Introduction to machine learning & Chemistry, or how I learned to be trendy

Clabaut Paul, Jiang Tao, Staub Ruben

ENS de Lyon

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Overview

1. Theory & Generalities
   - General principle of machine learning
   - Classification of machine learning
2. Application
   - Usages in chemistry
   - Limitations

Theory & Generalities

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What is machine learning ?

“A computer program 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.”

-Tom M. Mitchell

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What is machine learning ?

“Machine learning is glorified statistics”

“Machine learning is for Computer Science majors who couldn’t pass a Statistics course.”

“Machine learning is Statistics minus any checking of models and assumptions.”

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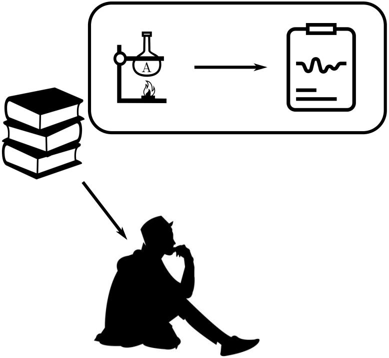
What is machine learning ?



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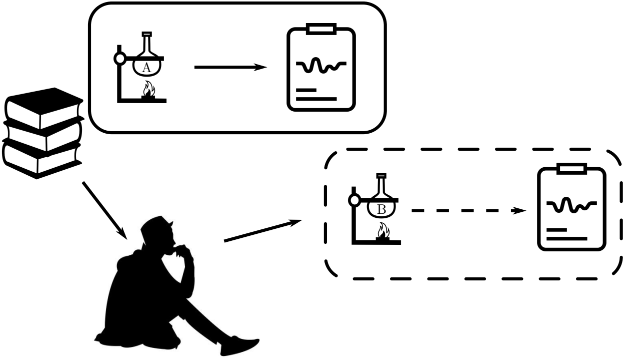

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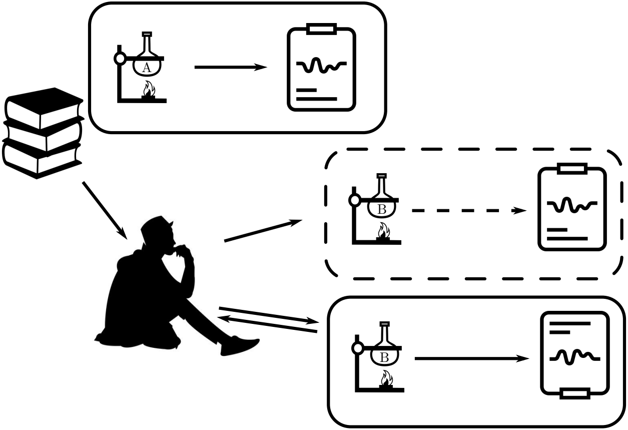

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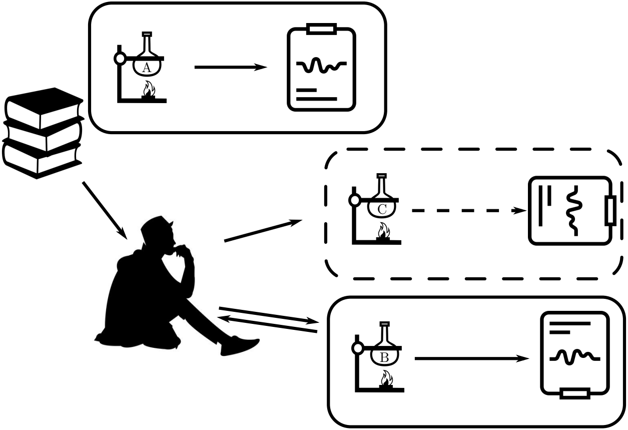

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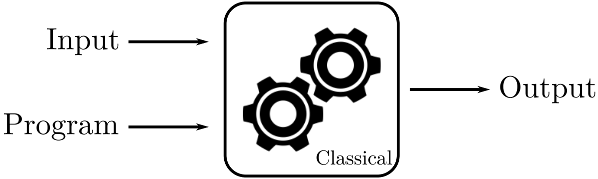

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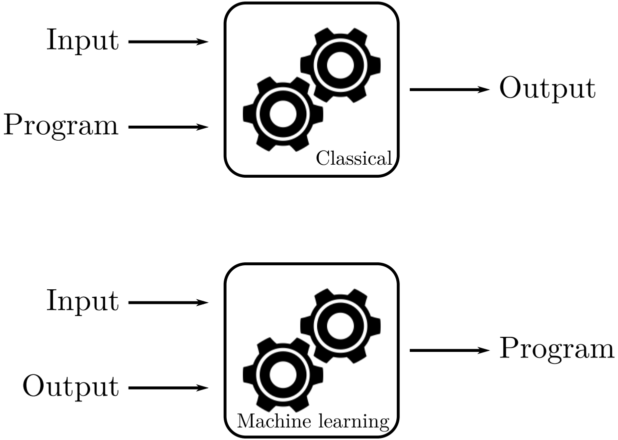

