From (chemical) data to information

Introduction to Machine learning for Chemistry Lecture 2

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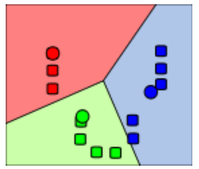
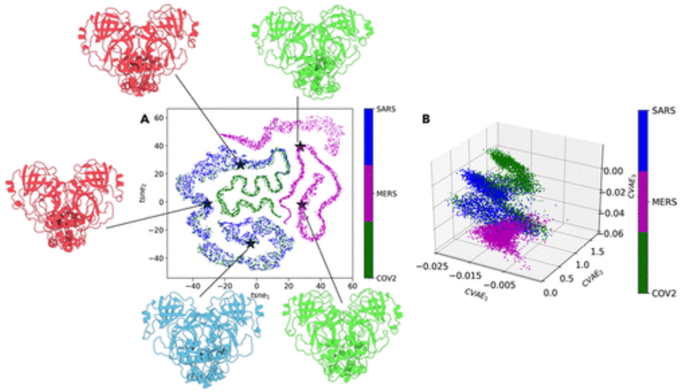
Room 214 JBB





Topics overview

Lecture 1

- What is machine learning?
- Examples of machine learning (in Chemistry)
- Introduction to **unsupervised learning**:
  - Clustering (k-means and others)
  - How does actual input data look like?
- Molecular fingerprints and nomenclature
- Introduction to **supervised learning:**
  - What is a classification problem?

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- Regressions
- Unsupervised learning continued:
  - Dimensionality reduction (PCA)
  - t-SNE
- Classifications in practice:
  - Random Forests
  - Multilayer perceptrons

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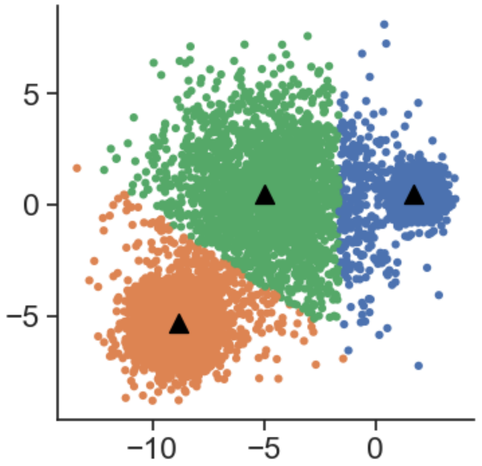
Learning outcomes:

- Understand the main pillars of machine learning
- Know about different clustering techniques as part of unsupervised learning
- Be able to use common nomenclature used in machine learning
- Use PCA to reduce the dimensions of your data set
- Understand how a regression problem can be cast as a machine learning problem
- Be aware of how random forests and multilayer perceptrons can be used in a classification problem

Recall from Lecture 1

Different clustering algorithm identify groups in datasets



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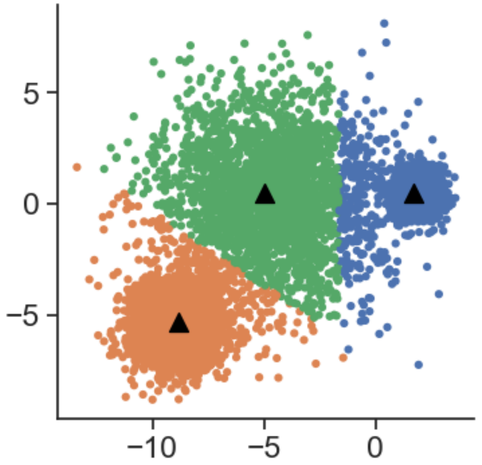
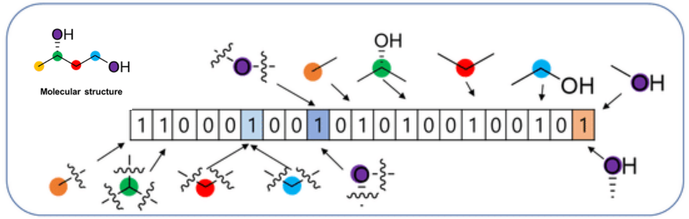


Features are used in input as feature vectors and can take many different forms



Original Morgan fingerprints

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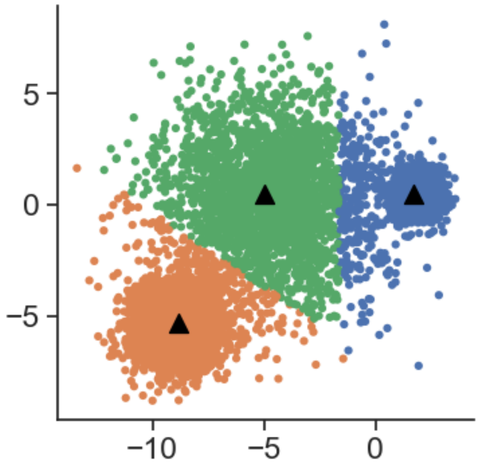

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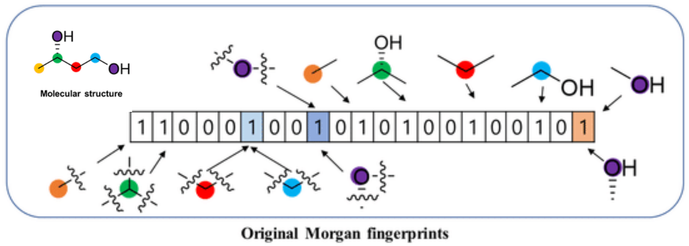
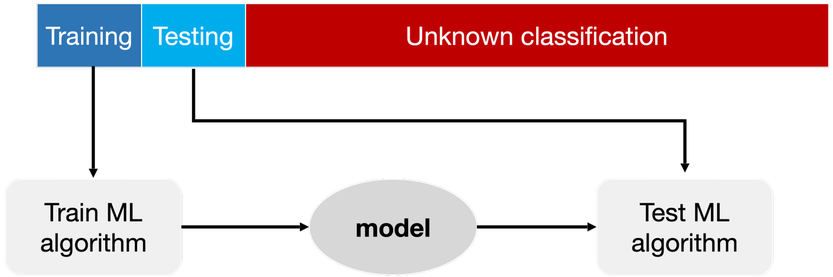


A classification model uses labelled data as input to train a model that can be used as a classifier



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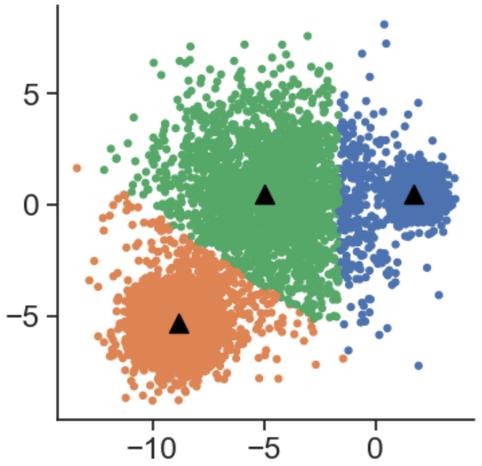

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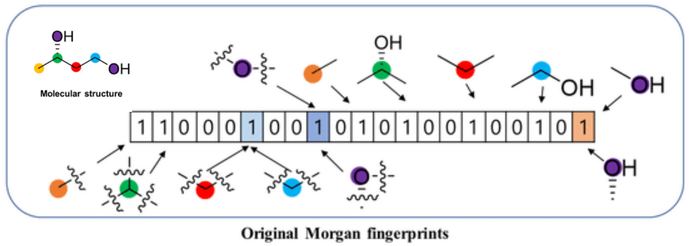

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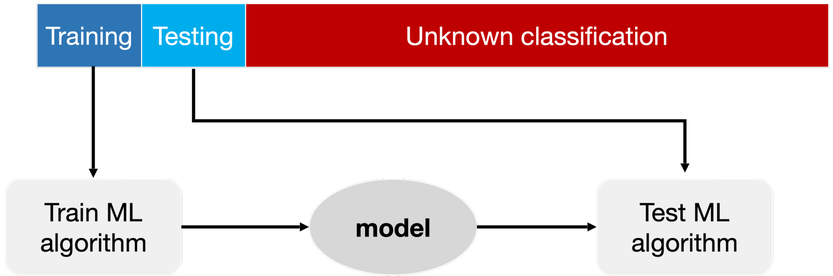
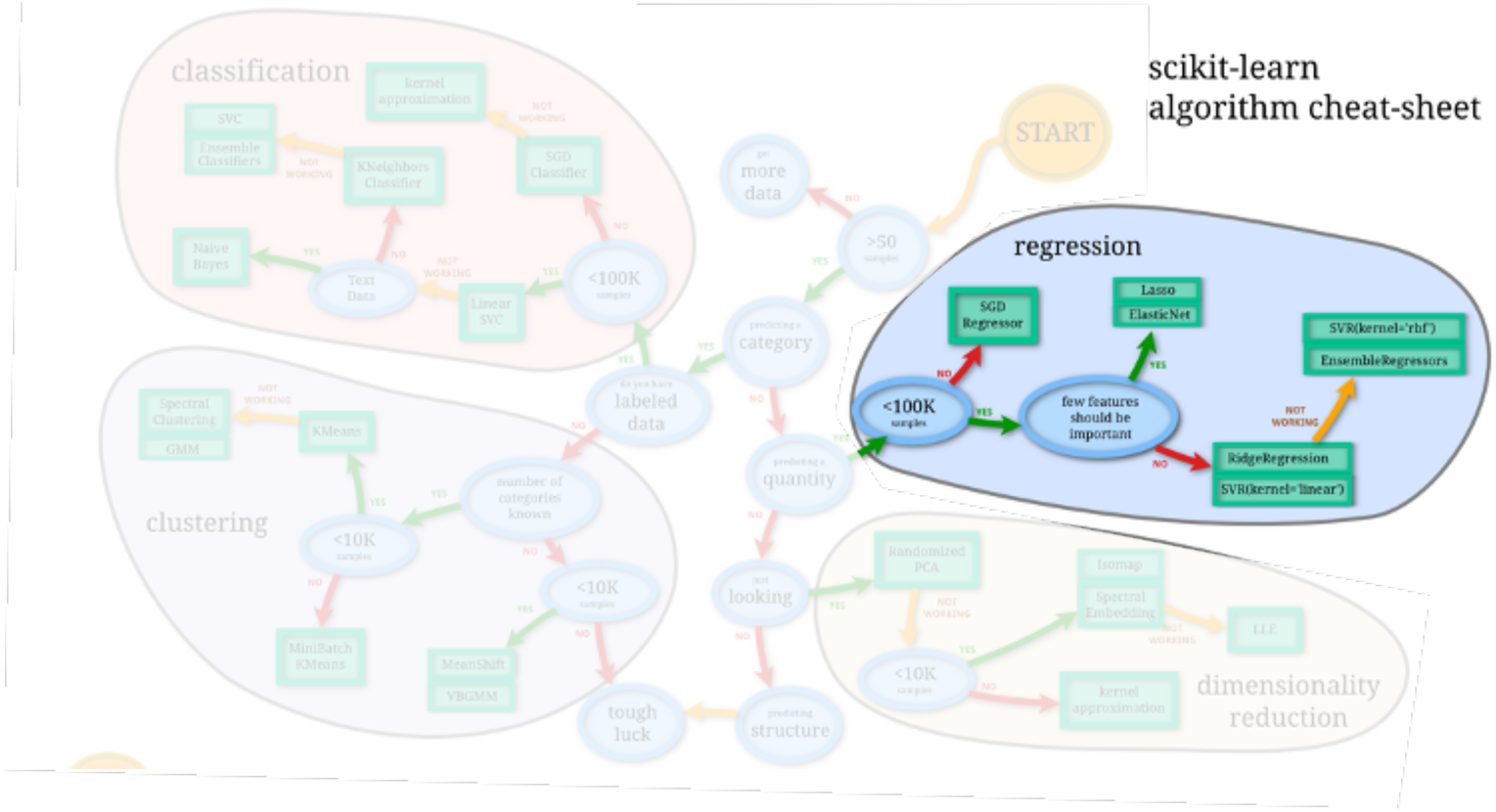


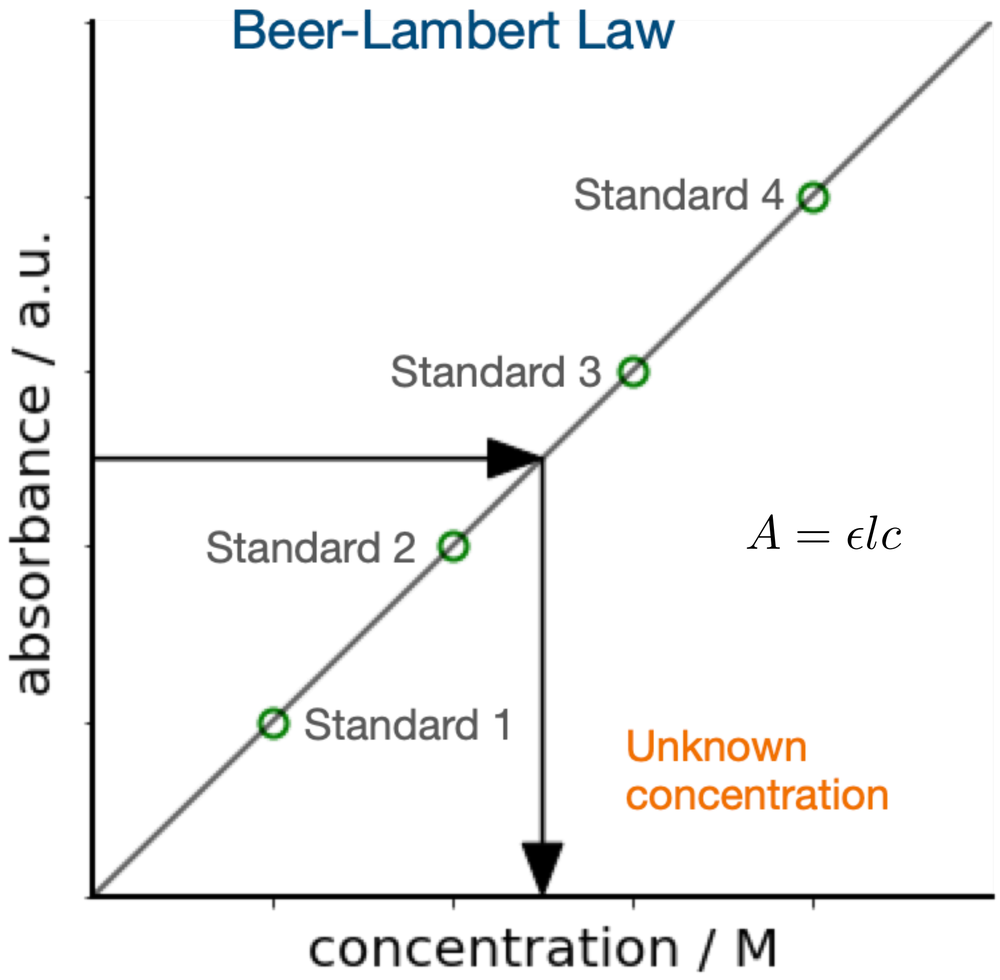
result \ real	Dog	Cat
Dog	90	10
Cat	12	88

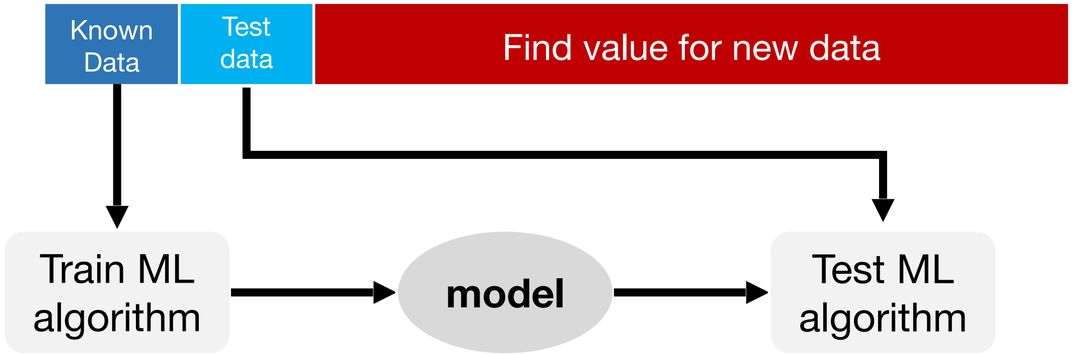
A confusion matrix allows the assessment of how good a model is.

The Data Mining World



Linear regression: an example





Now the model is the line of best fit that will allow us to identify an unknown concentration

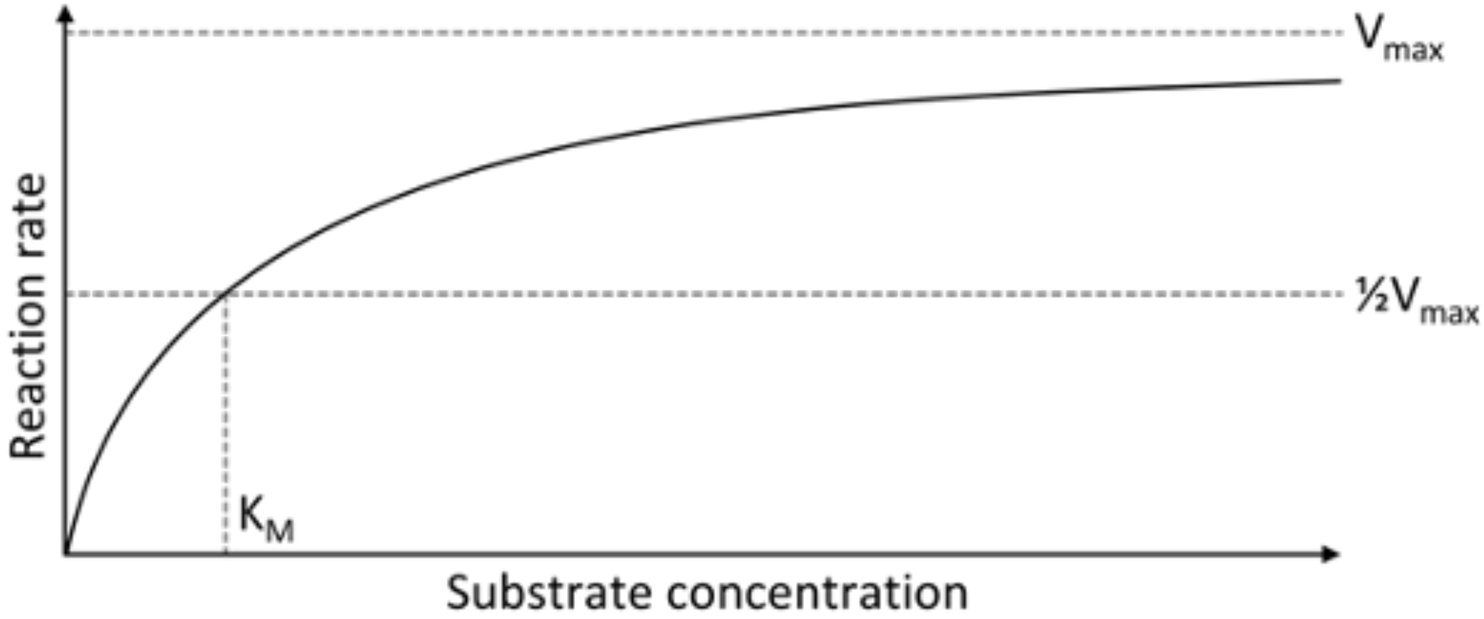
How do we find the line of best fit?

