervised Learning

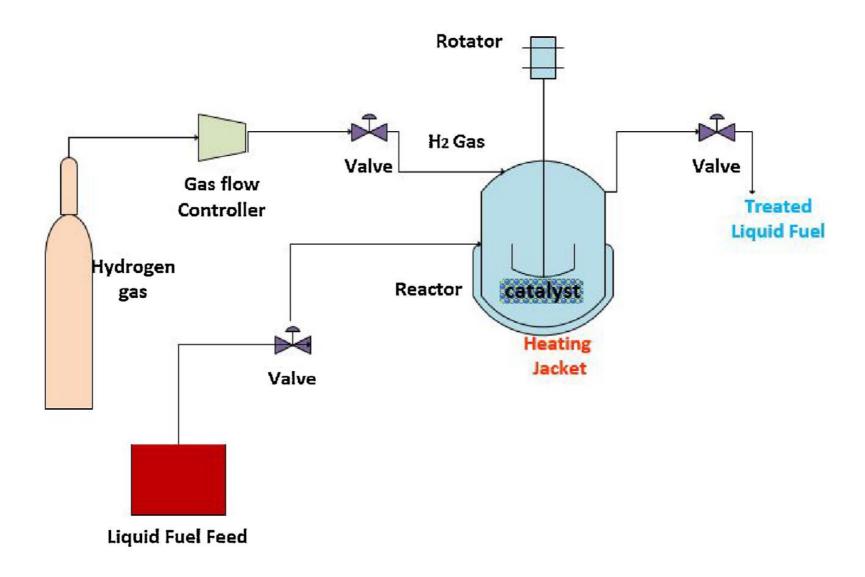
Phenomena under study: Objective distance







### Hidrodesulfuration



Temperature, Pressure, Hydrogen Flow rate, Inlet sulfur concentration, equipment operating days ...