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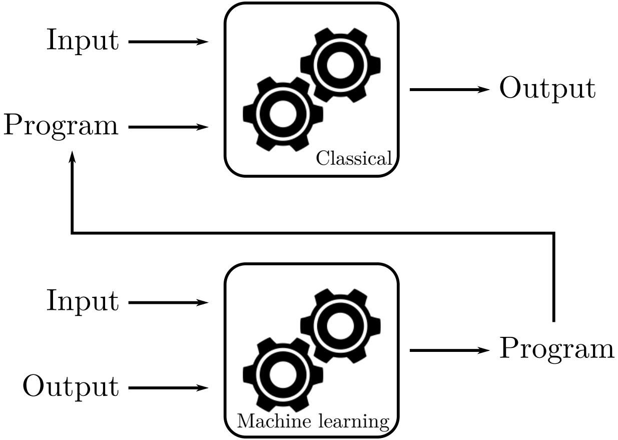

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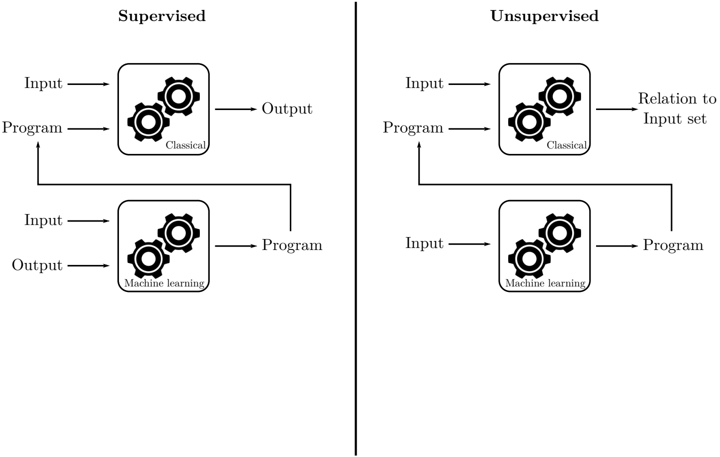
Supervised VS. Unsupervised



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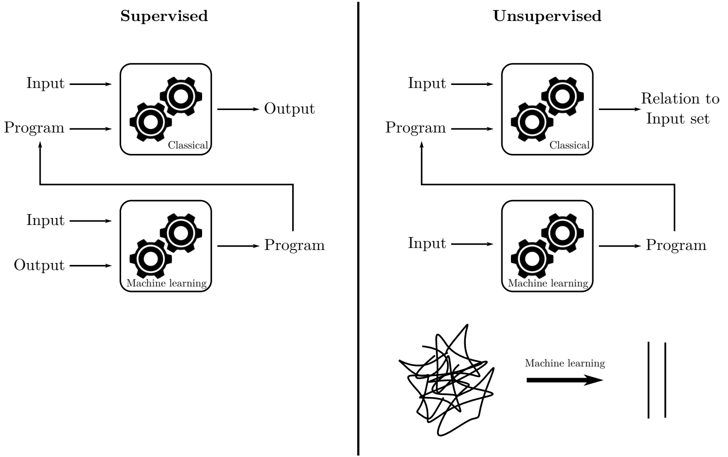

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Families of Supervised learning

Aim: finding a function (program) mapping features (input) to a target (output)

Linguistic distinction based on target type:

- Continuous target ⇒ **Regression** (e.g. E_{ads})
- Categorical target ⇒ **Classification** (e.g. active or not, cat or dog?)

Choose type of mapping function

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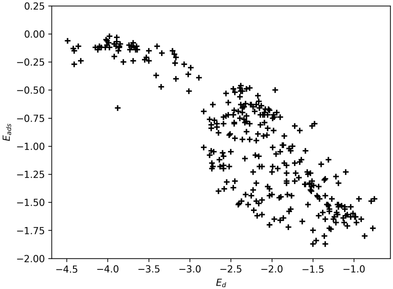
We all have done it a little before



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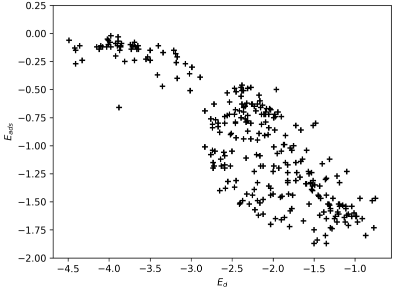

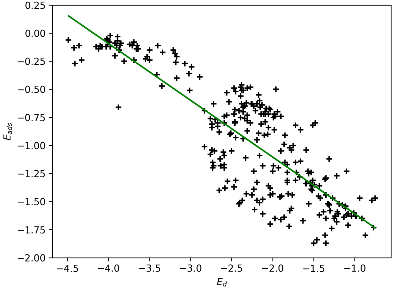

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Linear model (regression)