Non-linear Least squares

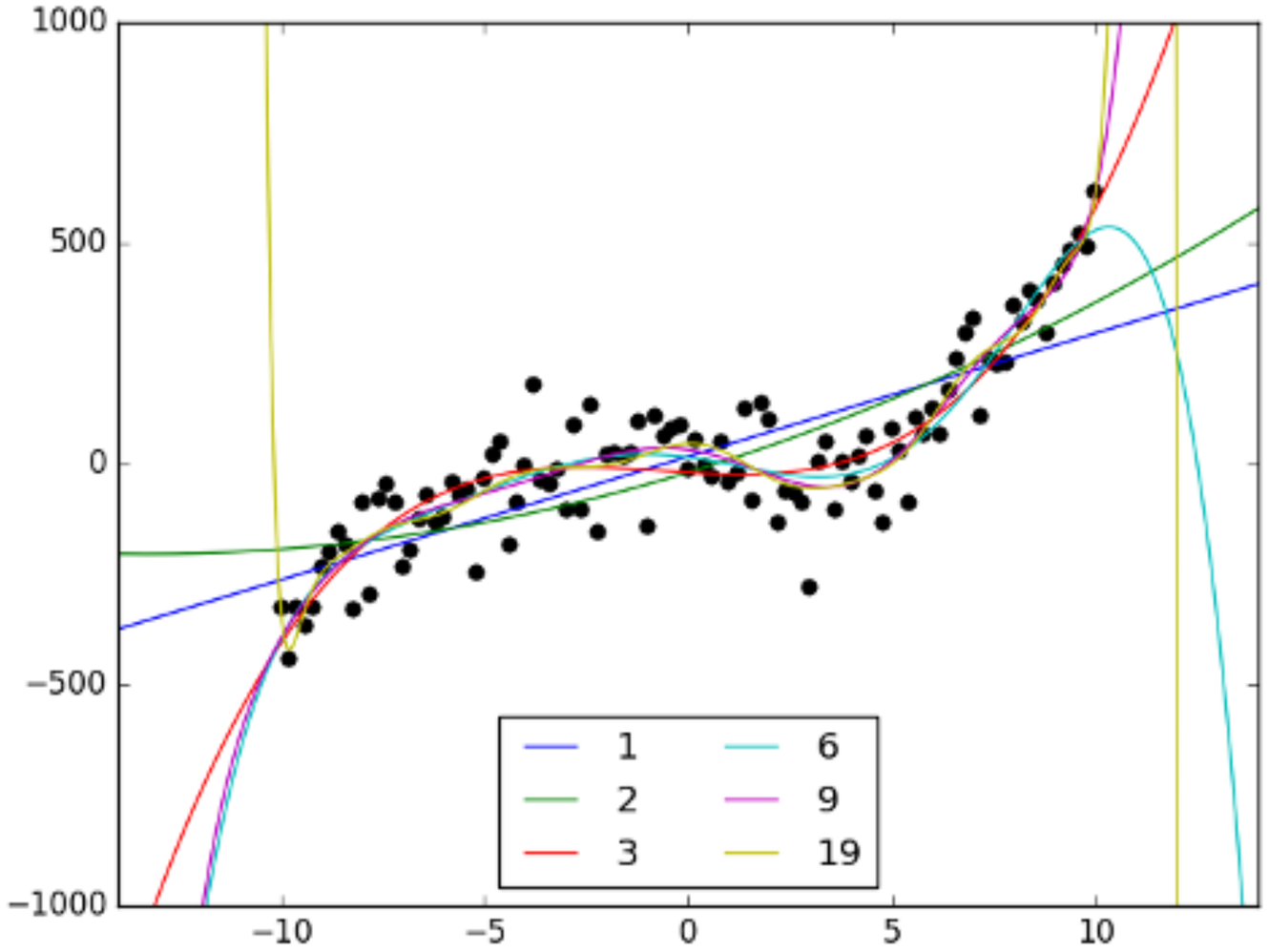
Non-linear combinations of model parameters, e.g. Michaelis Menten

$$\frac{d[P]}{dt} = \frac{V_{\max}[S]}{K_{\mathrm{M}} + [S]}$$

$$f(x, a, b) = \frac{ax}{b + x}$$



The more parameters the better the fit?



”With four parameters I can fit an elephant, and with five I can make him wiggle his trunk”

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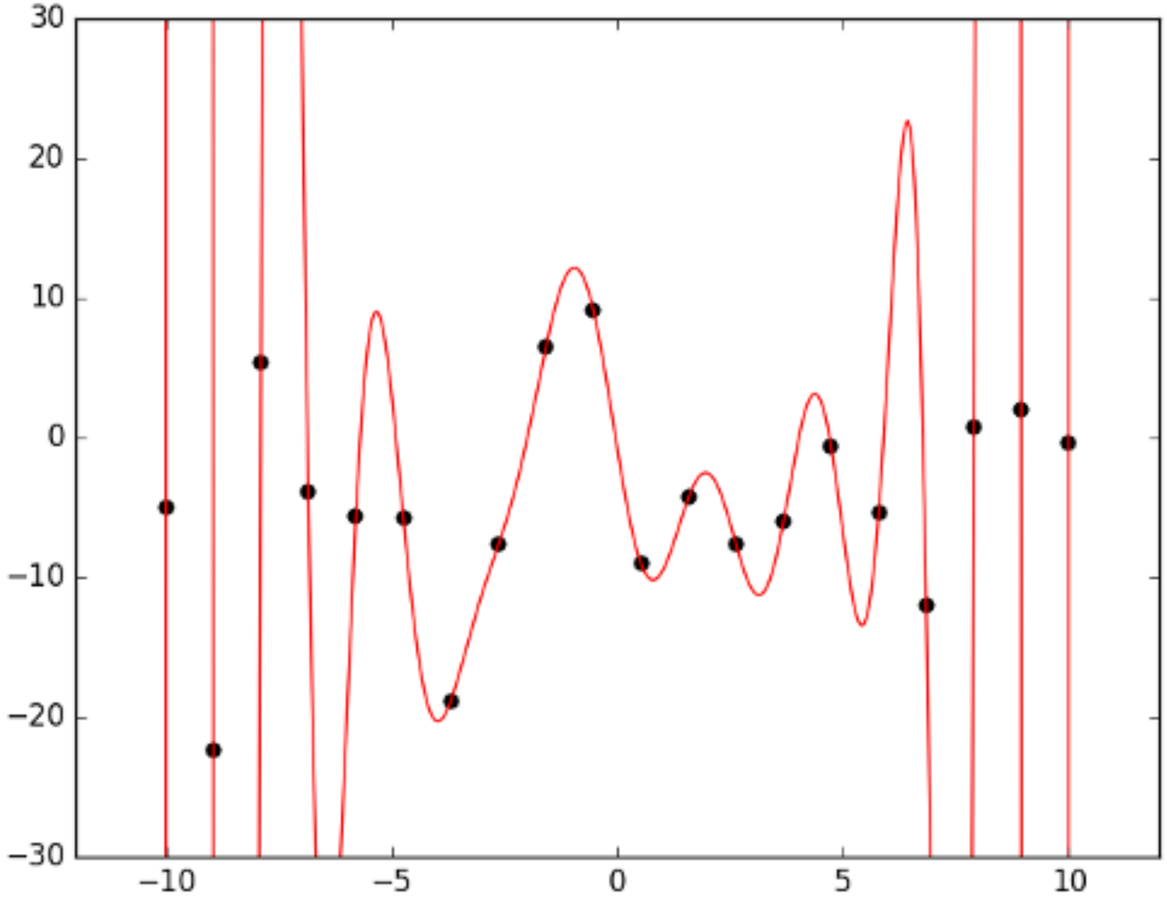

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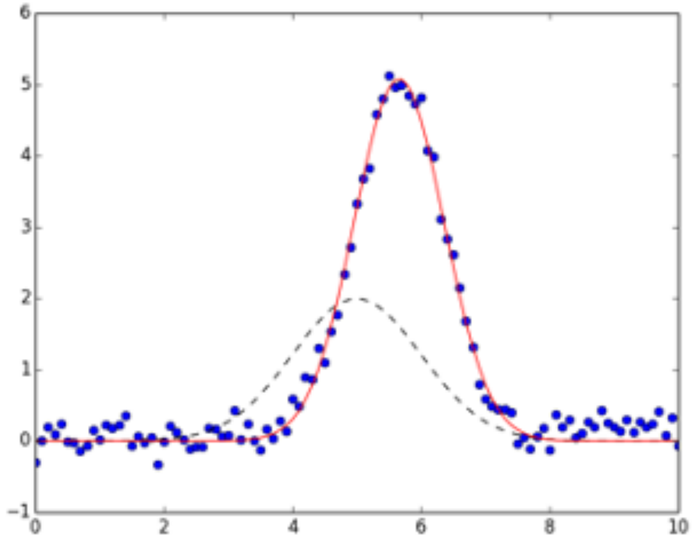
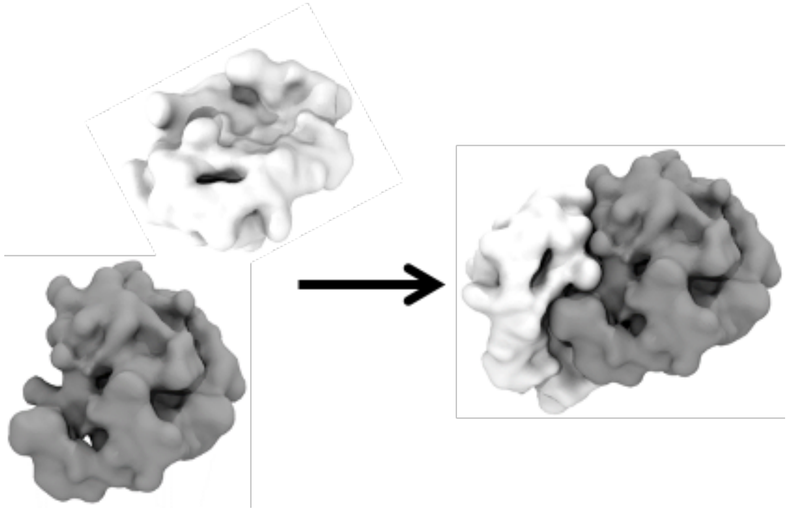
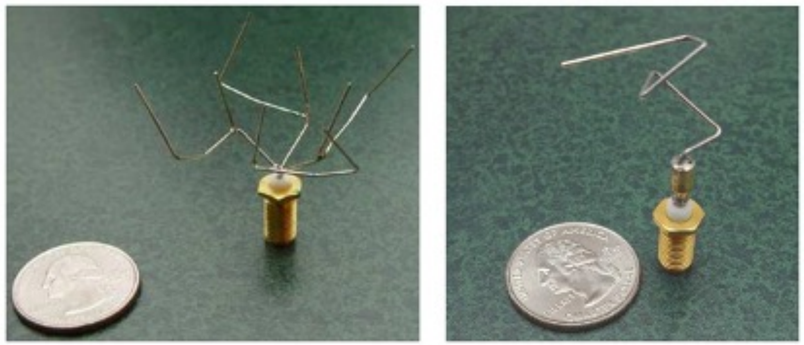
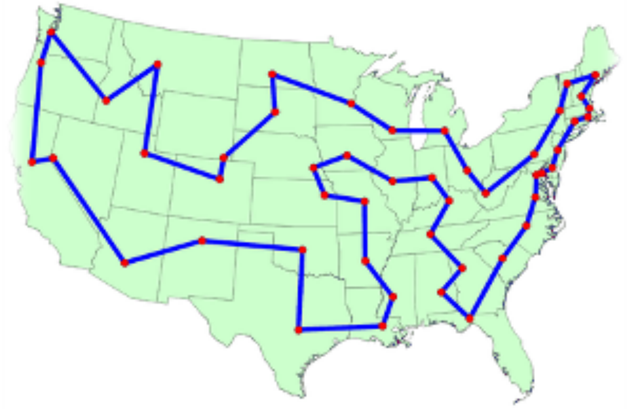
N points can be perfectly fitted with an N-1 order polynomial

Data Fitting is an Optimisation Problem









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Definitions:

- *parameters **x***: (sometimes) degrees of freedom
- *subset of Euclidean space*: search space
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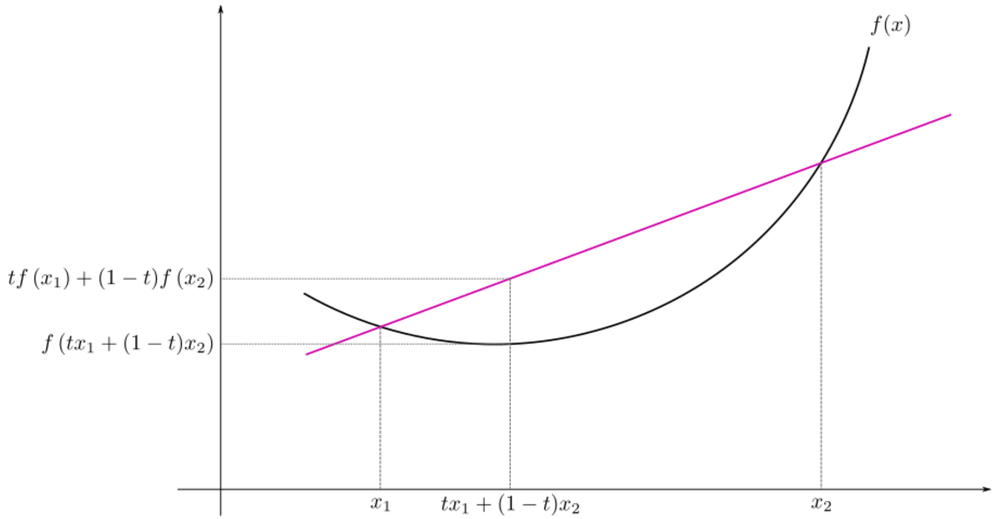
Convex function: iff the segments connecting any two points on the function, lie above it



the function has *only one* minimum

demonstrating that a problem is convex is a *big* deal!

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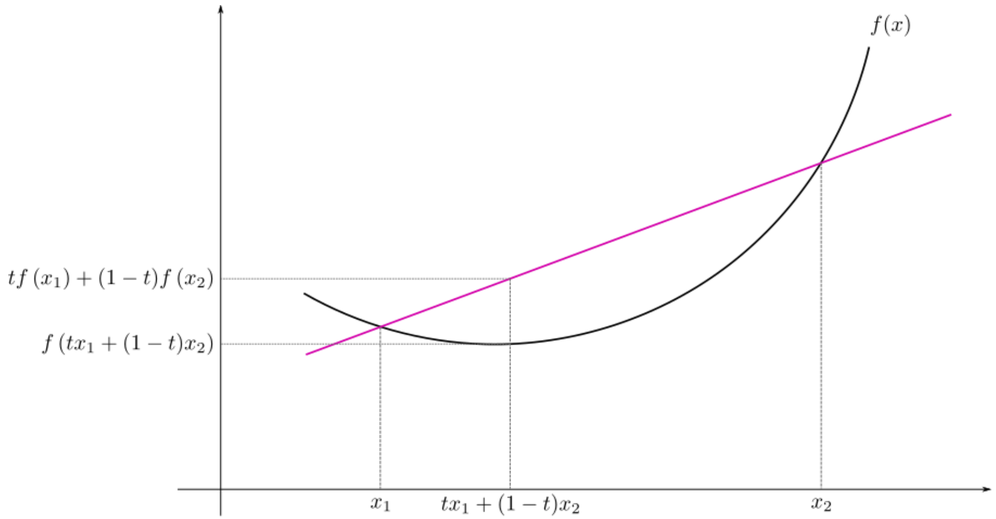

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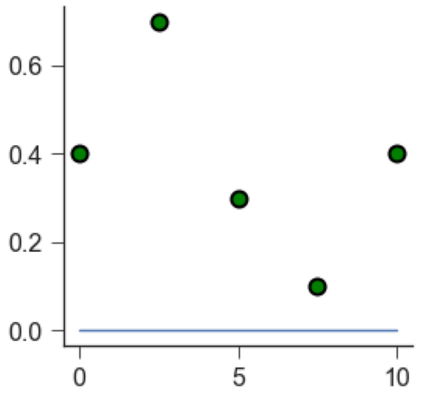
What is a good objective function?

Linear regression: in ML language



The blue line is meant to **fit** the green data points.

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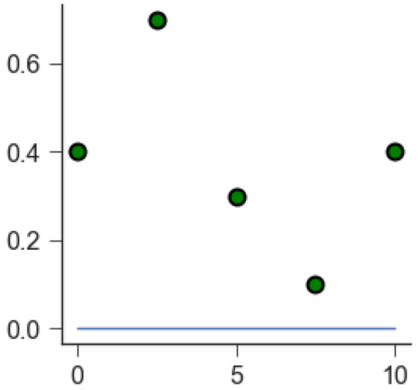

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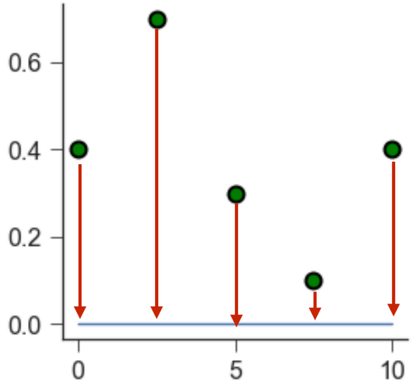

Red arrows are a called **residuals** and small arrows mean a good fit.

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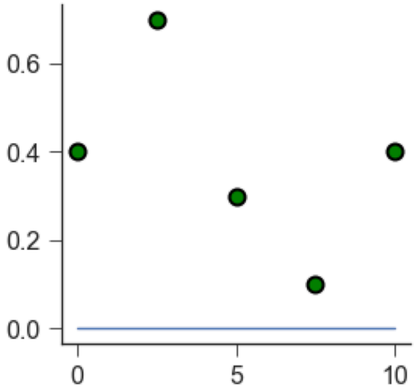

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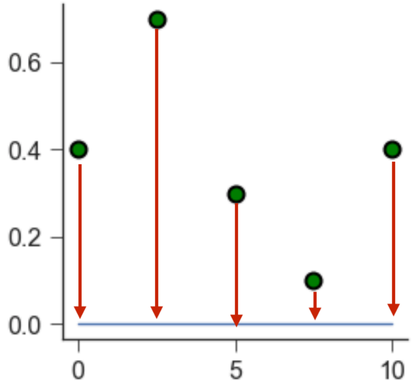

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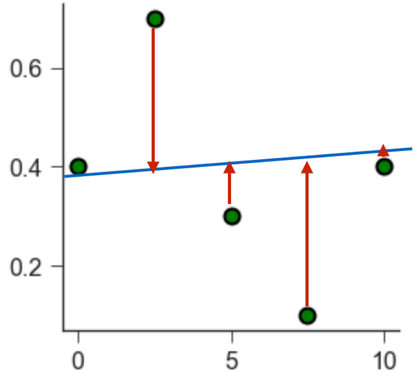

Mean square error is a good **loss function,** because it is **convex.**

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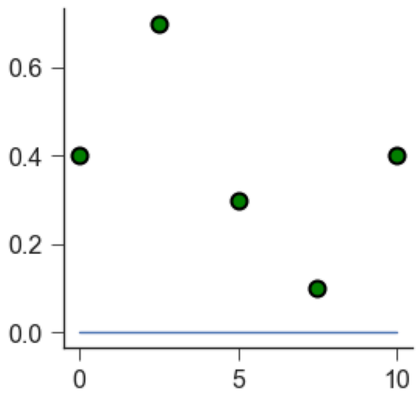

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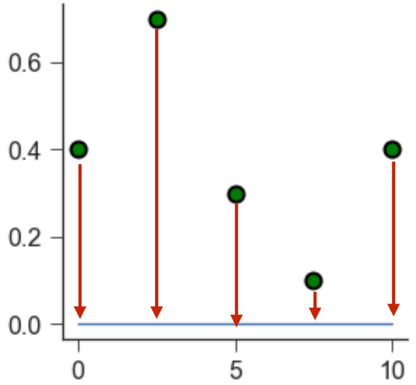

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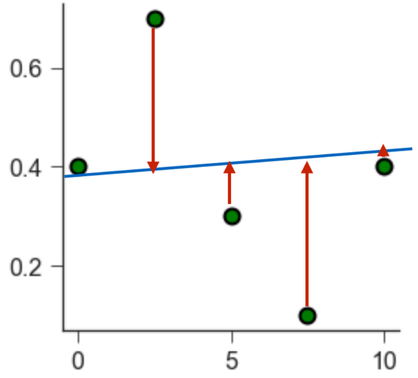

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$$\mathrm{MSE} = \frac{1}{n}\sum(Y_i - \hat{Y}_i)^2$$

n is the number of data points,
Y_i is the observed value (i.e. the measured data point),
$\hat{Y}_i$ is the predicted value (i.e. the value that lies on the line of best fit).