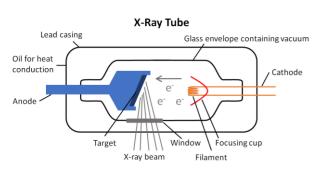
Output sulfur concentration

# Electromagnetic interaction \_\_\_\_\_ Energy



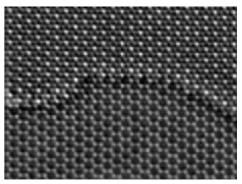






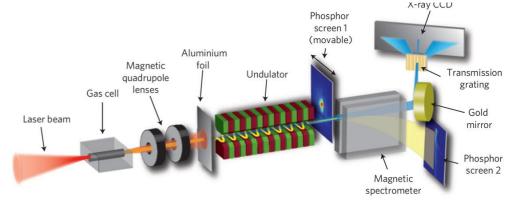










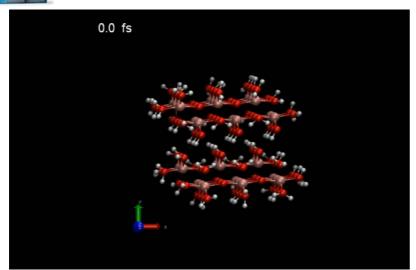


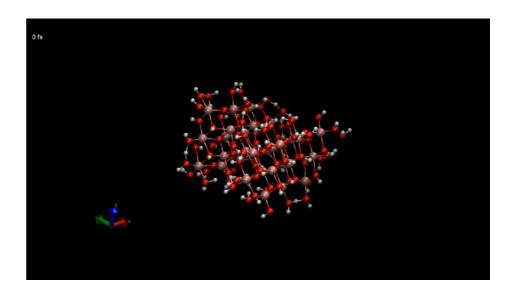


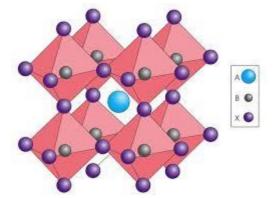
### Atomic distributions

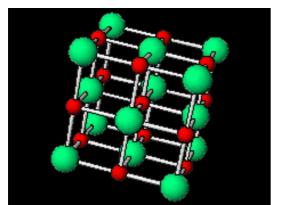


## Energy, Force





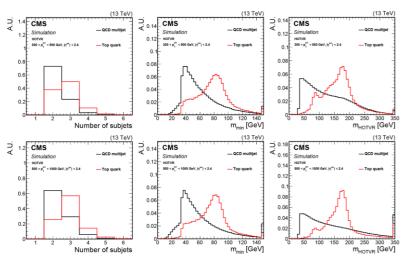






New compounds

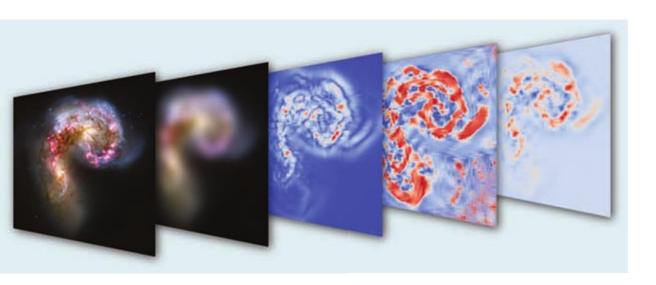
### High Energy Physics



**Figure 4.** Shape comparison of the main variables of the HOTVR algorithm for signal and background jets, in two different regions of the jet  $p_T$  as displayed in the plots.

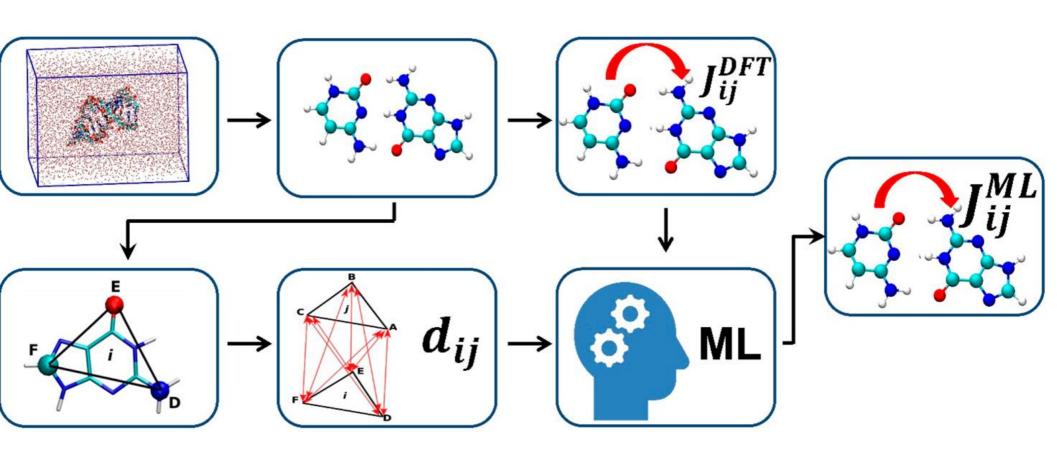
Detecting of heavy, energetic, Hadronically decaying particles

### Astronomy, Galaxies



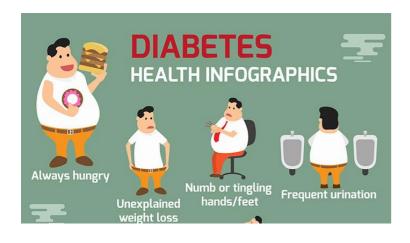
Galaxy inner structure

# Machine Learning Prediction of Electronic Coupling between the Guanine Bases of DNA



J. Phys. Chem. A 2020, 124, 7658-7664

#### Diabetes mortality

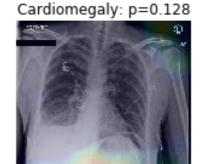


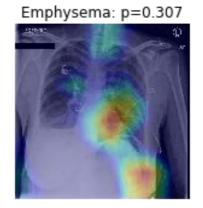
# Medical prognosis: Mortality after one year

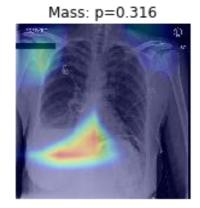
### Medical Diagnosis:

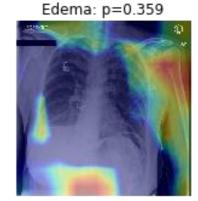
### **Pulmonary Diseases**

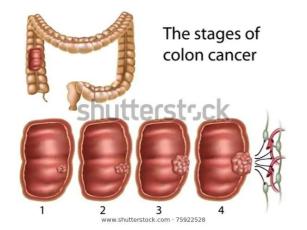
Original







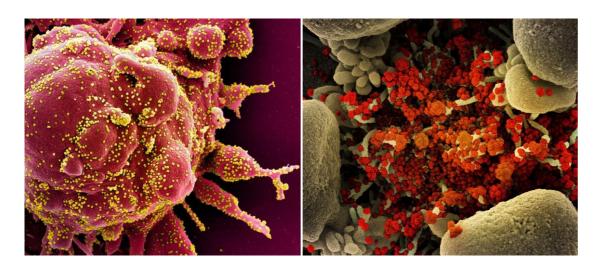




Medical treatment:

Effect of drugs combination

### Covid-19



Drug discovery and Vaccine development

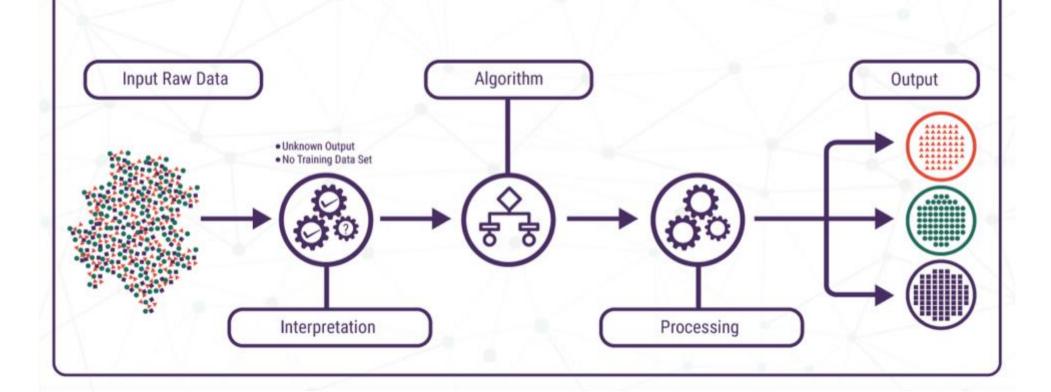
Automated extraction of chemical synthesis actions from experimental procedures

Nature communications, 11, 3601 (2020)

Thematic analysis of 18 years of physics education research conference proceedings using natural language processing

Phys. Rev. Phys. Education Research 16, 010142 (2020)

# UNSUPERVISED LEARNING

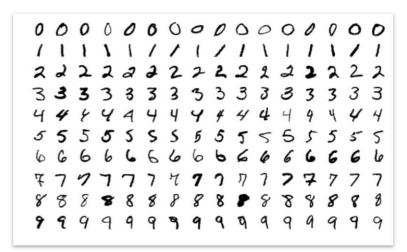




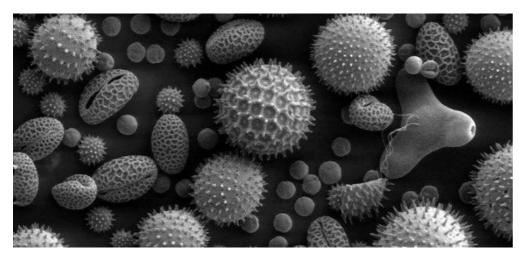


						25	15	9	2
1	2	7	8	7	0	3	S	0	8
4	5	8	0	2	3	2	9	7	7
3	Z	3	9		0		2	3	0
1	1	4	0	2	1	5	B	3	
8	6	ಳ	0	4	0	L	5	3	9
8	5				7	1	6	0	9
1	7	0	3			7		7	7
2	6	5	1	6	4	2	2	2	9
4	4	4	ર	0	6	9	4	8	3
- /	5	0	7	4	6	v	2	5	1

### Digits clustering





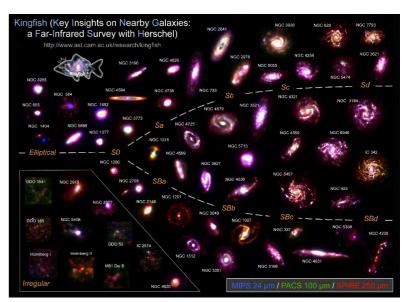


### Microstructure clustering





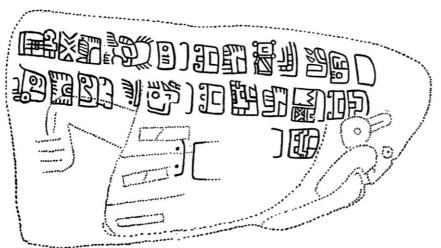














### K-means

### SOME METHODS FOR CLASSIFICATION AND ANALYSIS OF MULTIVARIATE OBSERVATIONS

**J.M<sub>AC</sub>QUEEN** (1987)

The main purpose of this paper is to describe a process for partitioning an N dimensional population into k sets on the basis of a sample. The process, which is called 'k-means,' appears to give partitions which are reasonably efficient in the sense of within-class variance.