Input: m features, 1 target

$$
\begin{array}{cccc}
 & \text{Features} & & \text{Target} \\
 & (x_1\ x_2\ \cdots\ x_m) & \rightarrow & y \\
\hline
 & (x_{11}\ x_{12}\ \cdots\ x_{1m}) & \rightarrow & y_1 \\
\text{Training set} & (x_{21}\ x_{22}\ \cdots\ x_{2m}) & \rightarrow & y_2 \\
 & \vdots & & \\
 & (x_{n1}\ x_{n2}\ \cdots\ x_{nm}) & \rightarrow & y_n
\end{array}
$$

Model: m parameters $w_1, w_2, \ldots, w_m$

$$\sum_i^m w_i x_i \approx y$$

Pros: easily to understand

Cons: restricted to linear relations

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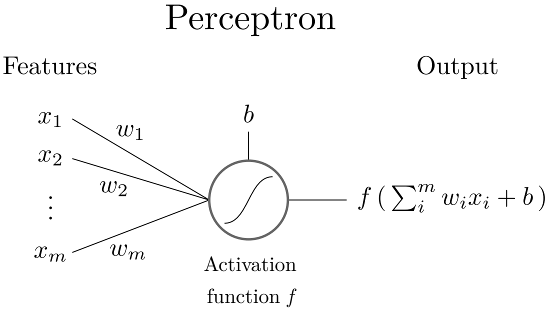
Neural network (regression)

Simplest neural network



Parameters: $w_1, w_2, \ldots, w_m, b$

Equivalent to linear model if we use $f : x \mapsto x$

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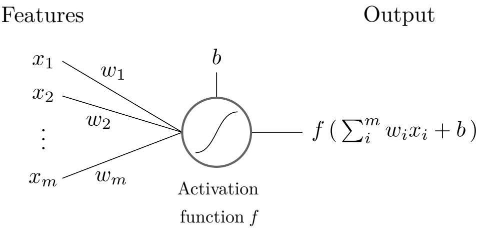
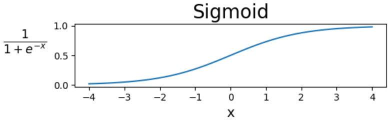
Neural network (regression)

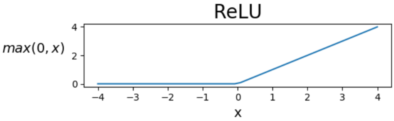
Simplest neural network

Perceptron



Common activation functions:





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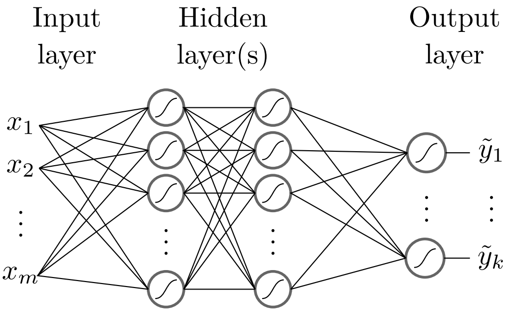
Neural network (regression)

Input: *m* features, *k* targets



Parameters: weights + bias of each neuron

Pros: fast to train, fast to predict, good fitting properties, trendy

Cons: black box, design tuning

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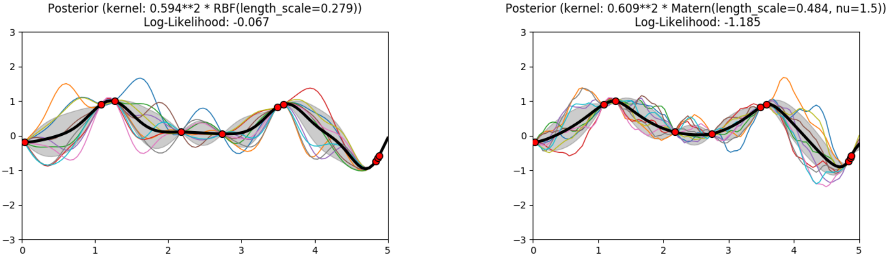
Gaussian process regression (regression)

Assume fitted target is a Gaussian process with given smoothness, use Bayesian inference to estimate probability distribution for prediction



Intuition: consider all possible fitted targets and extract probability distribution

Pros: native prediction confidence estimator

Cons: kernel-dependant, computationally costly training

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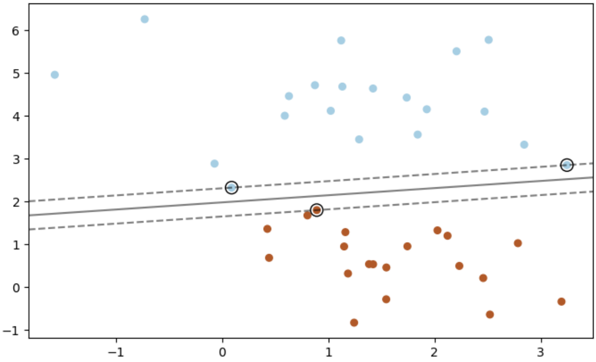
Support Vector Machine (classification)