Gradient Descent

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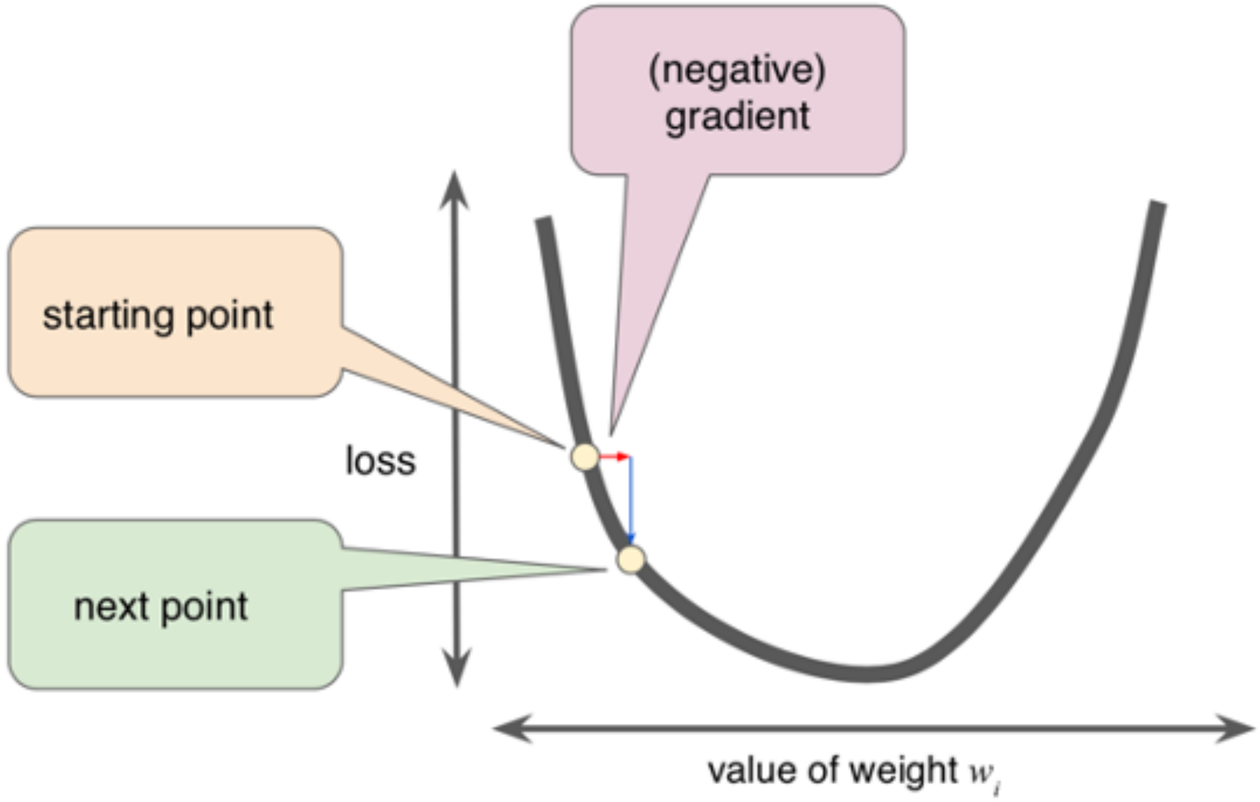
Objective: Find the minimum of the loss function (see optimisation problem)



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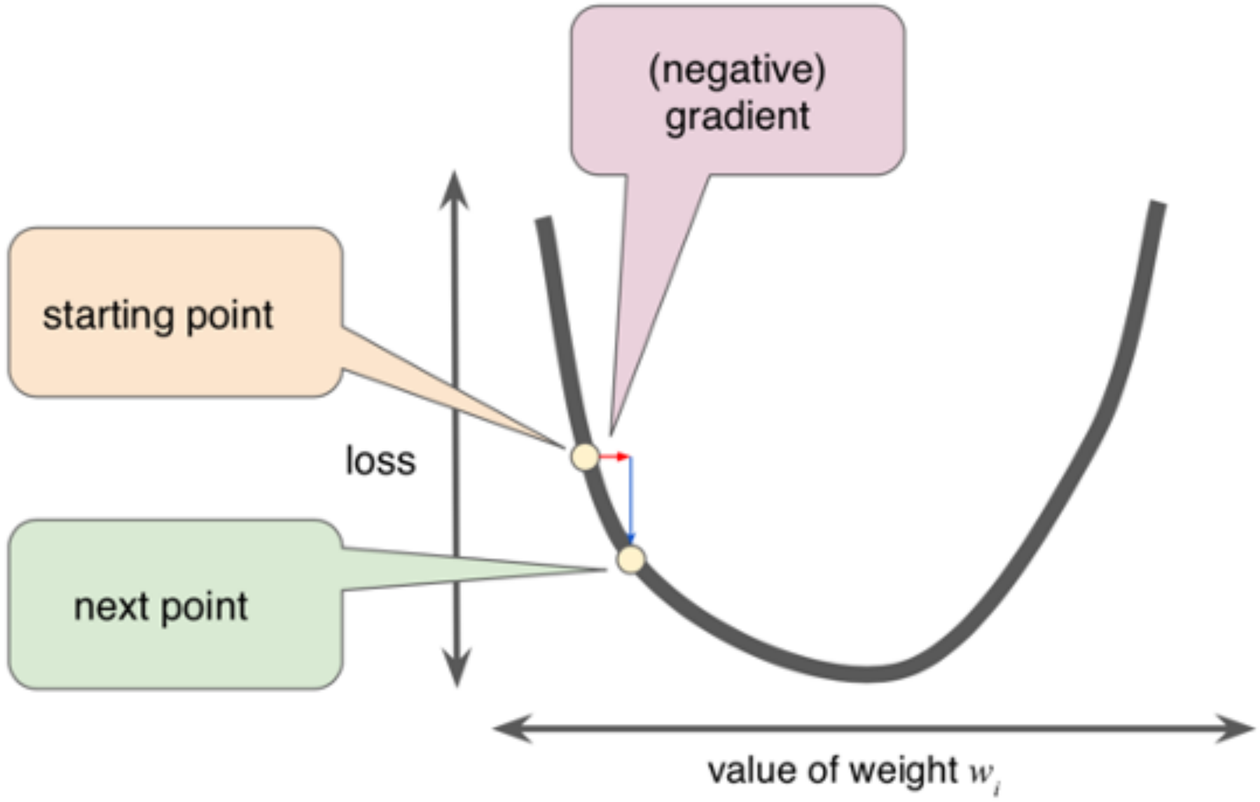
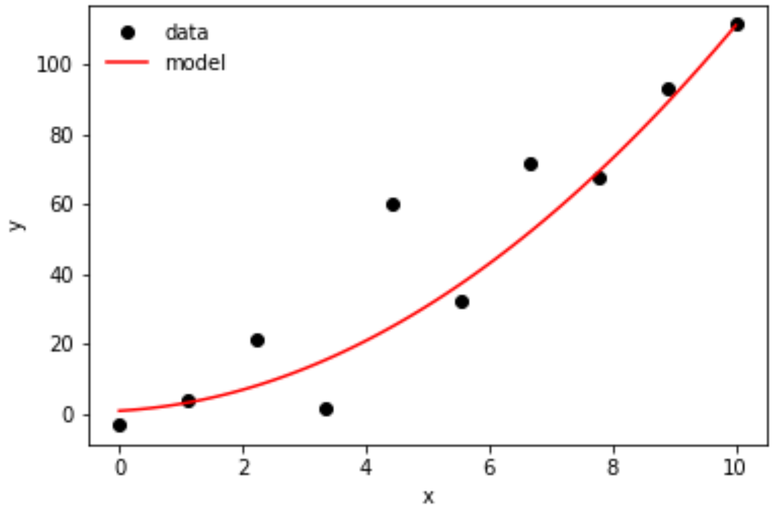


In machine learning, the step size of the gradient descent is called the **learning rate**

There is an *optimal learning* rate for every regression problem

Choosing the **best** optimiser is an optimisation problem in itself!

Linear Least Squares: A Summary



Model predicts values for each datapoint

$$\hat{y}_i = f(x_i; a, b, \ldots)$$

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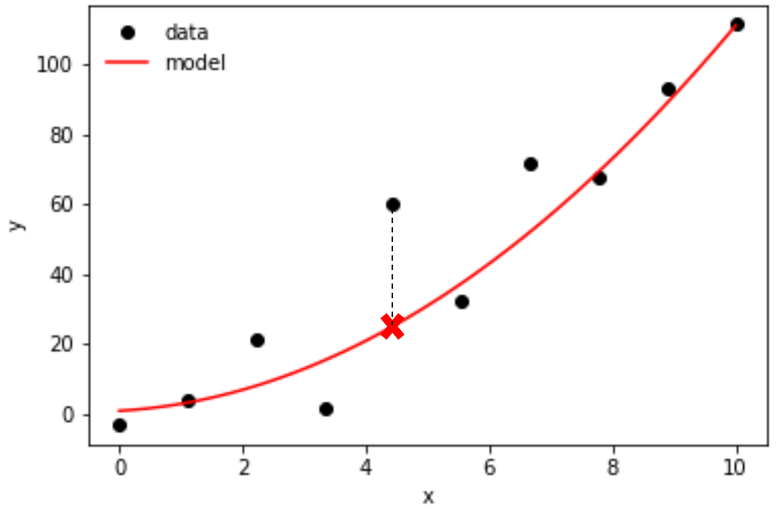

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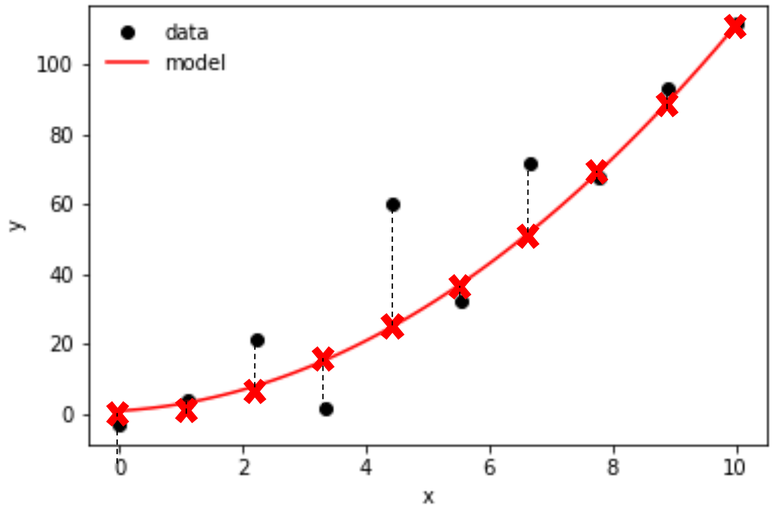

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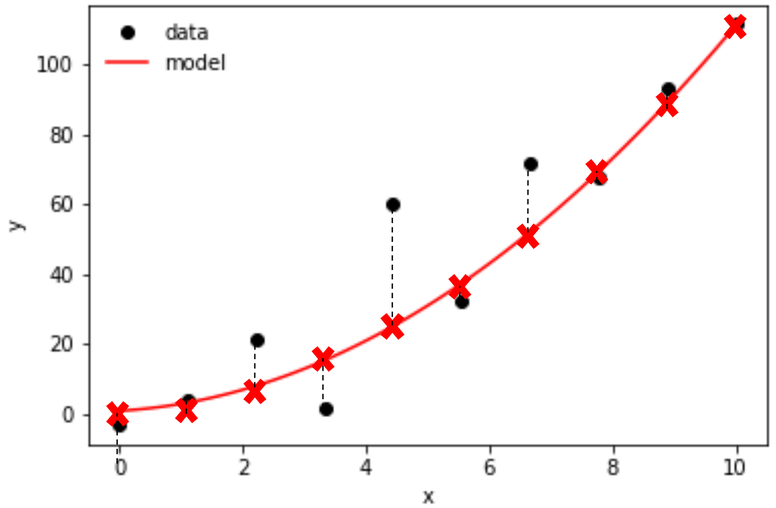

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The best model minimizes the sum of squared residuals (“loss function”)

$$E(a, b, \ldots) = \sum_{i=1}^{N} r_i^2$$

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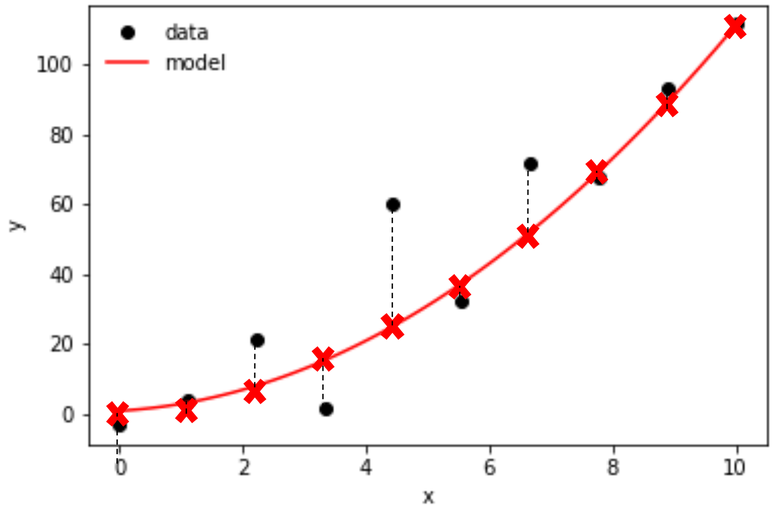

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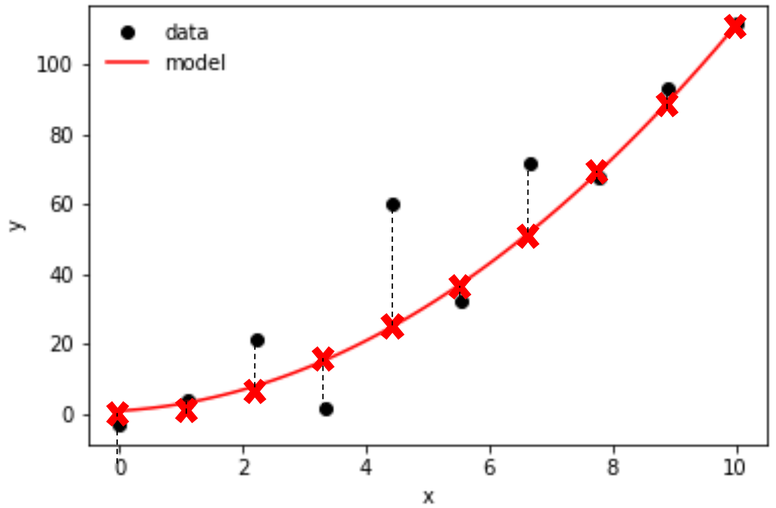
The best model minimizes the sum of squared residuals ("loss function")

$$E(a, b, \ldots) = \sum_{i=1}^{N} r_i^2$$

Solve: $\nabla E = 0$

-> find the minimum of the loss function
Note: This can be in many dimensions!

Linear Least Squares: A Summary



Model predicts values for each datapoint

$$\hat{y}_i = f(x_i; a, b, \ldots)$$

Residuals quantify prediction error

$$r_i = y_i - f(x_i; a, b, \ldots)$$

The best model minimizes the sum of squared residuals ("loss function")

$$E(a, b, \ldots) = \sum_{i=1}^{N} r_i^2$$

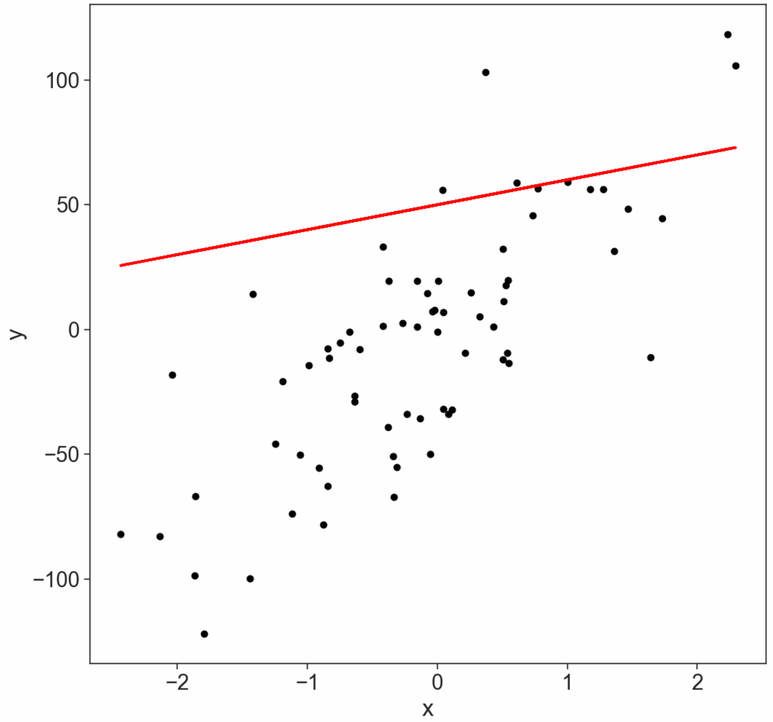
Solve: $\nabla E = 0$

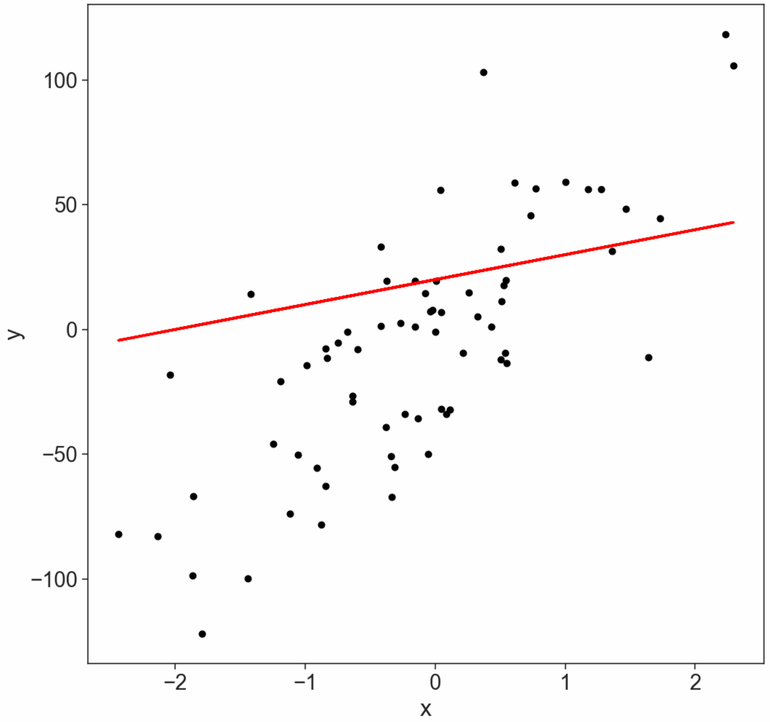
-> find the minimum of the loss function
Note: This can be in many dimensions!

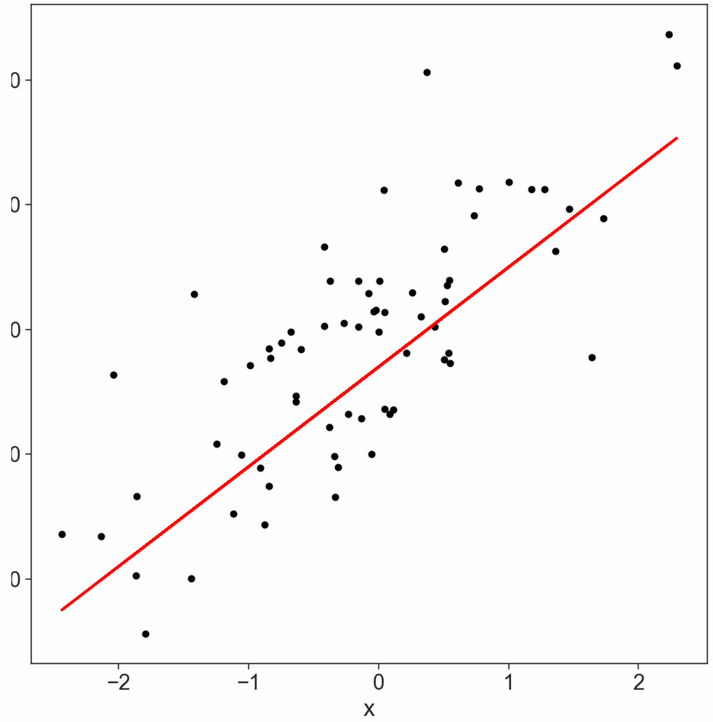
Use least squares (i.e. analytical solution) if:

- there are more data points than parameters (overdetermined)
- Model's parameters combine linearly (linear least squares)