#### The way kmeans algorithm works is as follows:

Specify number of clusters K.

Initialize centroids by first shuffling the dataset and then randomly selecting K data points for the centroids without replacement.

Keep iterating until there is no change to the centroids. i.e assignment of data points to clusters isn't changing.

Compute the sum of the squared distance between data points and all centroid s.

Assign each data point to the closest cluster (centroid).

Compute the centroids for the clusters by taking the average of the all data points that belong to each cluster.

The used metric to detect the clusters is:

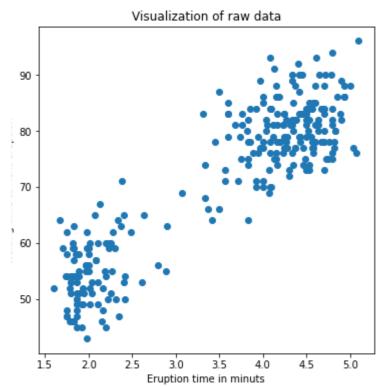
$$J = \sum_{i=1}^{m} \sum_{k=1}^{K} w_{ik} ||x^{i} - \mu_{k}||^{2}$$

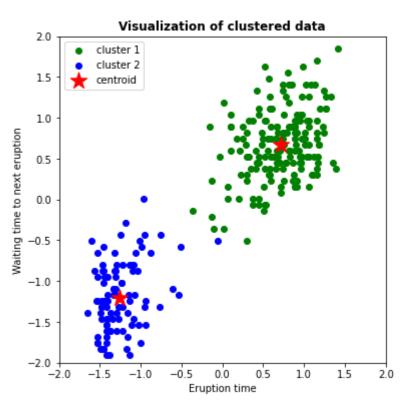
where  $w_{ik}$  = 1 for data point  $x_i$  if it belongs to cluster k; otherwise,  $w_{ik}$ =0. Also,  $\mu_k$  is the centroid of  $x_i$ 's cluster.



### **Geyser's Eruptions**

	eruptions	waiting
0	3.600	79
1	1.800	54
2	3.333	74
3	2.283	62
4	4.533	85







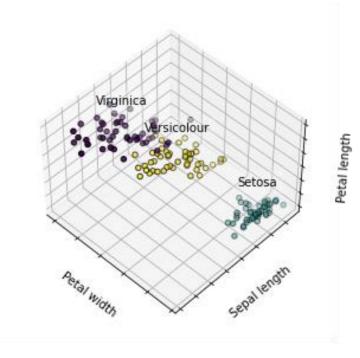
[[5.1 3.5 1.4 0.2]

[4.9 3. 1.4 0.2]

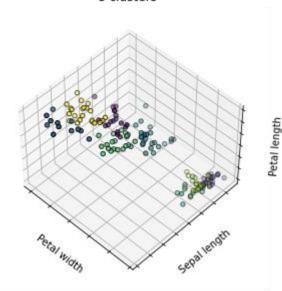
[4.7 3.2 1.3 0.2]

[4.6 3.1 1.5 0.2]

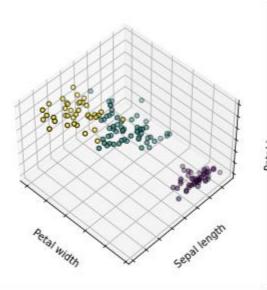
[5. 3.6 1.4 0.2]]



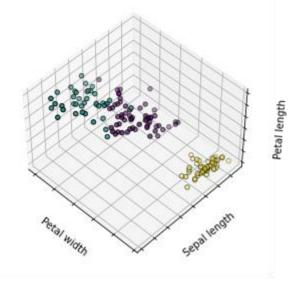
8 clusters



3 clusters

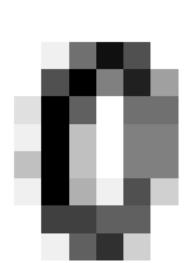


3 clusters, bad initialization



### Digits clustering

0.096	2	4.0000000000000000000000000000000000000				M.C.	S	1251015	8
4	57	8	0	2	3	2	9	7	7
3	B	3	9	5	0	3	2	3	0
1	1	4	0	2	1	5	S	3	6
8	6	४	0	4	0	4	5	3	9
8	5	4	2	2	7	1	6	0	9
1	チ					7			7
2	6	7	7	6	4	2	2	2	9
4	4	4	ર	0	6	9	4		
1	5	0	3	4	6	8	2	5	1



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