Input: m features, 1 categorical target



Intuition: Find best splitting hyperplane

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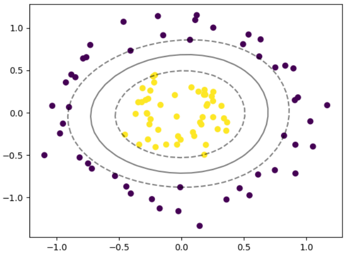
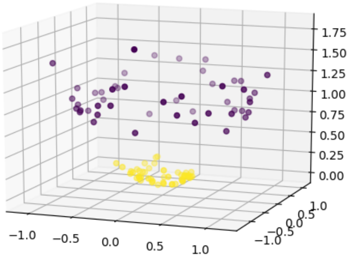
Support Vector Machine (classification)

Change the metric through a non-linear kernel → embedding into higher-dimensional space where separation could be possible.





Pros: adapted for high-dimensionality

Cons: kernel-dependant, computationally costly training

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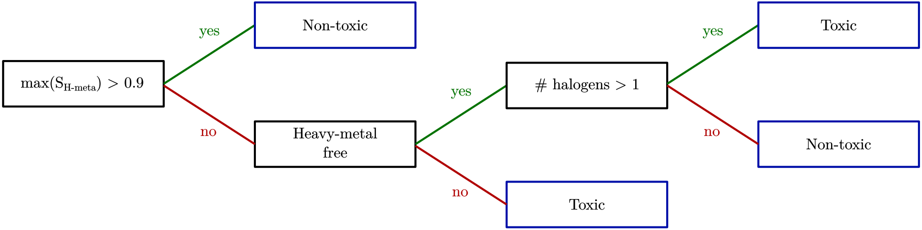
Decision tree (classification)

Input: *m* features, 1 categorical/continuous target



Intuition: Find best (feature+threshold) splitting on each node
Pros: easy interpretation (relevant features, ...), very fast prediction
Cons: requires balanced classes, optimal solution is NP-hard

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Decision tree (classification)

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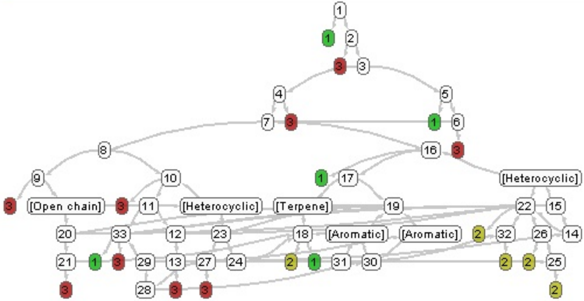

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Families of Unsupervised learning

Aim: Without consulting the target/output (sometimes absent), finding the structure in the input data itself.

Useful in certain cases:

* No prior knowledge of how many/what classes is the data divided into.

* Find out the most important features of the input data before feeding it to a machine.

Typical methods:

Clustering: k-means clustering, hierarchical clustering

Dimensionality reduction: PCA, Autoencoder

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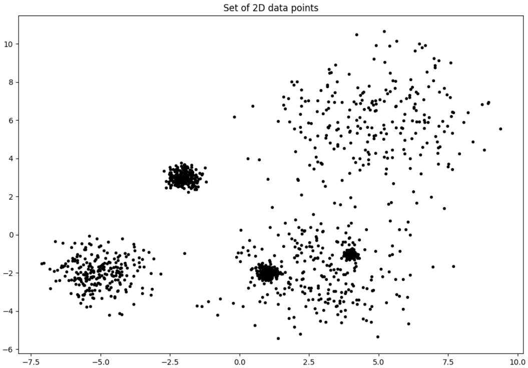
Clustering illustration

Clustering is partitioning into groups of close points
Non trivial task: How many clusters do you identify?



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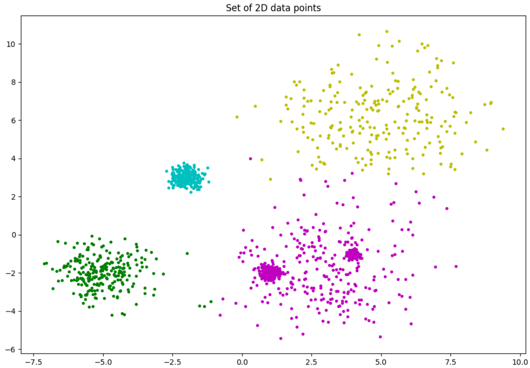

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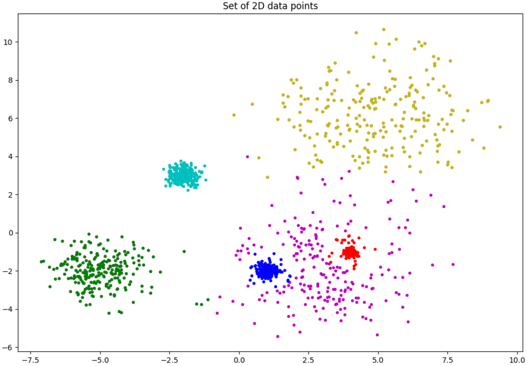