Gradient Descent: learning rate and initial conditions

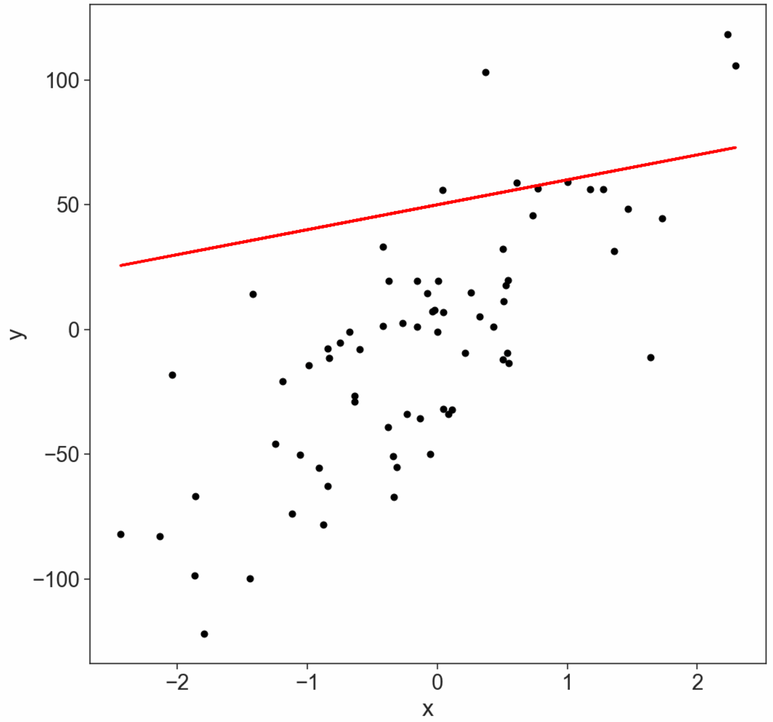


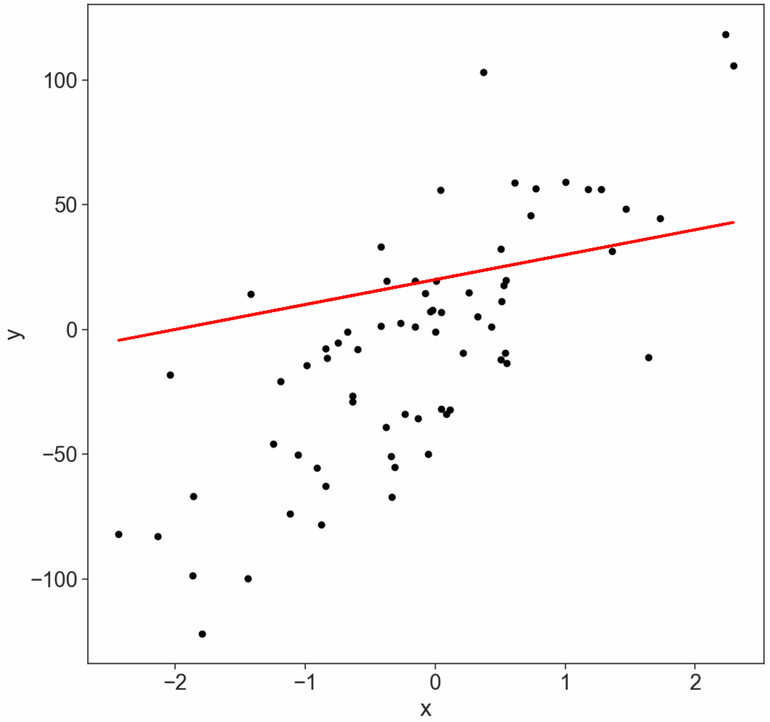


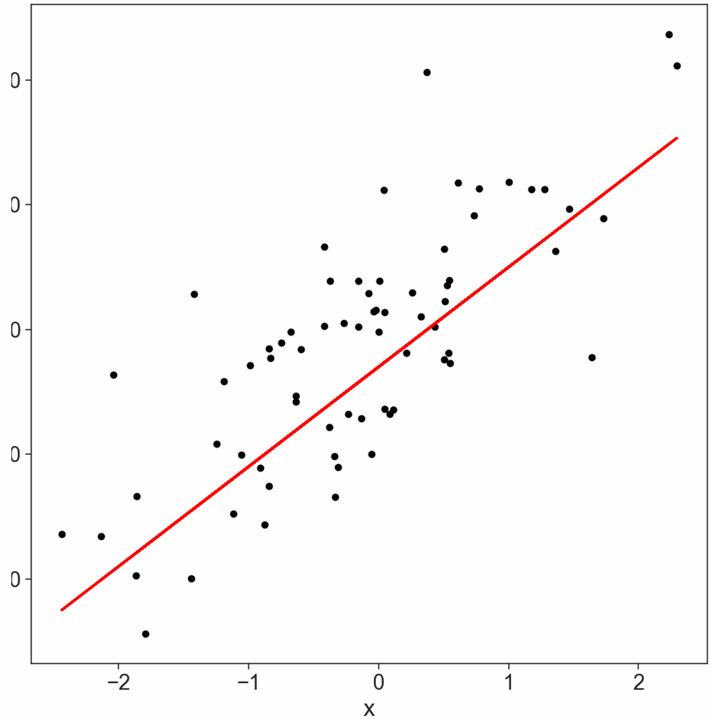


Low learning rate
bad starting point
424 steps

Gradient Descent: learning rate and initial conditions







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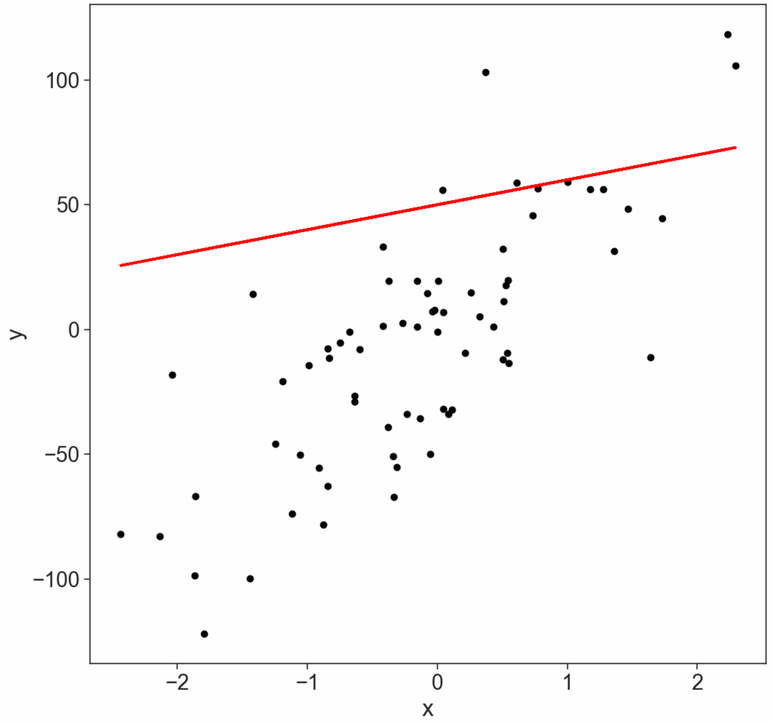
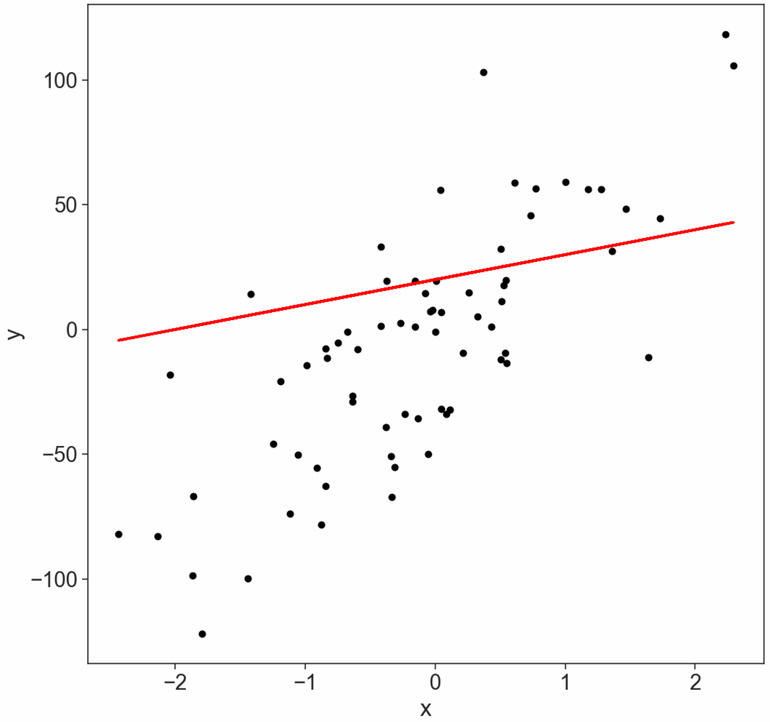
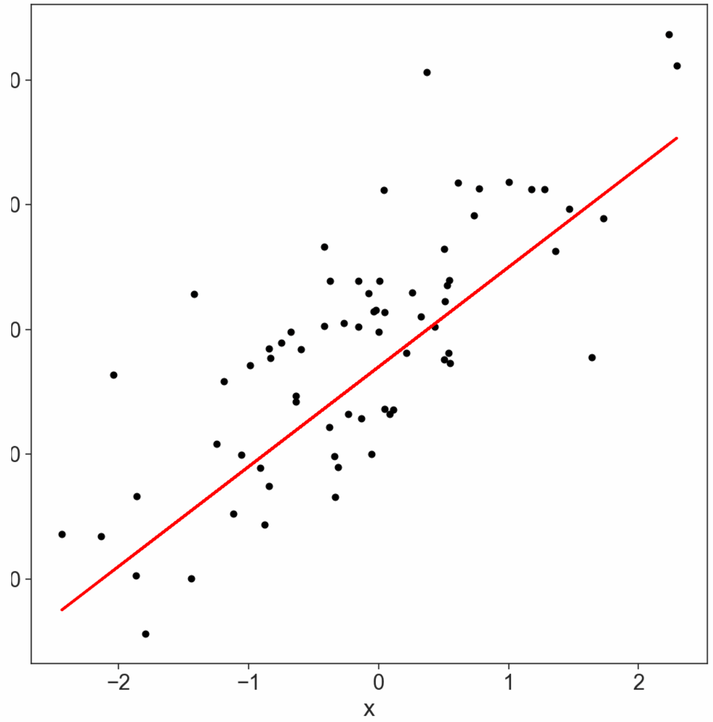
Gradient Descent: learning rate and initial conditions







Low learning rate
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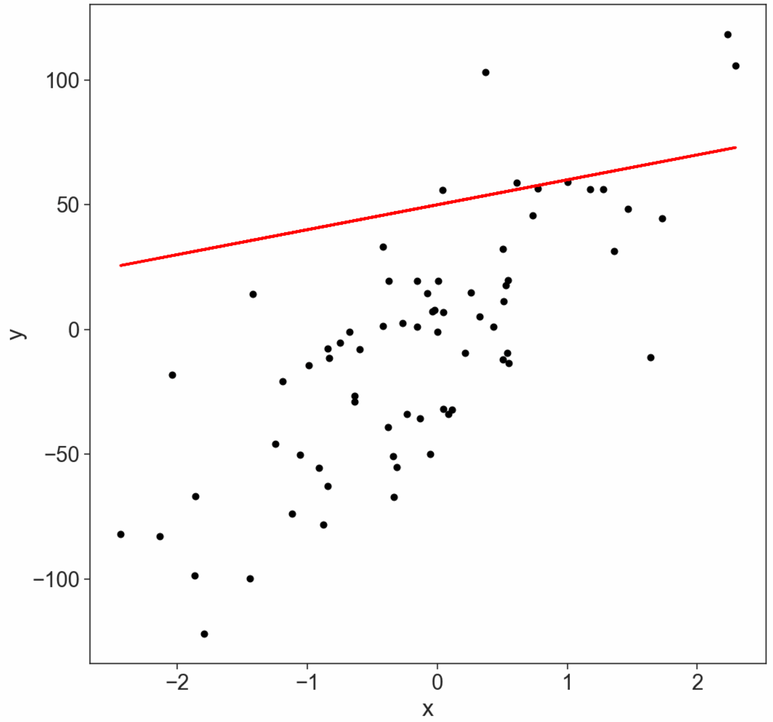
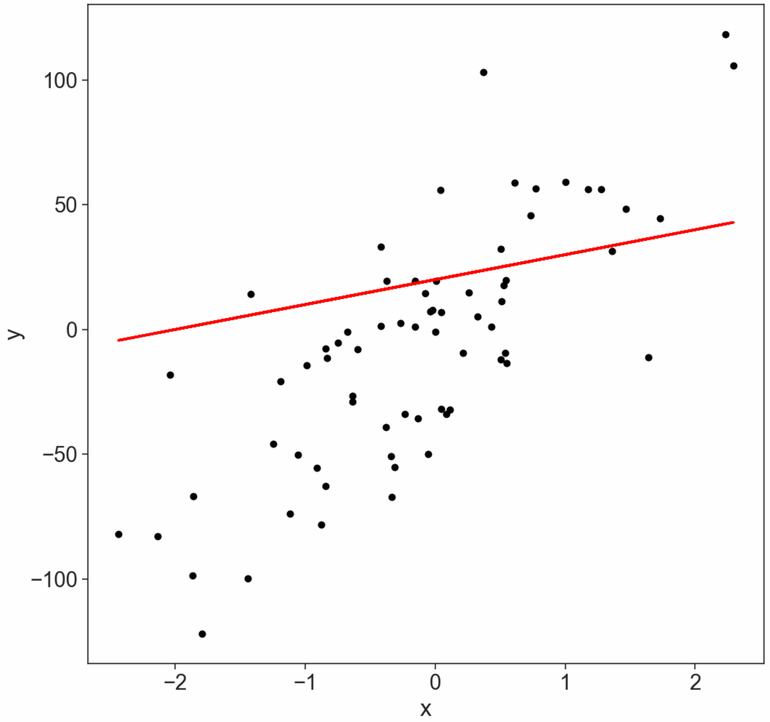
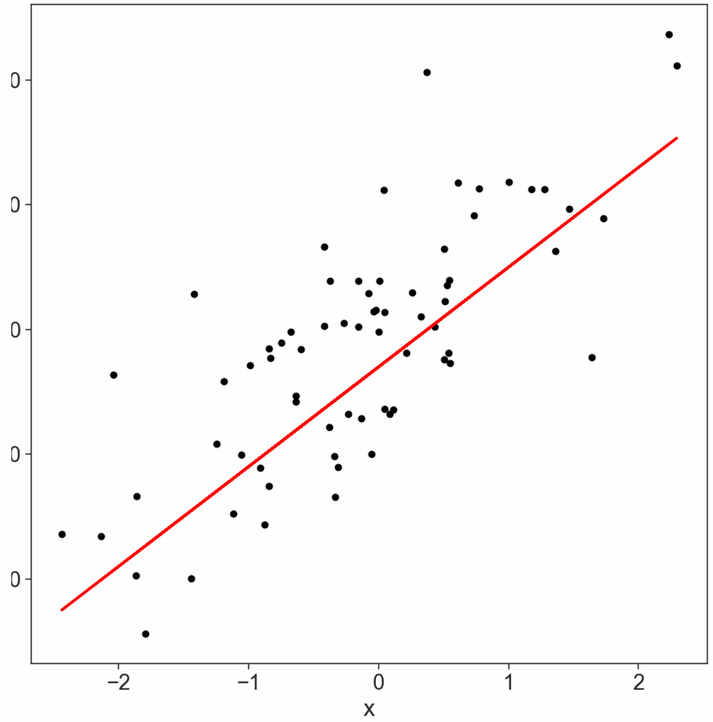
Gradient Descent: learning rate and initial conditions



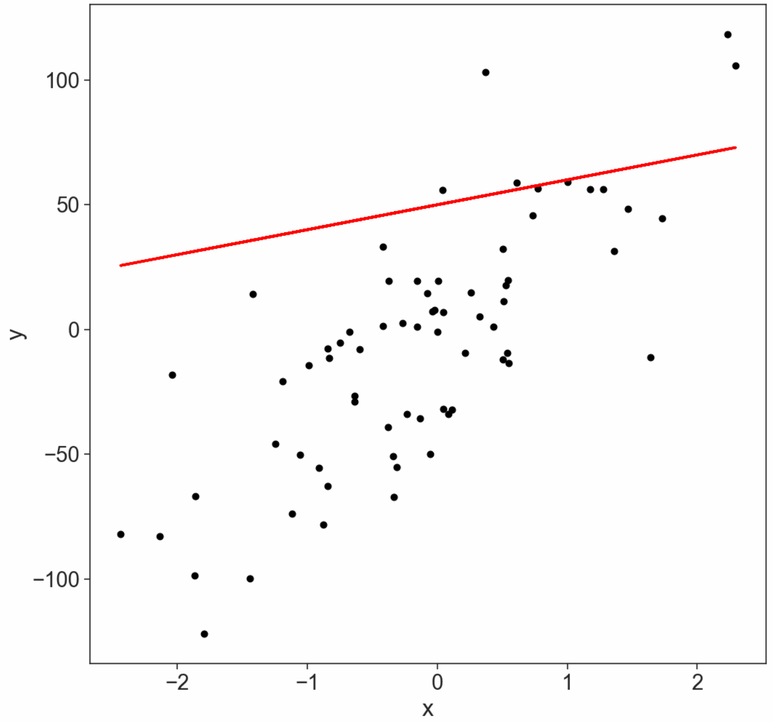
Low learning rate
bad starting point
424 steps



High learning rate
bad starting point
52 steps



Gradient Descent: learning rate and initial conditions



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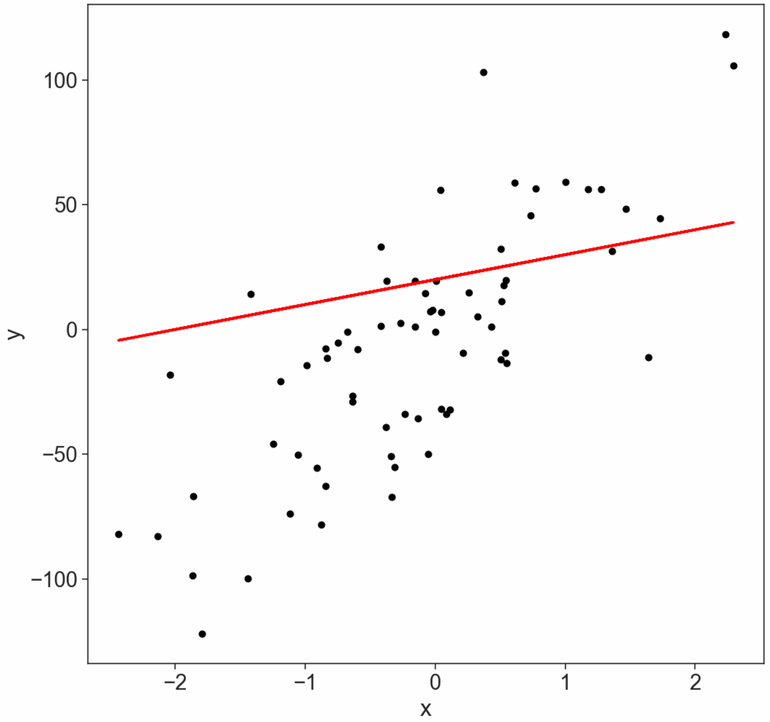

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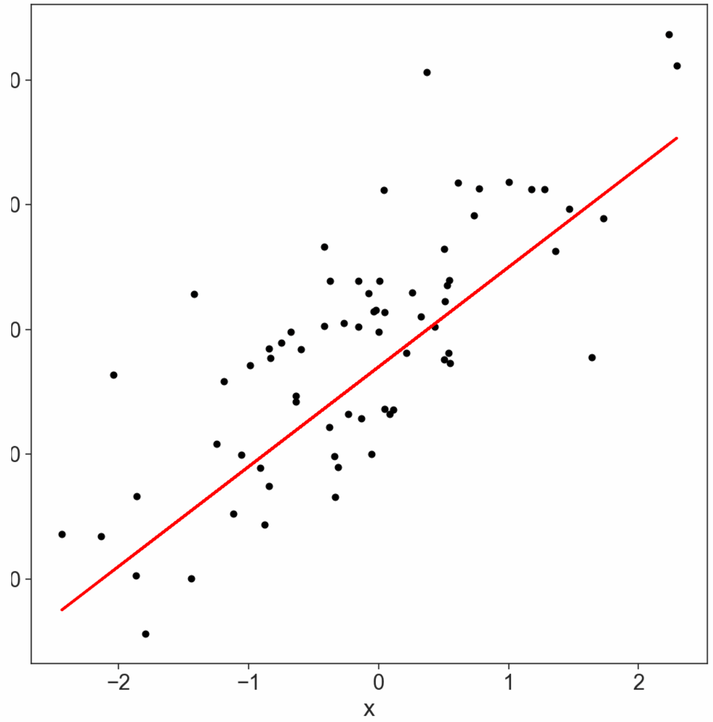

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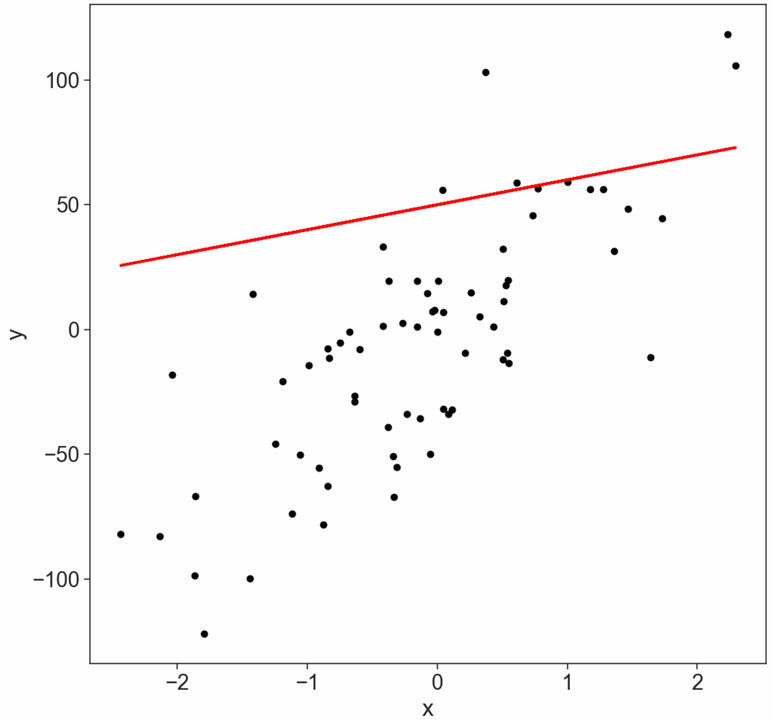

Low learning rate
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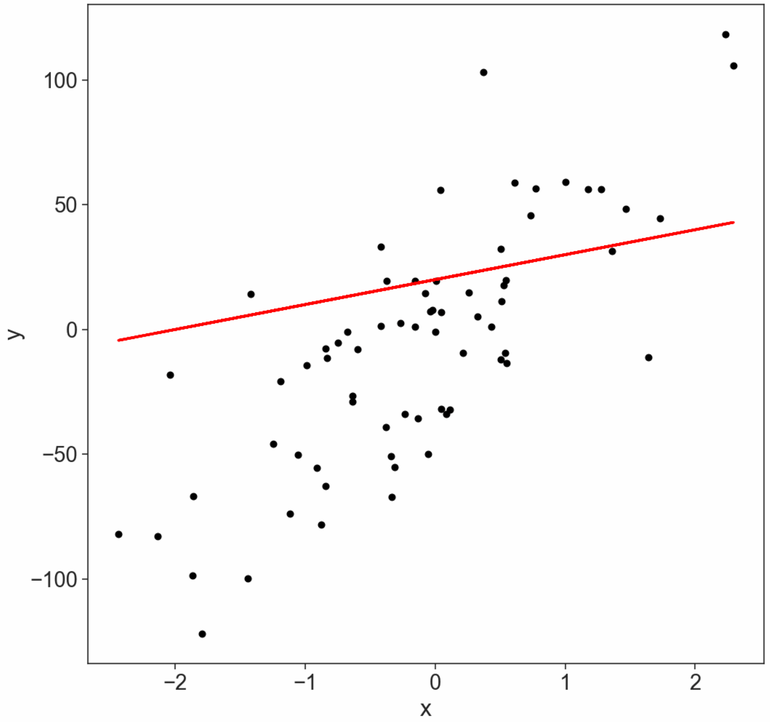
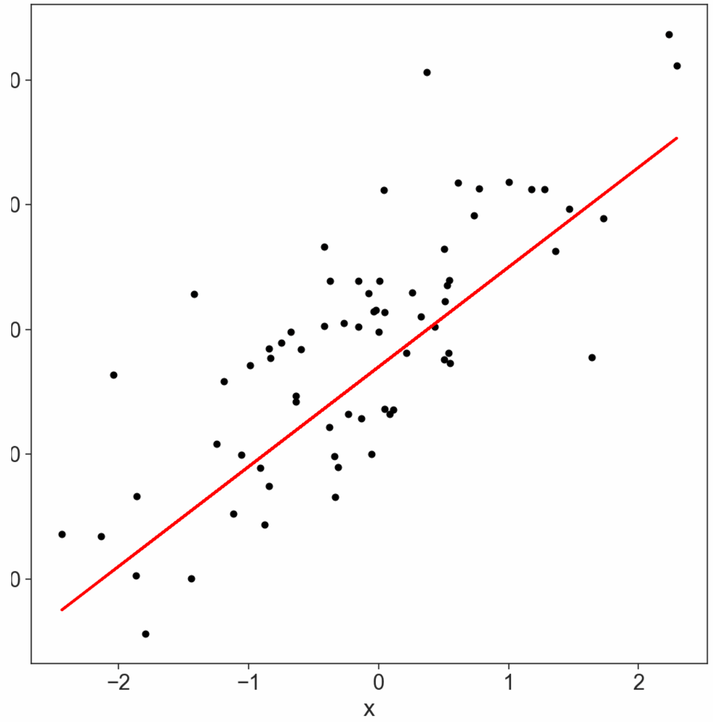
424 steps



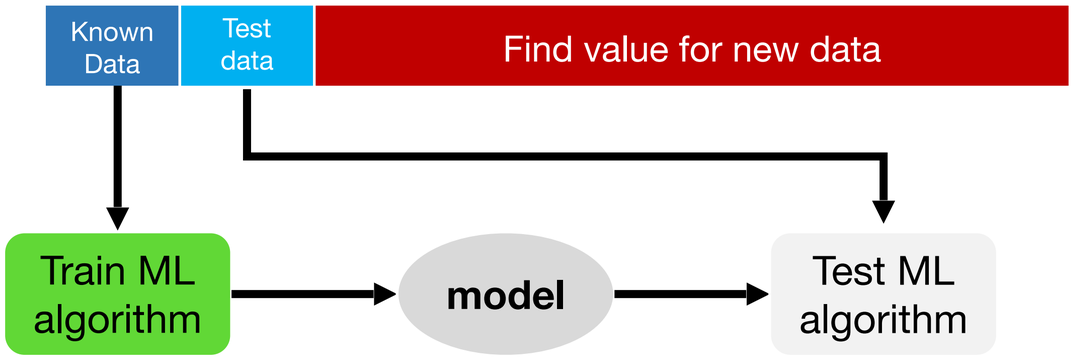
High learning rate
bad starting point
52 steps



Low learning rate
Good starting point
379 steps

Learning Algorithms for regression problems

- Decision Tree Regression (DT)
- Random Forests (RF)
- Neural Network Regressions (ANN)
- Support Vector Machine (SVM)
- **Linear Regression (LR)**
- *Non-Linear Regression*
- K Nearest Neighbor (KNN)
- Gaussian Regression
- ...

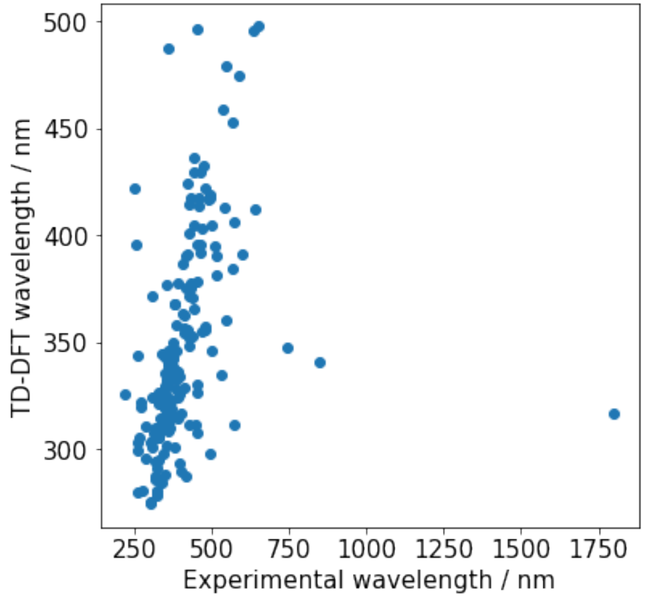


Linear and non-linear examples in chemistry

Can you think of linear/non-linear regression models you have used in your degree?

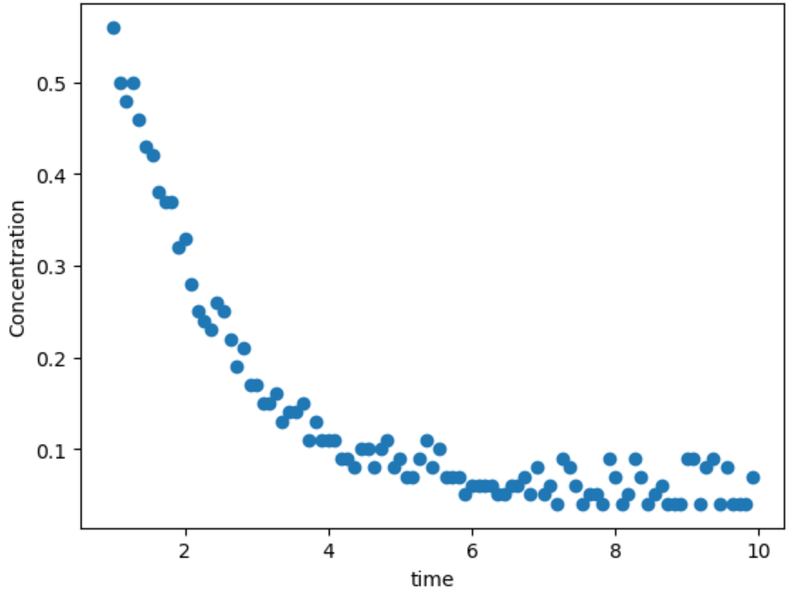
Can you think of examples in multiple dimensions?

Comparing experimental UV-Vis data with DFT calculations



$$f(x) = mx + b$$

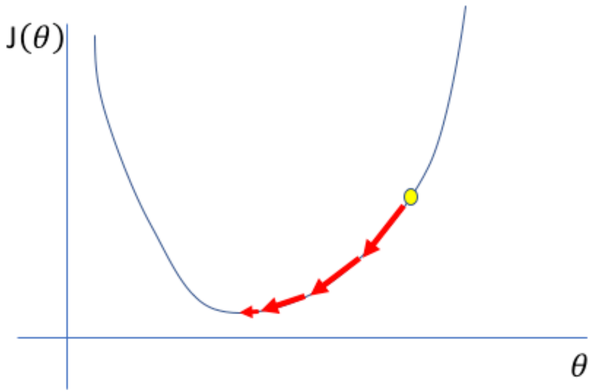
Variation of the concentration of a drug molecule in blood over time



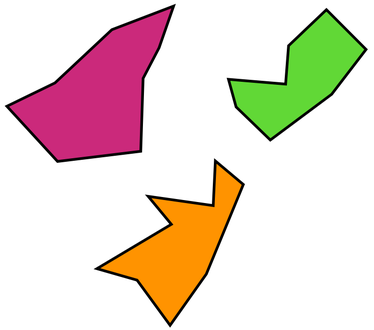
$$f(x) = a\exp(kx) + b$$

Hyper parameters open up an array of modelling choices

Learning rate

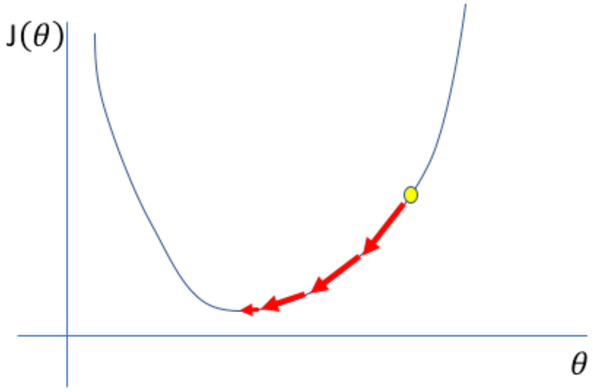


Hyper parameters open up an array of modelling choices

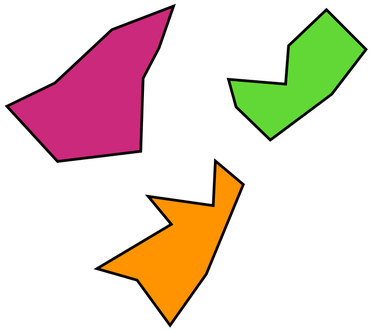


N-clusters

Learning rate



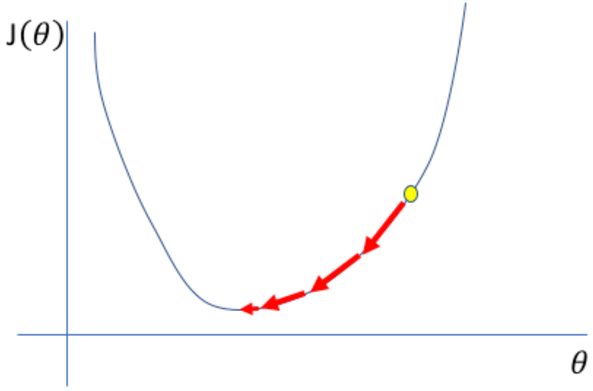
Hyper parameters open up an array of modelling choices



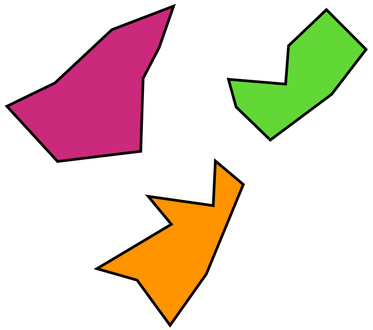
N-clusters

How many dimensions for reduction

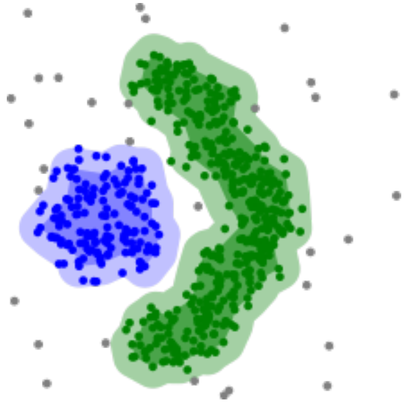
Learning rate



Hyper parameters open up an array of modelling choices



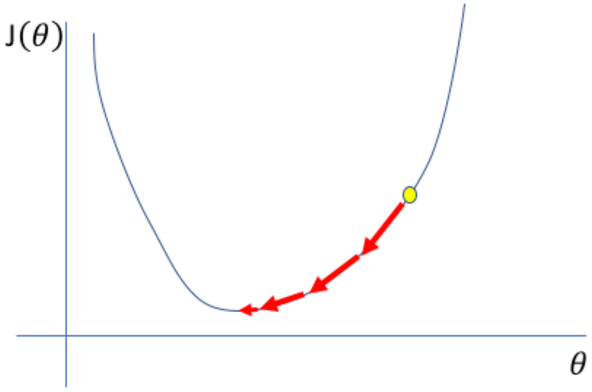
N-clusters



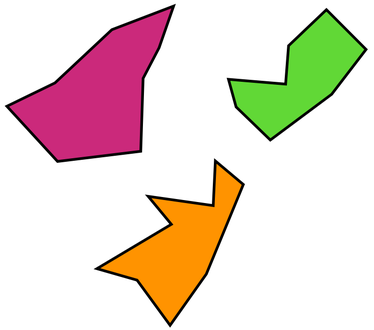
epsilon

How many dimensions for reduction

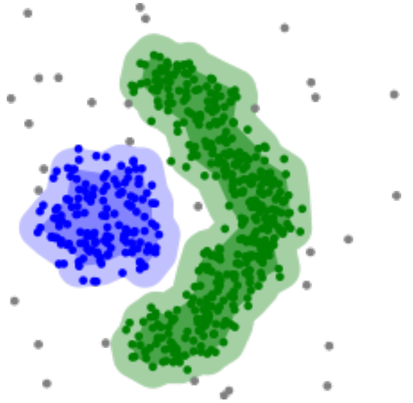
Learning rate



Hyper parameters open up an array of modelling choices



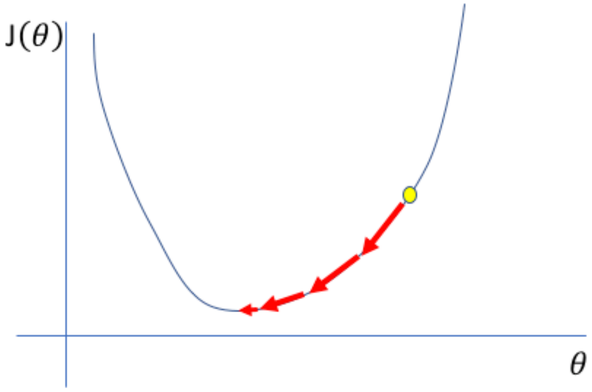
N-clusters



epsilon

How many dimensions for reduction

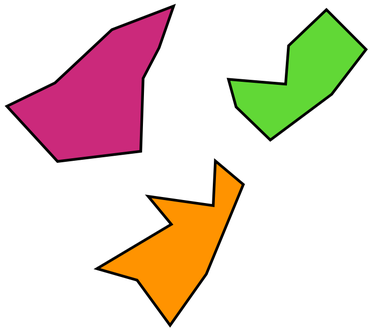
Learning rate



Optimiser	Year	Learning Rate	Gradient
Momentum	1964		✓
AdaGrad	2011	✓	
RMSprop	2012	✓	
Adadelta	2012	✓	
Nesterov	2013		✓
Adam	2014	✓	✓
AdaMax	2015	✓	✓
Nadam	2015	✓	✓
AMSGrad	2018	✓	✓

Choice of optimiser to minimise the loss

Hyper parameters open up an array of modelling choices



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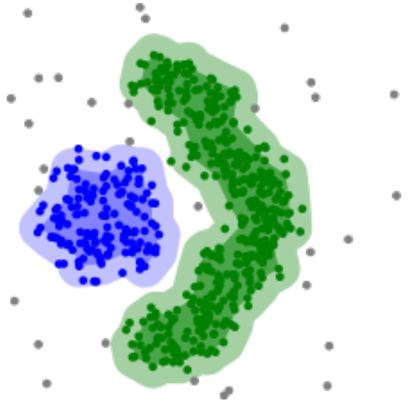
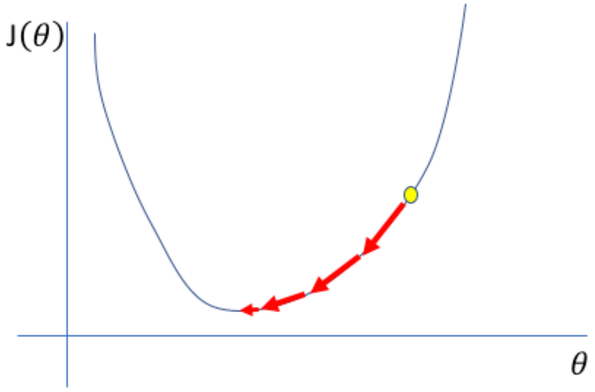


Choice of loss function

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

Learning rate



How many dimensions for reduction

epsilon

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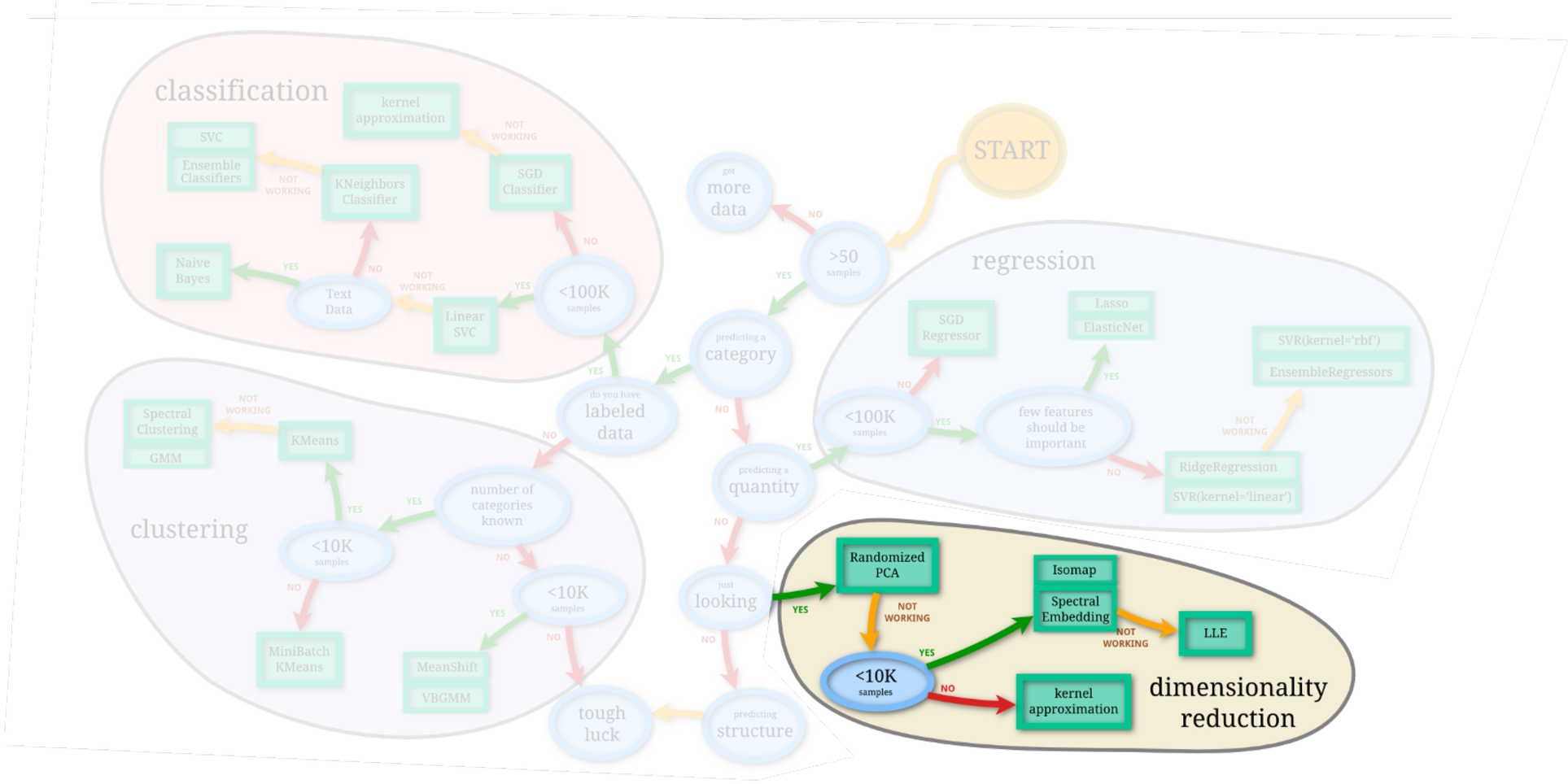
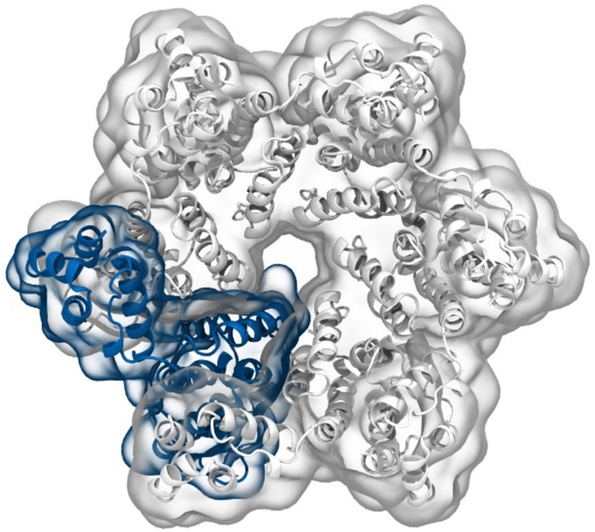
Choice of optimiser to minimise the loss

The Data Mining World — Dimensionality Reduction



From **scikit-learn.org**

What are the ‘dominant’ dimensions?