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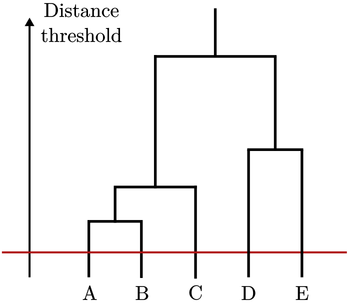
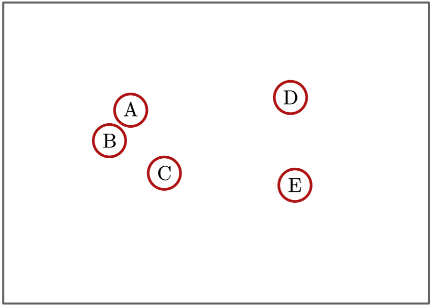
Hierarchical clustering (clustering)

Input: metric between clusters, data points

Explore clusters generated for every threshold, produce dendrogram





Pros: easy to interpret, good overview

Cons: need user-defined metric between clusters, threshold selection

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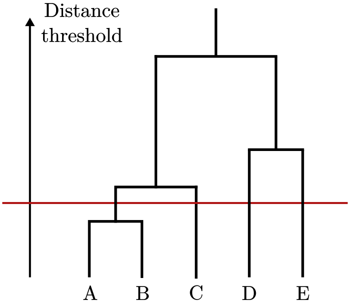

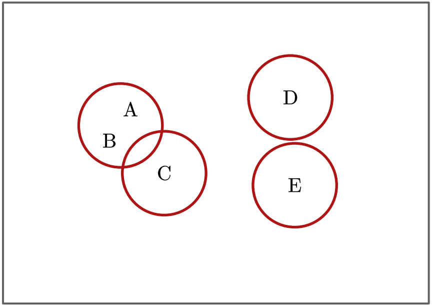

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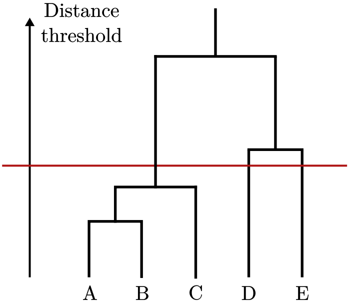

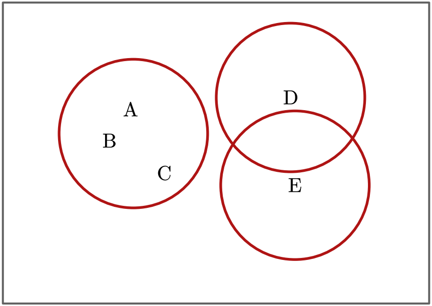

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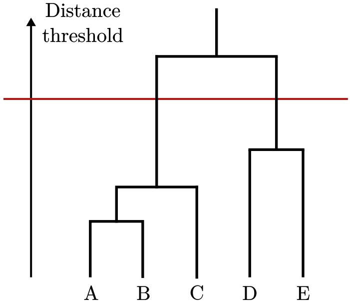

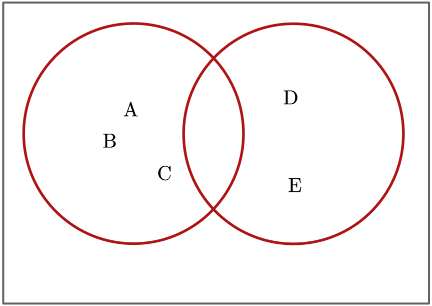

Pros: easy to interpret, good overview

Cons: need user-defined metric between clusters, threshold selection

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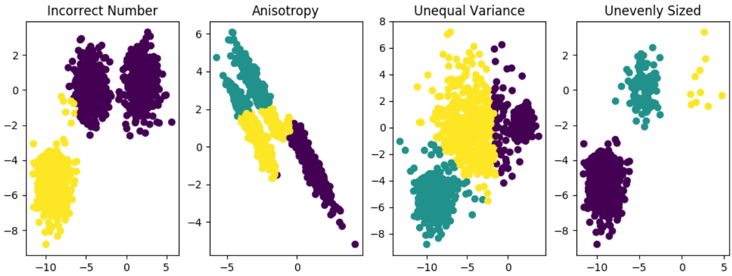
K-means clustering (clustering)

Input: number of clusters, distance between data points

Find centroids that minimize the within-cluster sum-of-squares



Pros: easy to understand

Cons: stochastic, assume convex and isotropic, poor high-dimensionality support

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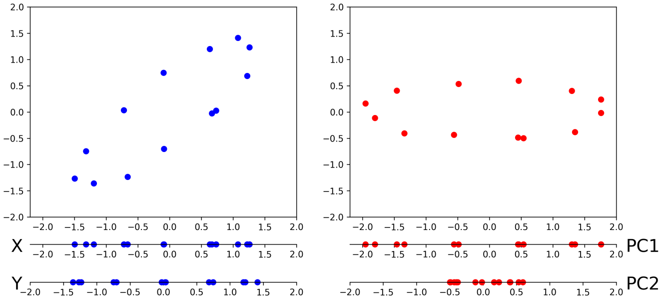
PCA (dimensionality reduction)



Emphasize variation and bring out strong patterns in a dataset.

Useful for finding important features in high dimensional dataset.

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PCA (Wine chemistry)

Feature No.	Composition
1	Alcohol
2	Malic acid
3	Ash
4	Alcalinity of ash
5	Magnesium
6	Total phenols
7	Flavanoids
8	Nonavanoid phenols
9	Proanthocyanins
10	Color intensity
11	Hue
12	OD280/OD315
13	Proline

Class	Number of wines
1	59
2	71
3	48

https://archive.ics.uci.edu/ml/datasets/Wine, Accessed: 2019-11-29

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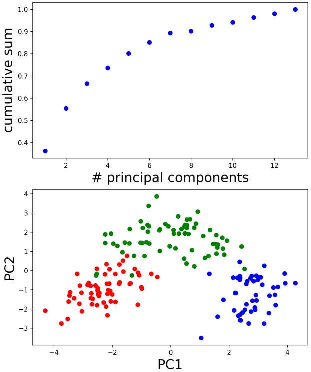

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Manifold (dimensionality reduction)

Non-linear dimensionality reduction:

- Kernel PCA (use kernel instead of covariance)
- MDS (preserve distances)
- Isomap (preserve geodesic graph-based distances)
- Self-organizing maps (preserve topology)
- ...

Application

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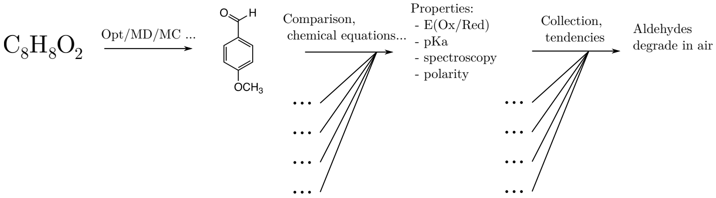
Categories of applications in chemistry

Substitute to computation algorithm, Direct property prediction, Data analysis



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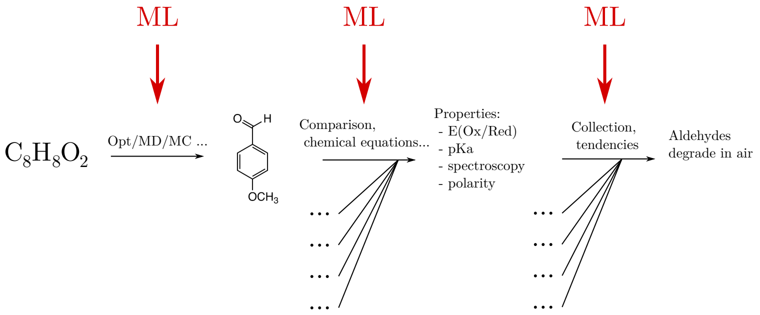

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Application: Water/Platinum potential: Goal

DFT

500 ps of 20$\AA$ thick water layer on 3*3*4 Pt (111) slab
$\rightarrow$ 8 yrs on 100 processors

MM

$$E = E_{slab} + \sum_{wat}(E_{wat} + E_{slab/wat}) + \sum_{wat}\sum_{wat}(E_{wat/wat} + E_{slab/wat/wat}) + \sum_{wat}\sum_{wat}\sum_{wat}(\ldots) + \ldots$$

Neural Network

$$E = \sum_{atoms} E_{NN}(environement) \rightarrow \text{Might just work !}$$

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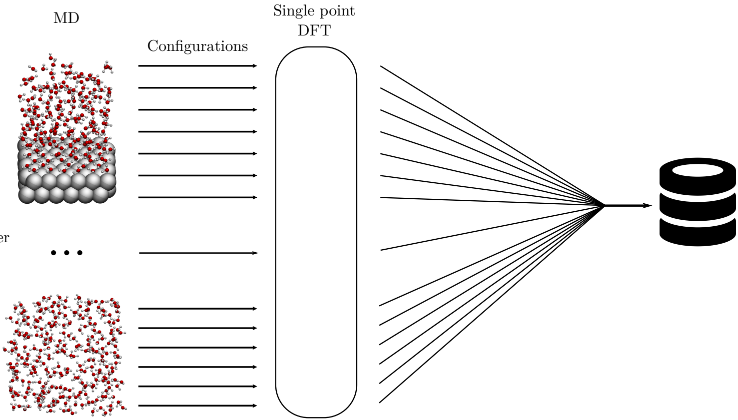
Step 1 Gathering data

- large/small slabs
- hot/cold dynamics
- thick/thin water layer
- with/without void
- with/without slab
...