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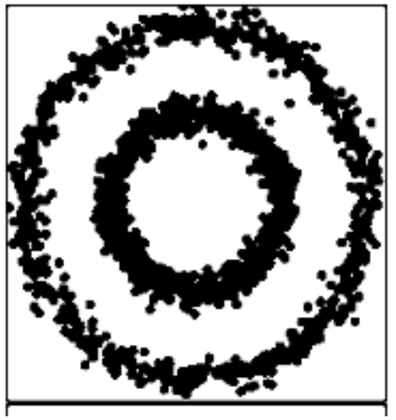
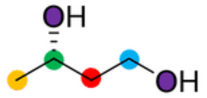


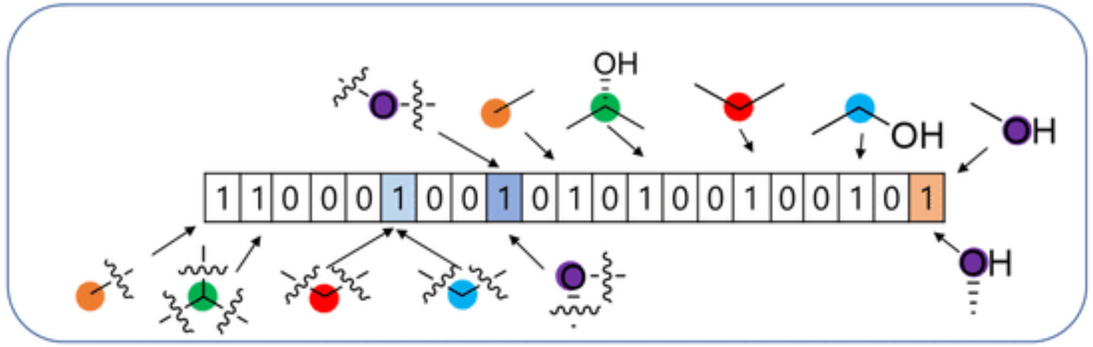
Dimensionality reduction

Feature vectors

```
['ATOM:ACE 1 CH3 1 x',
 'ATOM:ACE 1 CH3 1 y',
 'ATOM:ACE 1 CH3 1 z',
 'ATOM:ACE 1 C 4 x',
 'ATOM:ACE 1 C 4 y',
 'ATOM:ACE 1 C 4 z',
 'ATOM:ACE 1 O 5 x',
 'ATOM:ACE 1 O 5 y',
 'ATOM:ACE 1 O 5 z',
 'ATOM:ALA 2 N 6 x',
 'ATOM:ALA 2 N 6 y',
 'ATOM:ALA 2 N 6 z',
 'ATOM:ALA 2 CA 8 x',
 'ATOM:ALA 2 CA 8 y',
 'ATOM:ALA 2 CA 8 z',
 'ATOM:ALA 2 CB 10 x',
 'ATOM:ALA 2 CB 10 y',
 'ATOM:ALA 2 CB 10 z',
 'ATOM:ALA 2 C 14 x',
 'ATOM:ALA 2 C 14 y',
 'ATOM:ALA 2 C 14 z',
 'ATOM:ALA 2 O 15 x',
 'ATOM:ALA 2 O 15 y',
 'ATOM:ALA 2 O 15 z',
 'ATOM:NME 3 N 16 x',
 'ATOM:NME 3 N 16 y',
 'ATOM:NME 3 N 16 z',
 'ATOM:NME 3 C 18 x',
 'ATOM:NME 3 C 18 y',
 'ATOM:NME 3 C 18 z']
```



Molecular structure

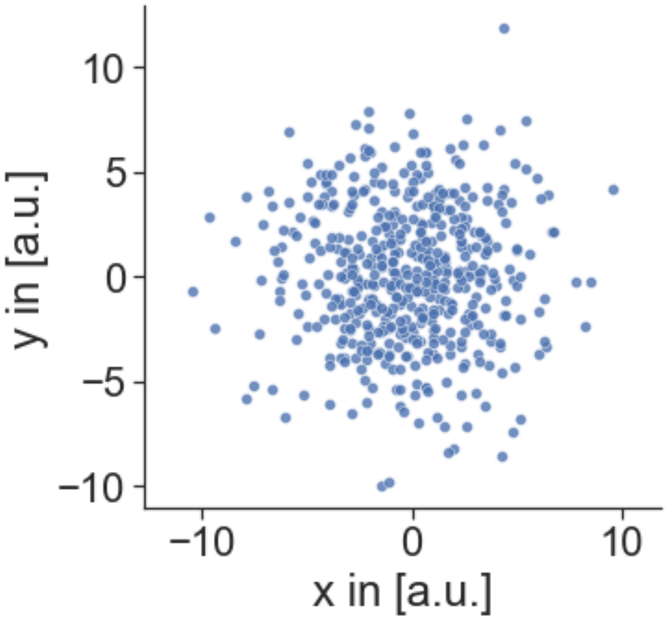


Original Morgan fingerprints

- Clustering on high dimensional data is difficult because often **not enough data is available.**
- How can you identify the **most important features before e.g. clustering?**

Principal component analysis (PCA)

- Principle component analysis finds the **dominant component** in the feature space
- A regression finds the **correlation** of the data in feature space



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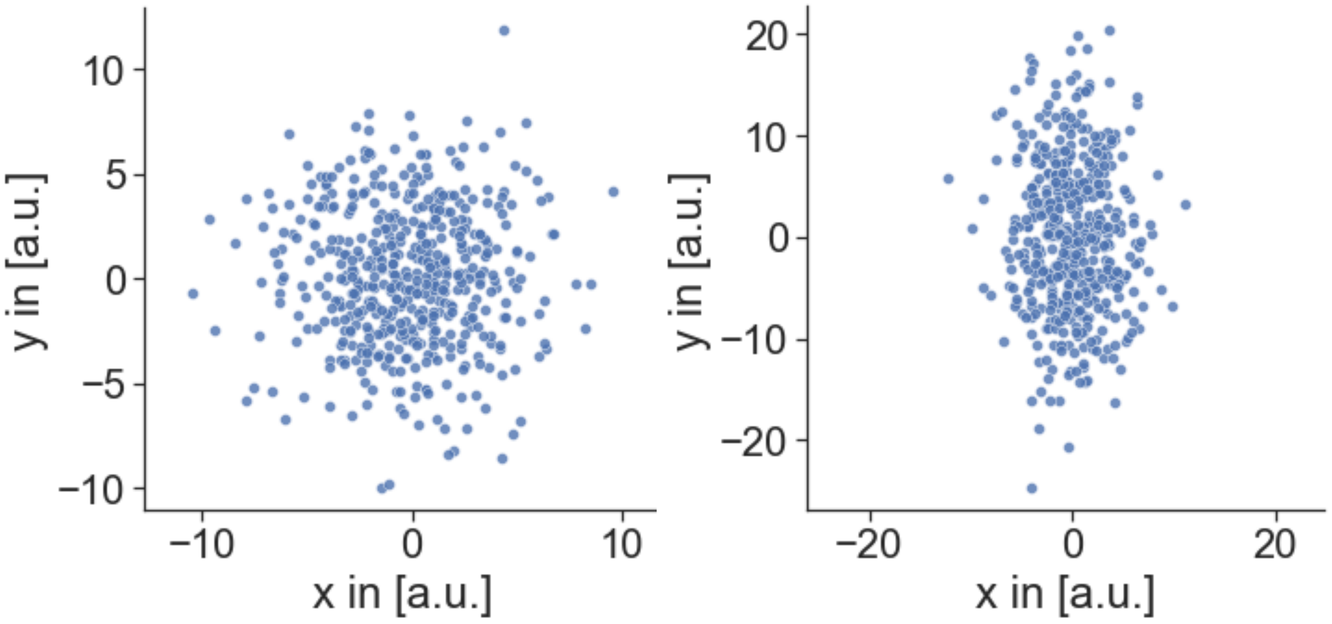

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- Principle component analysis finds the **dominant component** in the feature space
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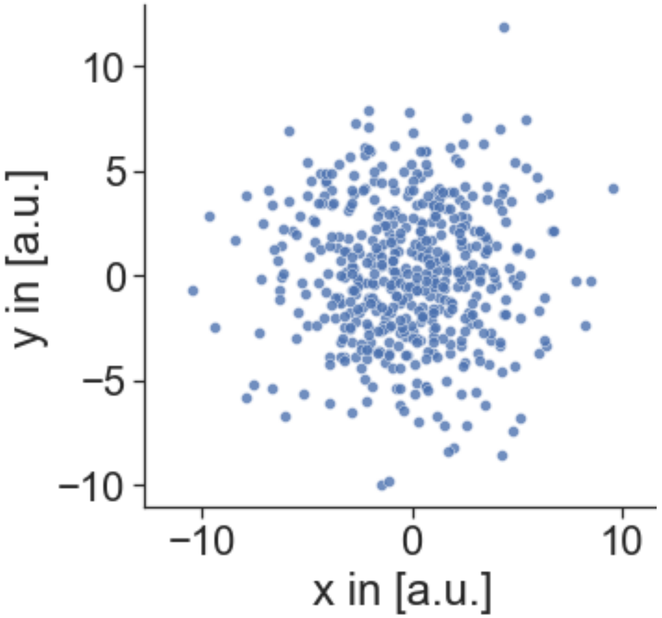

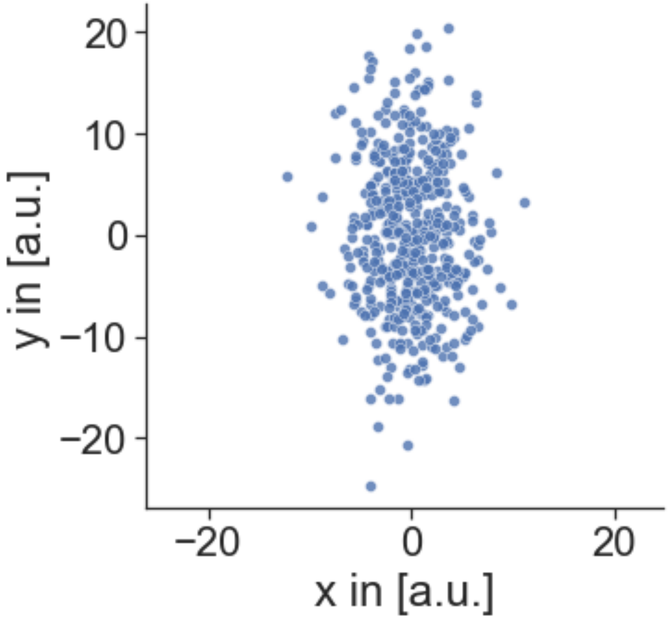

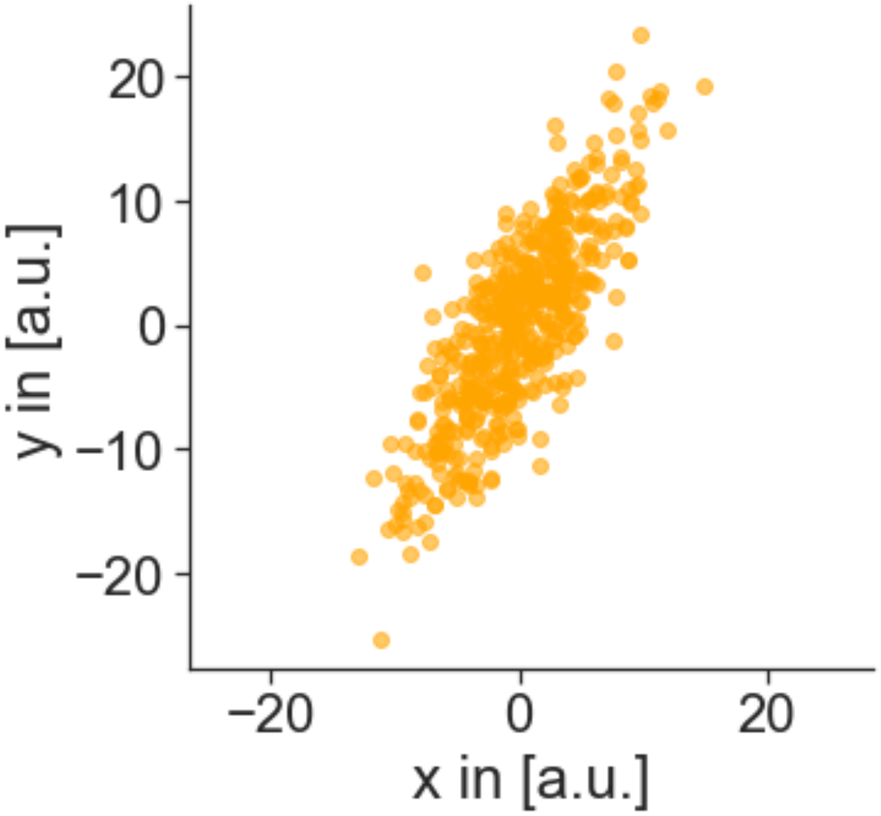

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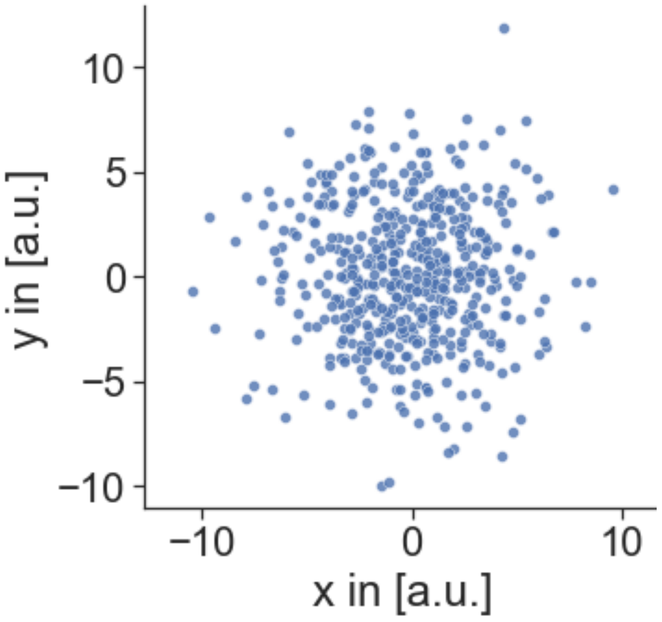

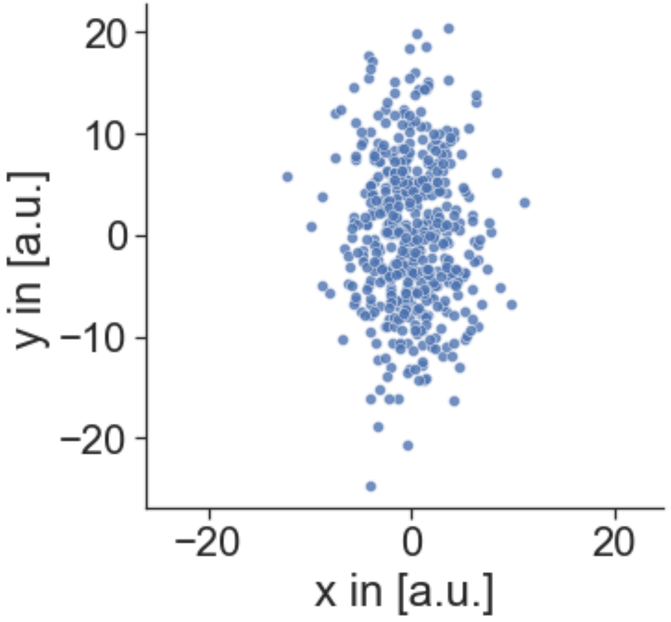

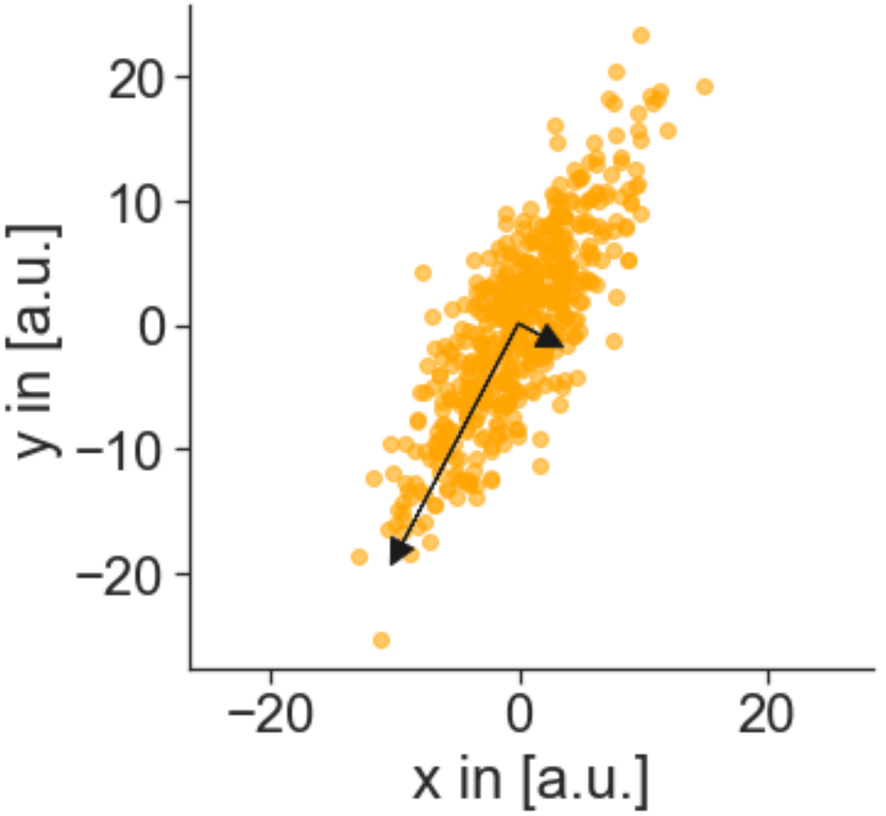

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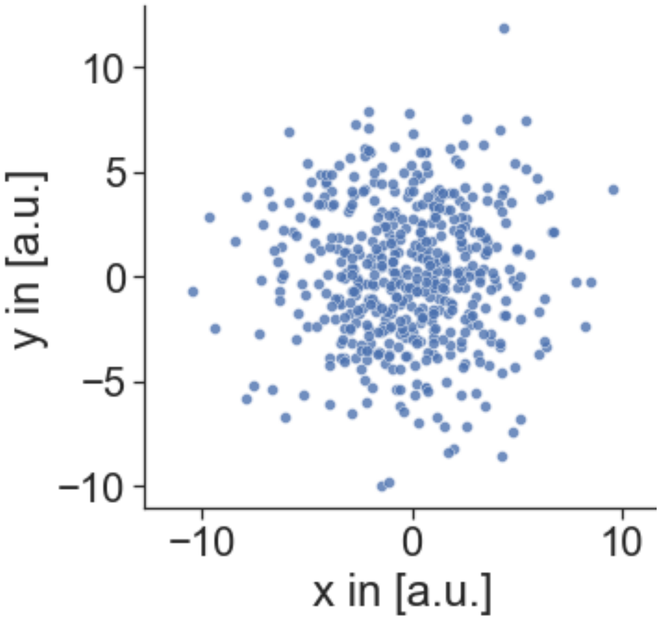

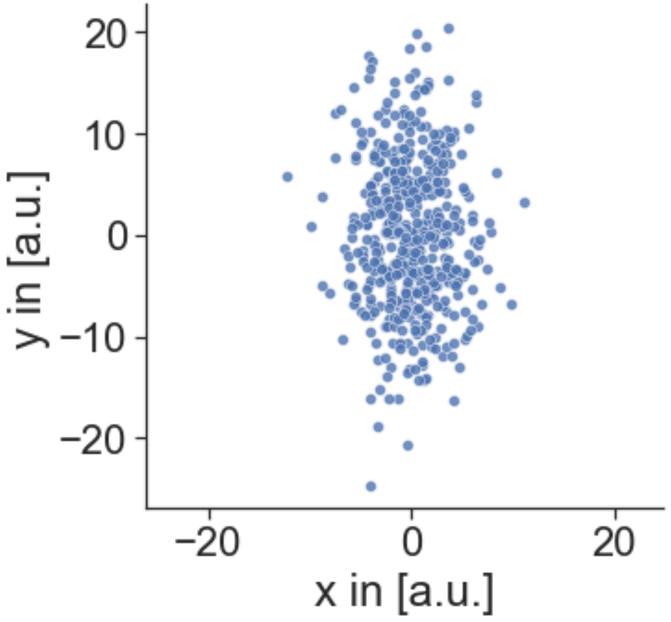

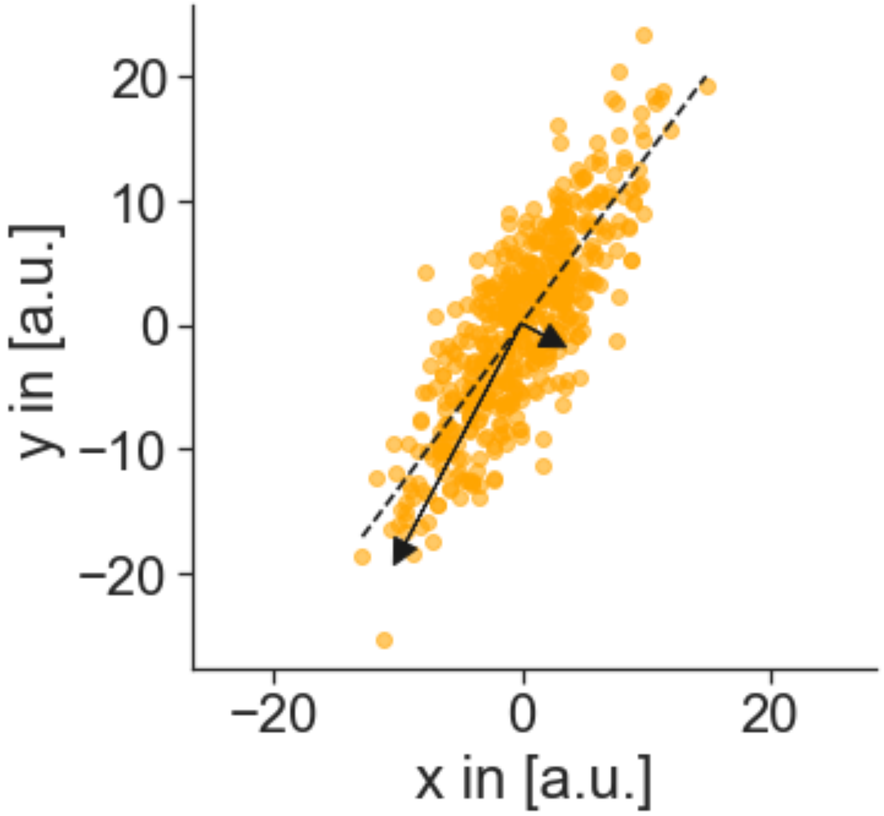

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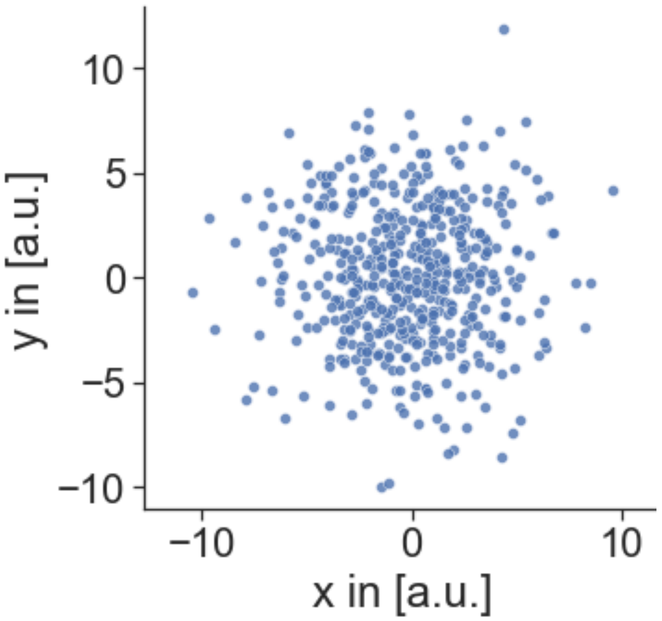

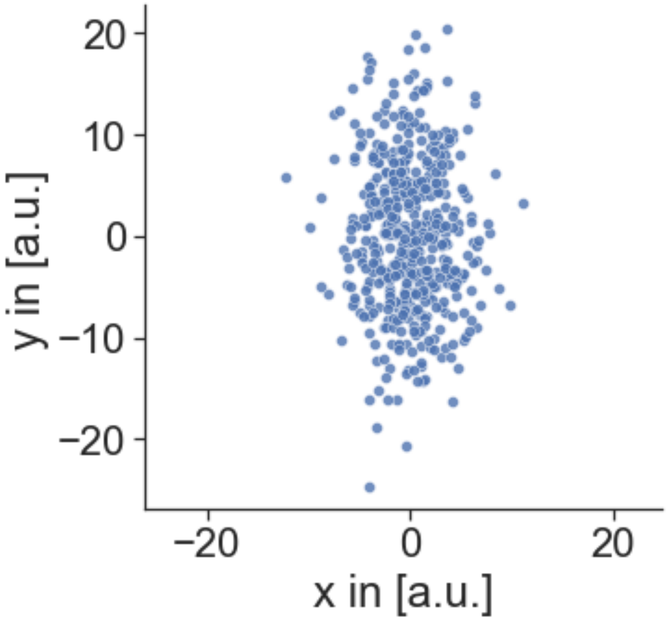

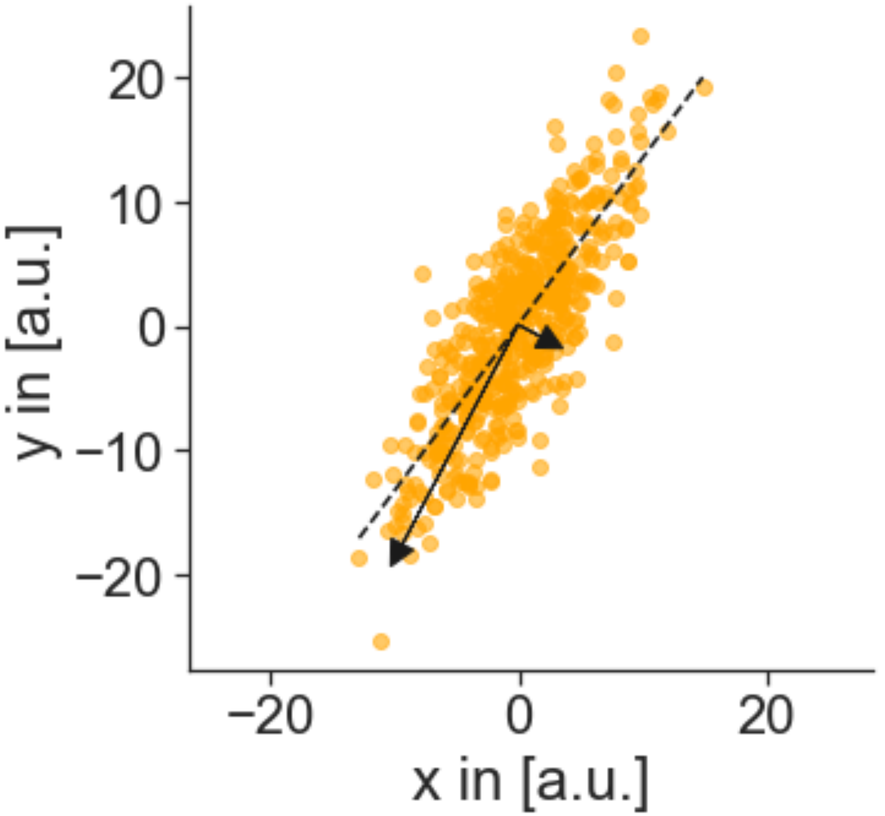

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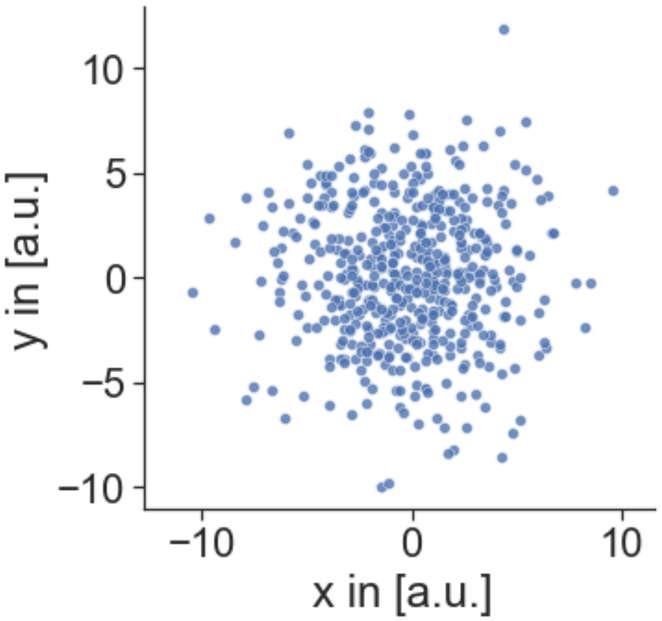

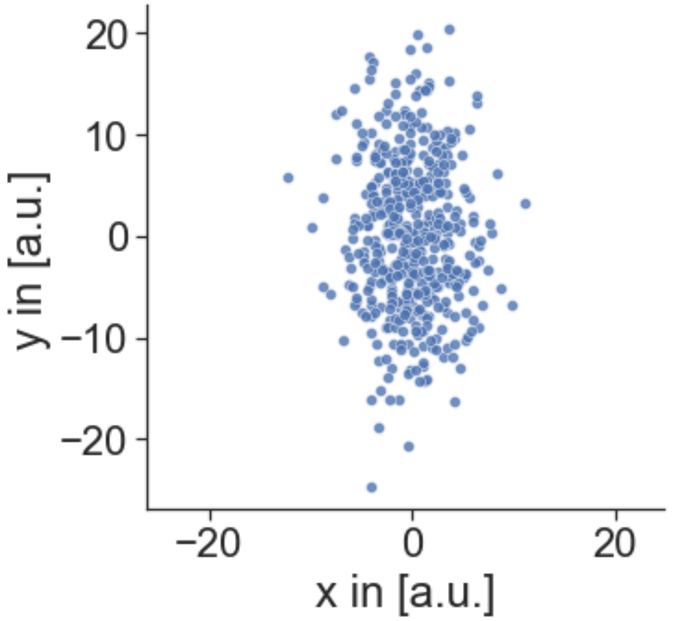

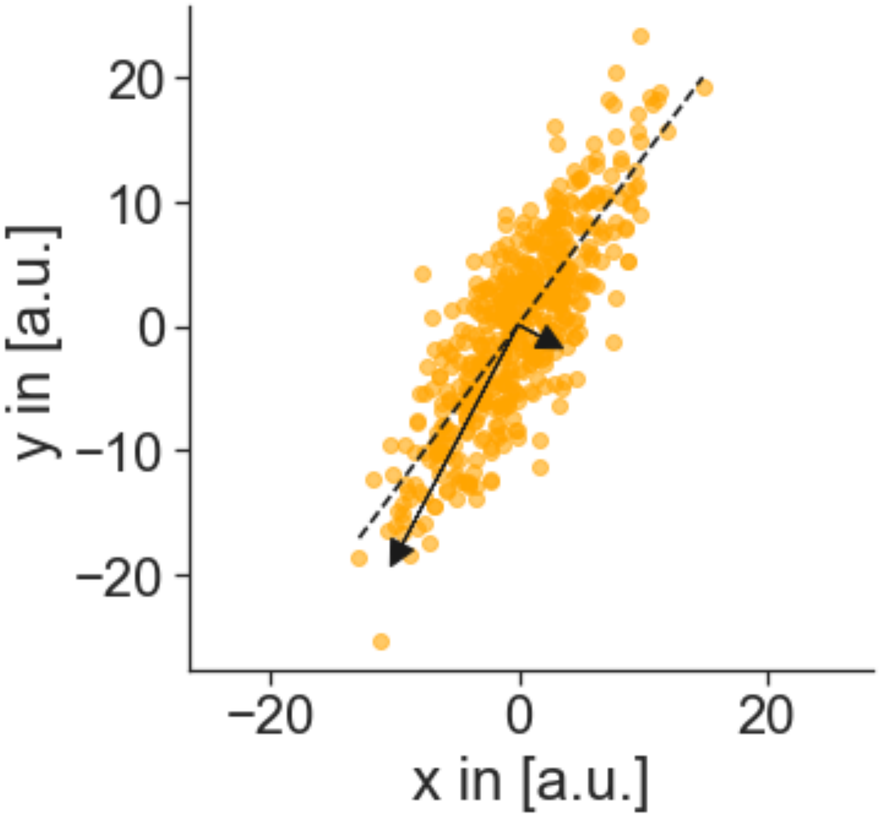

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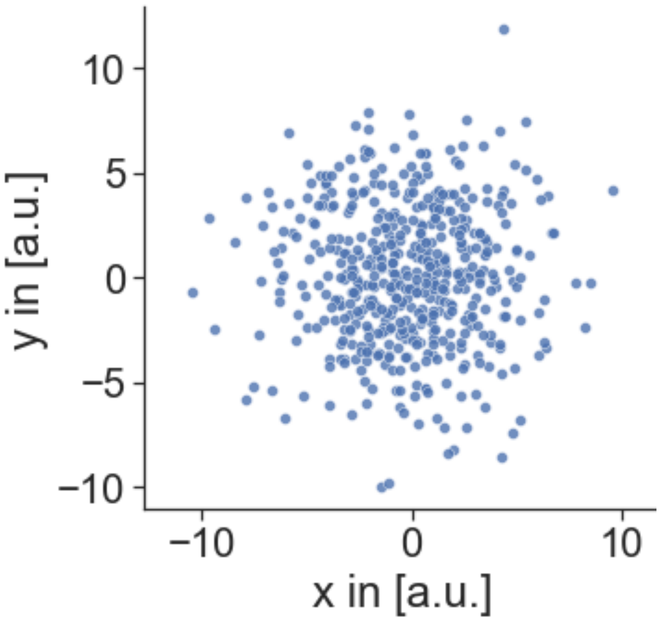

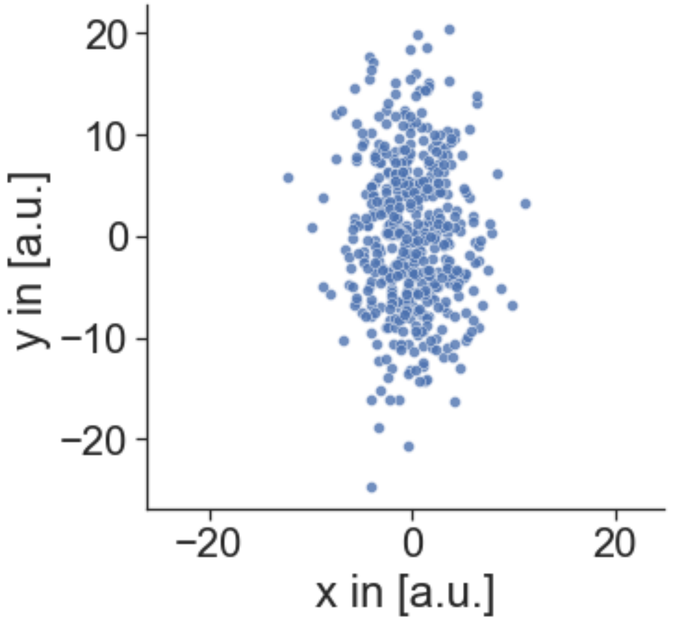

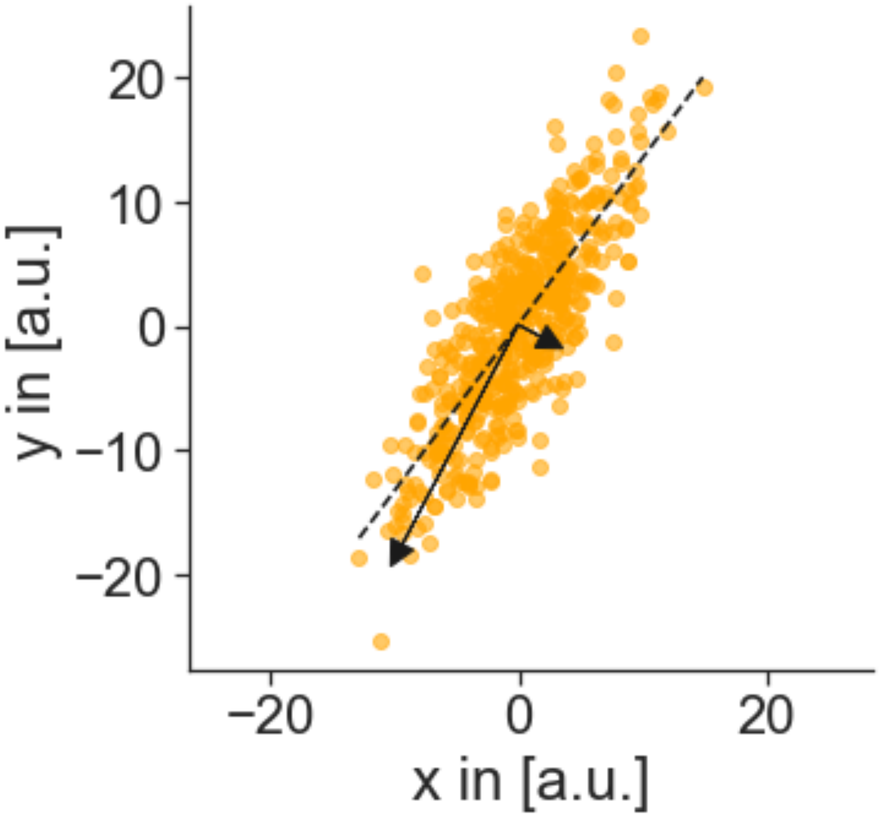

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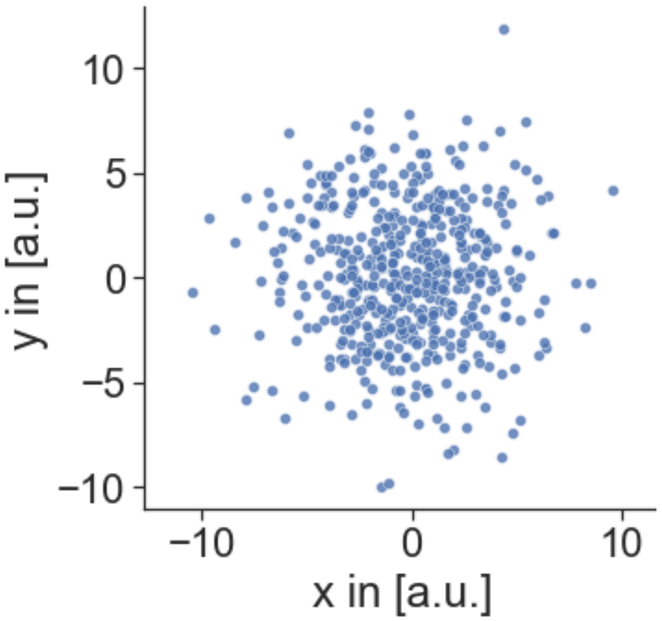

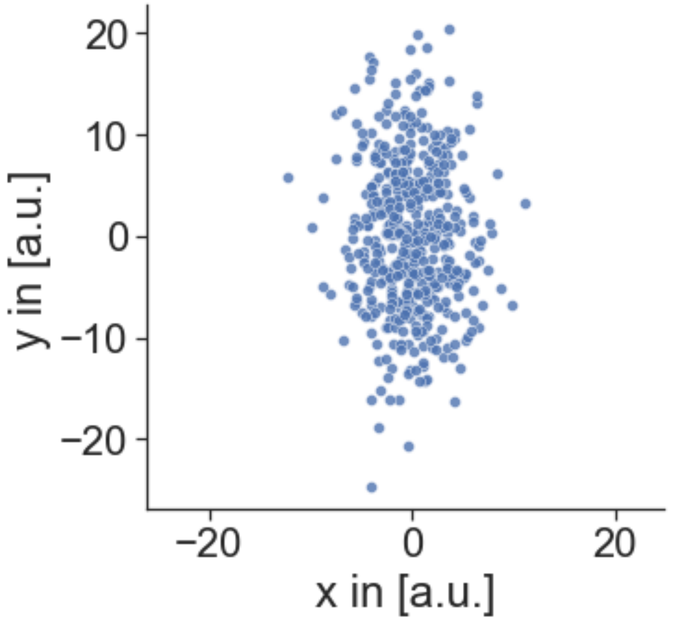

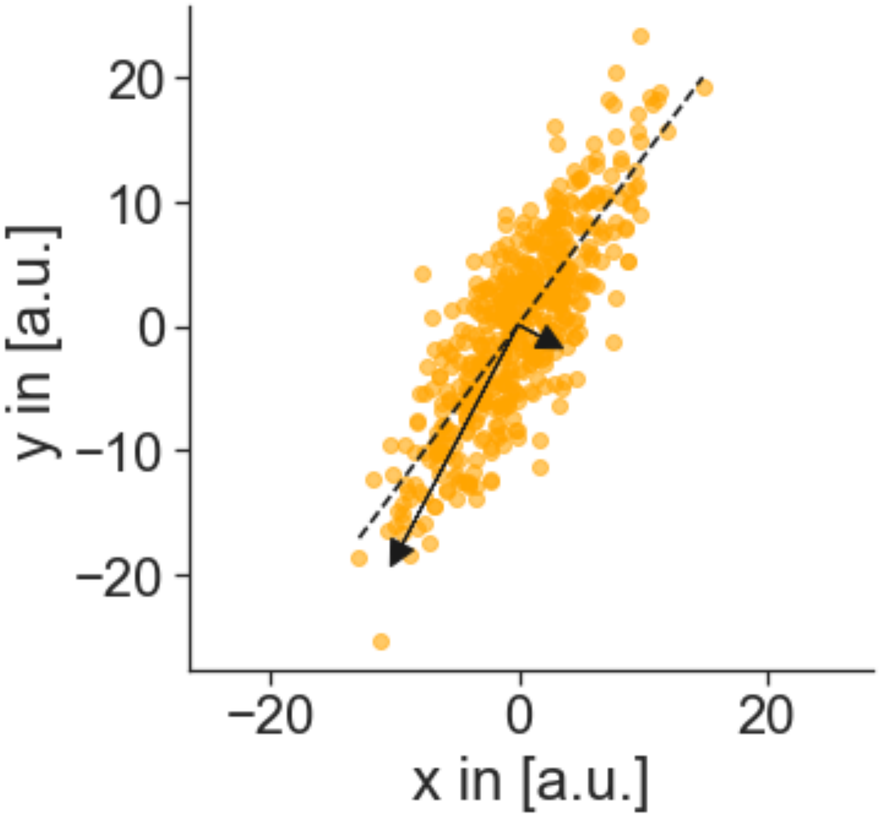

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Solving the generalised eigenvalue problem

$$\mathbf{C}(0)\mathbf{W} = \mathbf{W}\boldsymbol{\Sigma}$$

Gives an eigenvector matrix **W** that will allow the transform of the original data **X** onto a new basis **T** that maximises the variance.