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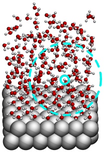
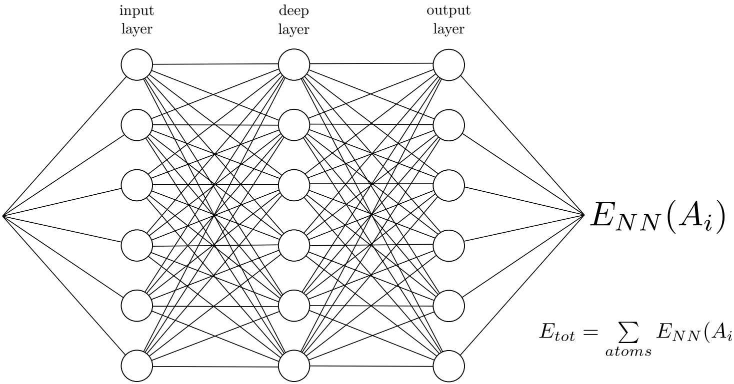
Step 2 Input and Training the Neural Network





$$E_{tot} = \sum_{atoms} E_{NN}(A_i)$$

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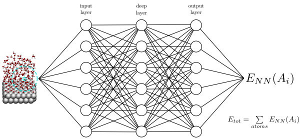
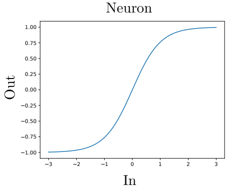
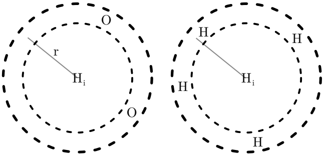
Step 2 Input and Training the Neural Network





input layer <=>
ensemble of symetry function



$$F_{radial}(H_i, r, O) = 2$$

$$F_{radial}(H_i, r, H) = 4$$

$N_{coefficient}$

$= (N_{input\_function} * N_{neuron,layer1} + N_{neuron,layer1} * N_{neuron,layer2} + N_{neuron,layer2}) * 3$ (O,H,Pt)

Artrith, N.; Behler, J. *Physical Review B* **2012**, *85*, DOI: 10.1103/PhysRevB.85.045439

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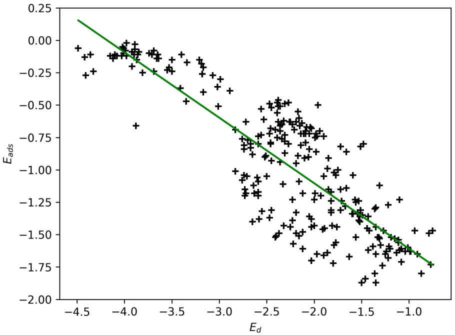
The adsorption energy example



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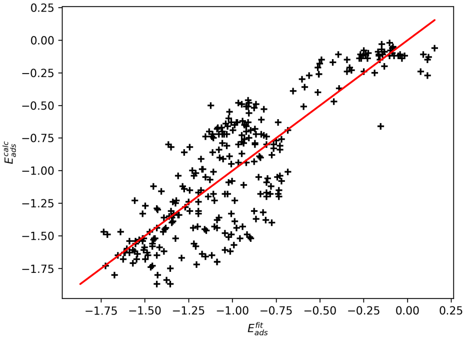
Linear fit vs calculation



Only one descriptor (E_d) is not good enough!
Even if it is based on a physical model (tight binding model)

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What if we consider more descriptors?

f	:	Filling of a d-band
E_d	:	Center of a d-band
W_d	:	Width of a d-band
γ_1	:	Skewness of a d-band
γ_2	:	Kurtosis of a d-band
W	:	Work function
r_0	:	Atomic radius
r_d	:	Spatial extent of d-orbitals
IE	:	Ionization potential
EA	:	Electron affinity
χ_0	:	Pauling electronegativity
χ	:	Local Pauling electronegativity
V_{ad}^2	:	Interatomic d coupling matrix element

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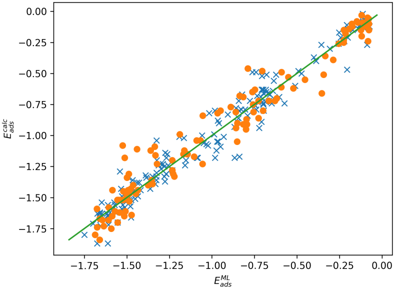
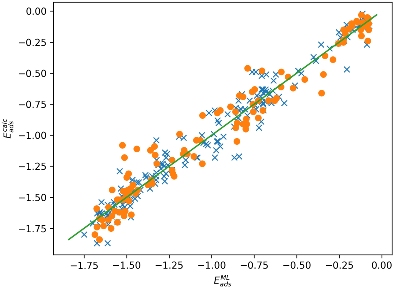
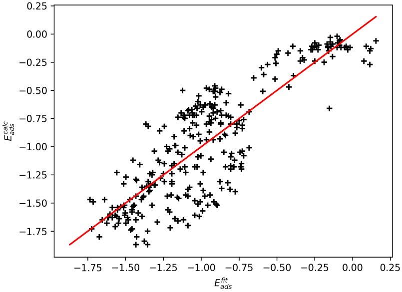
ML vs calculation



Ma, X. et al. *The Journal of Physical Chemistry Letters* **2015**, *6*, 3528–3533





ML significantly improves the fit by utilizing many descriptors.

ML needs input with chemistry insight in it.

ML is a tool, not magic.

Ma, X. et al. *The Journal of Physical Chemistry Letters* **2015**, *6*, 3528–3533

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Domain of applicability

Models must be treated with care

Beware of **overfitting**:

- Especially with high-dimensionality
- Quality estimator: **cross-validation** is a good starting point

Learned models are meant for **interpolation**, not extrapolation:

- Would require physico-chemical justification
- Training set should cover your subsequent usage

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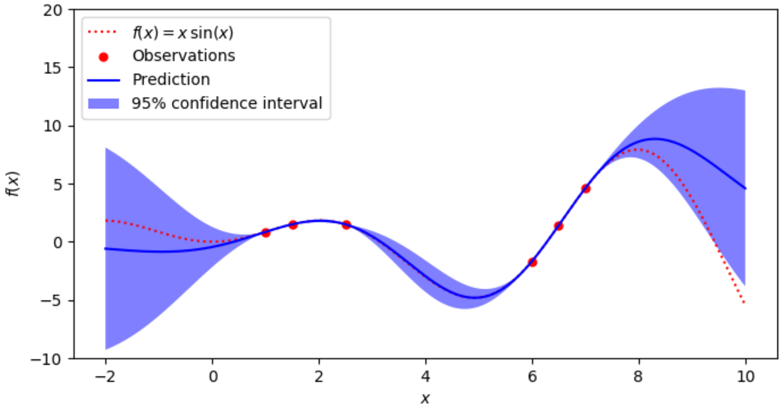
Extrapolation illustration



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Checking assumptions

Theorem (No free lunch)

Any two optimization algorithms are equivalent when their performance is averaged across all possible problems

$\Rightarrow$ There cannot exist a machine learning algorithm that outperforms all other algorithms on every problem

$\Rightarrow$ A machine learning algorithm can be better than an other **only** under specific assumptions

The moral being: compare and select the algorithm that fits the best your problem

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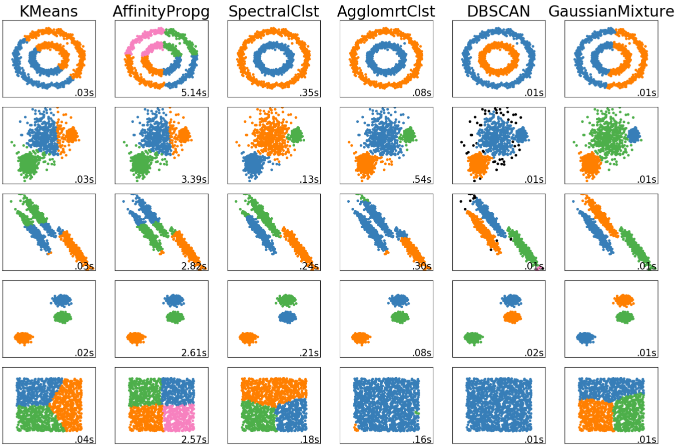
Clustering comparison



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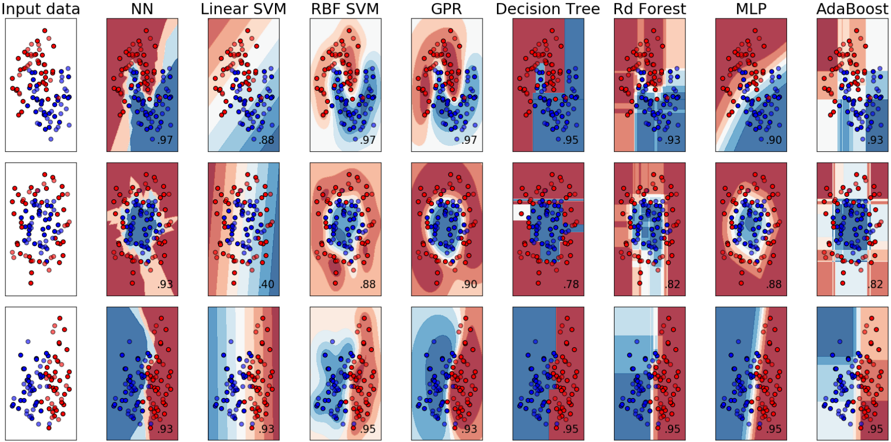
Classifiers comparison



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Another paradigm?

Third basic paradigm of machine learning: **reinforcement learning**

Aim: apply best policy to minimize regrets, without initial expertise (learn policies on the fly)

Trade-off between exploration and exploitation

Applications: decision making, global minimization, ...

Algorithms: MCTS, genetic algorithms, ...

Grandmaster level in StarCraft II using multi-agent reinforcement learning.png

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Oriol Vinyals, Igor Babuschkin, [...] David Silver

Nature **575**, 350–354(2019) | Cite this article

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The Singularity is Near