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It is possible to choose m eigenvectors to project onto by only using the first m-columns of **W**.

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The would be the 'dominant' features!

PCA example

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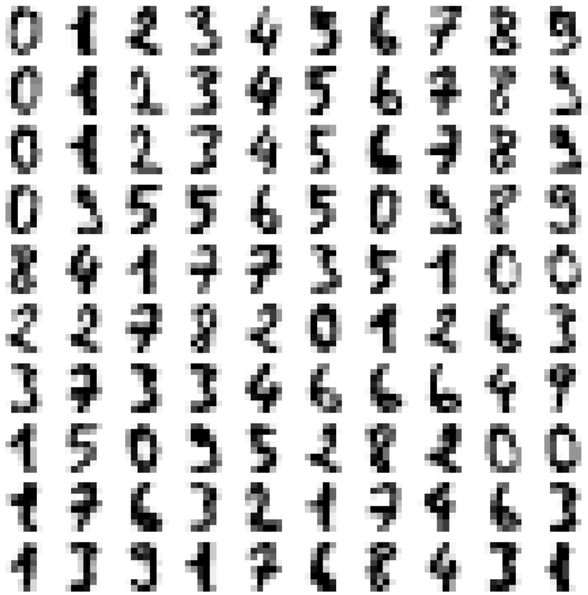
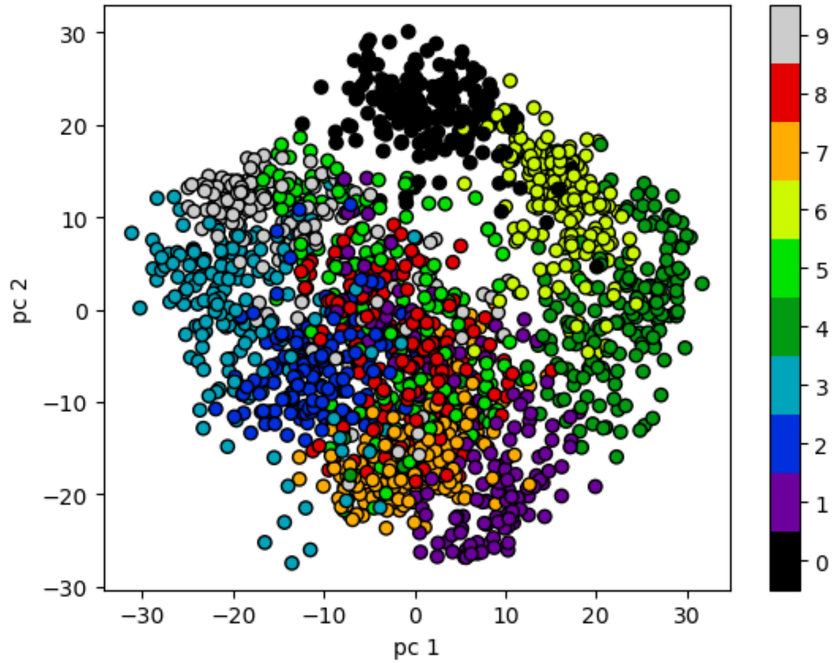
MNIST database of written digits



Input is a vector of 64 dimensions 8x8 pixel digits



2 principle components manage to project a few of the digits in a similar area of space!

PCA example

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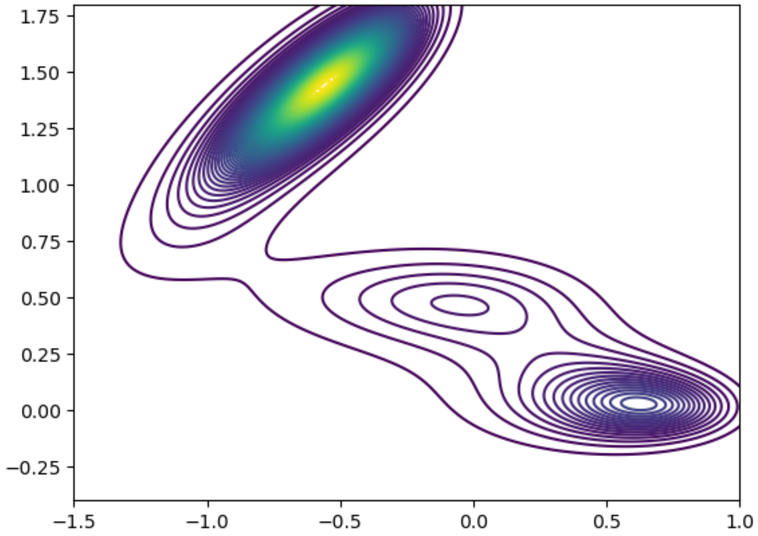
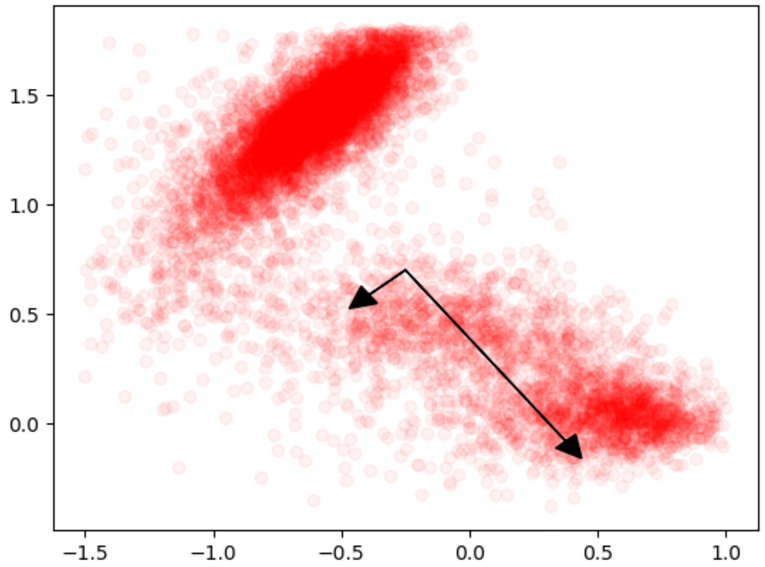


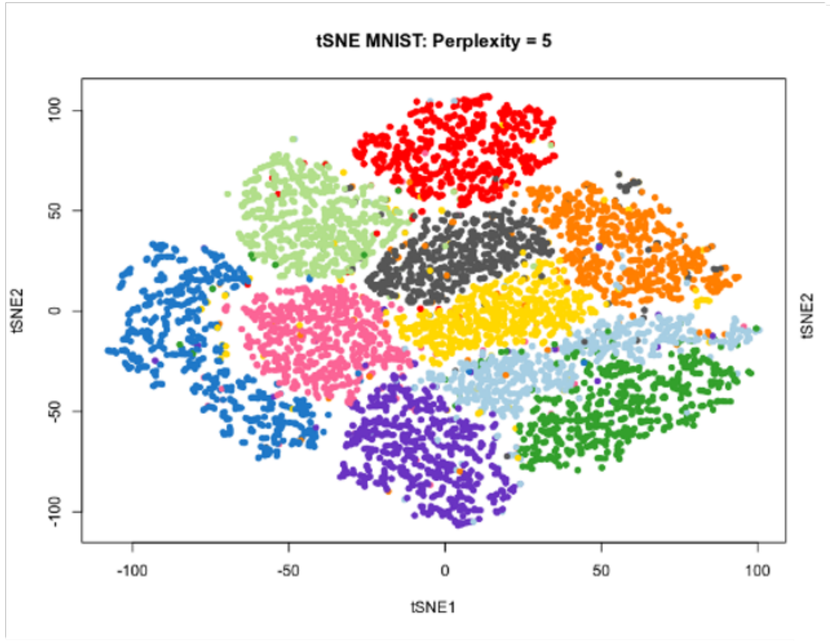


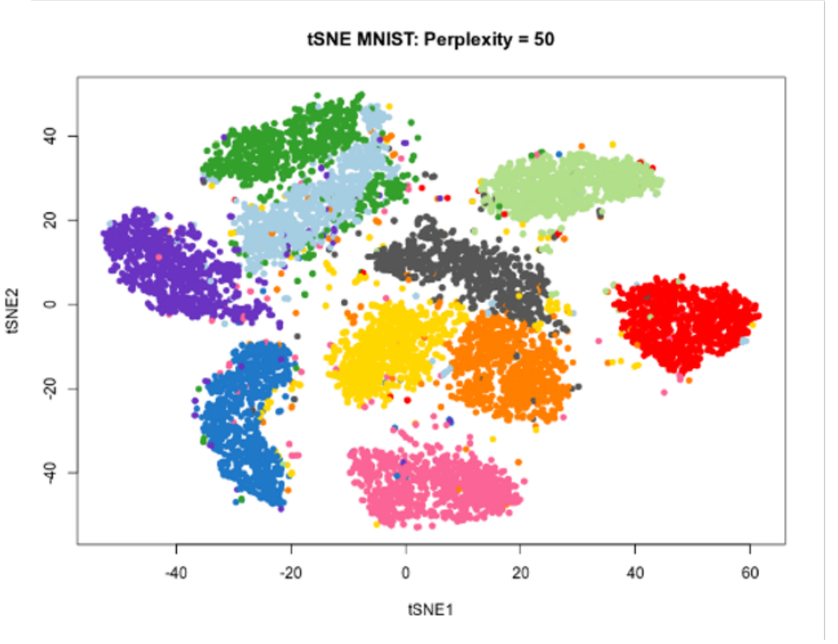
Finding the dominant reaction coordinate of a potential energy surface of a reaction!

T-distributed Stochastic Neighbour Embedding (t-SNE)

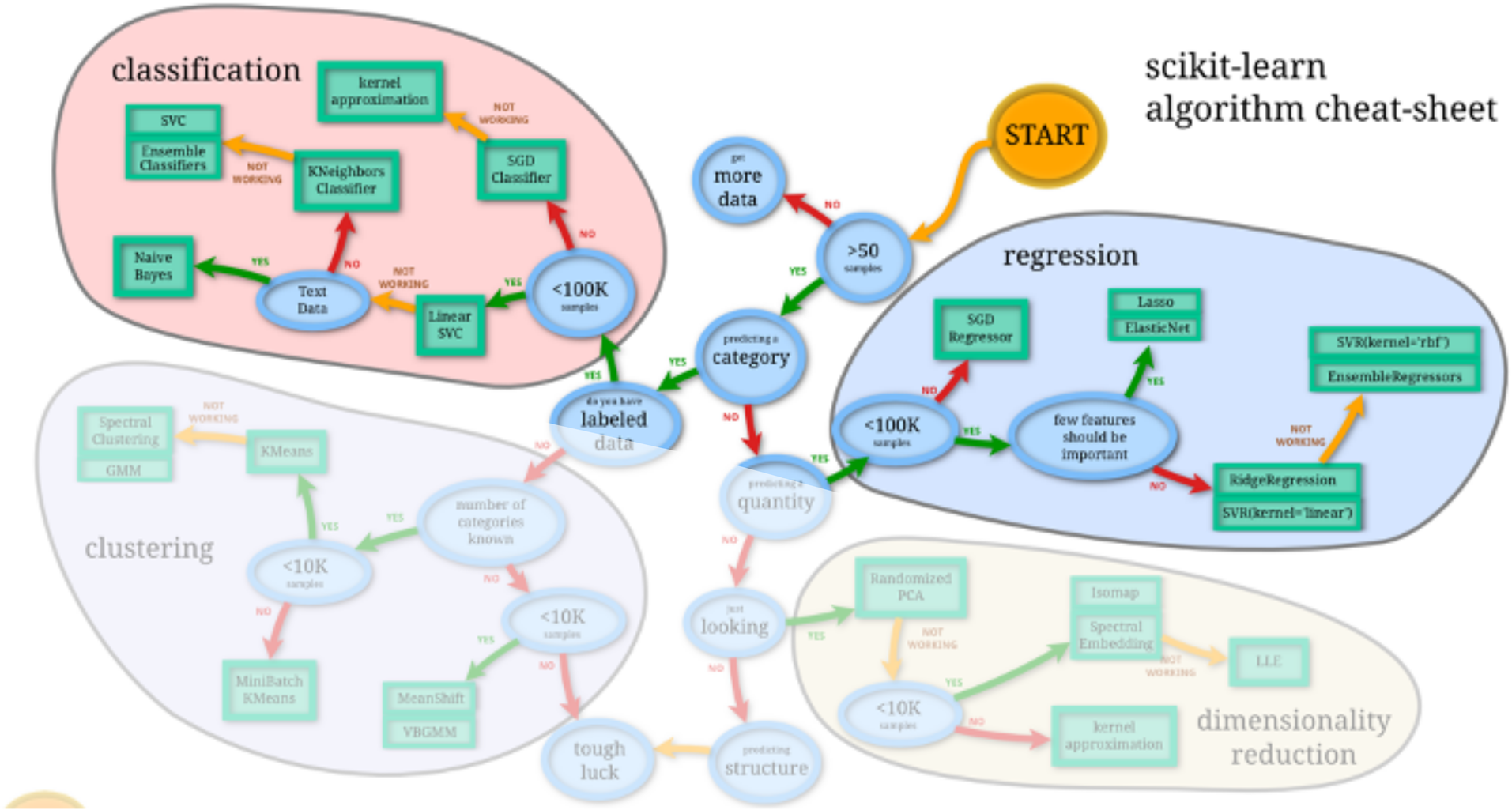
- Useful for visualisation, project high-dimensional data in 2 or 3 dimensions.
- Controlled by one main parameters: “perplexity”
- Relative distance between points not quantitatively meaningful

MNIST: database of written digits





ML Algorithms for classification and regression



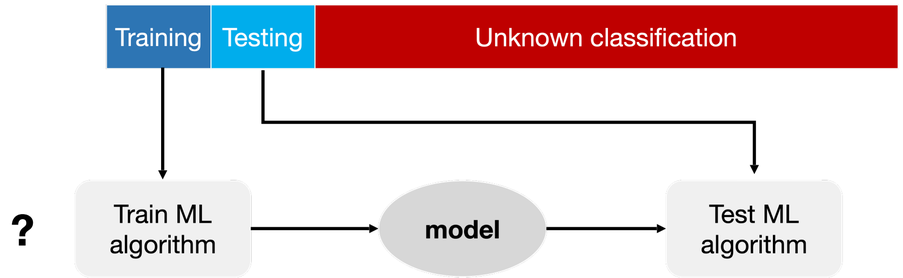
Learning Algorithms

Classification task

- **Decision Tree (DT)**
- **Random Forests (RF)**
- **Artificial Neural Network (ANN)**
- Support Vector Machine (SVM)
- Logistic Regression (LOGRES)
- Naïve Bayes (NB)
- K Nearest Neighbor (KNN)
- ...

Regression task

- **Decision Tree Regression (DT)**
- **Random Forests (RF)**
- **Neural Network Regressions (ANN)**
- Support Vector Machine (SVM)
- Linear Regression (LR)
- K Nearest Neighbor (KNN)
- Gaussian Regression
- ...



How do I pick the best learning algorithm?

Learning algorithms quality criteria:

- **accuracy**: percentage of correct classification

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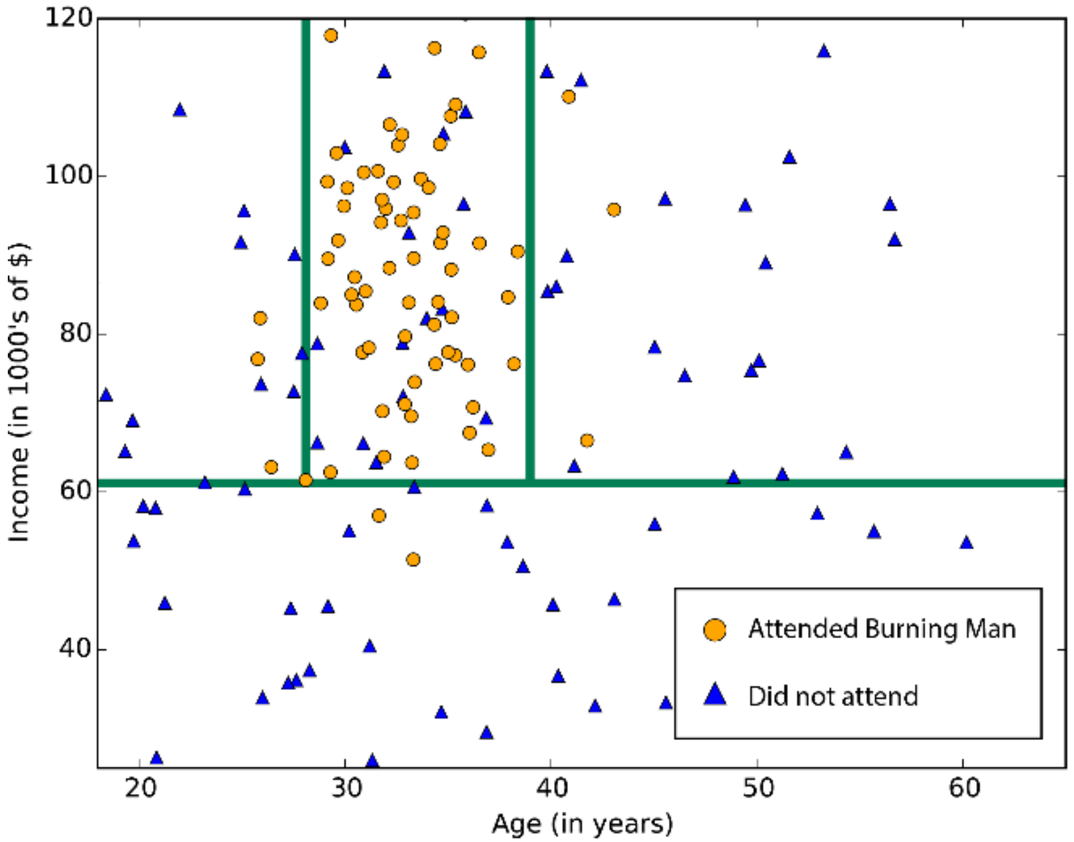
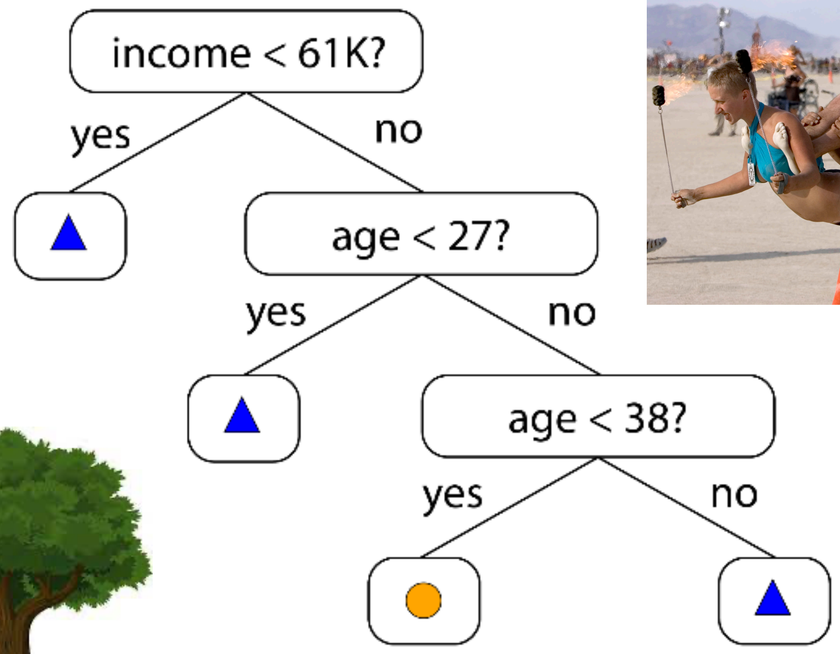
Learning algorithms quality criteria:

- **accuracy**: percentage of correct classification
- **robustness**: handling noise and missing values
- **efficiency**: time to construct and use the model
- **scalability**: efficiency in memory requirements
- **interpretability**: how much the model is understandable

Decision Trees (DT)





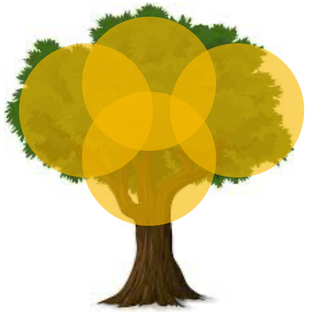
- Subdivides features space in sectors
- Can overfit if space subdivision becomes too fine

azure.microsoft.com/en-us/documentation/articles/machine-learning-algorithm-choice

Bootstrap Aggregating (Bagging)

training set *D* with *m* examples

D= | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |



L. Breiman, *Bagging Predictors,* in *Machine* Learning, Springer, 1996

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A weighted sum of weak classifiers creates a single strong classifier

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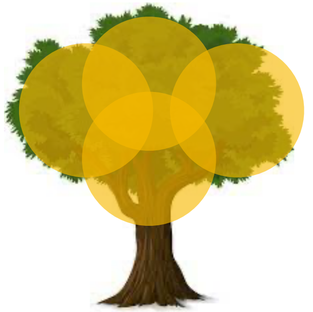

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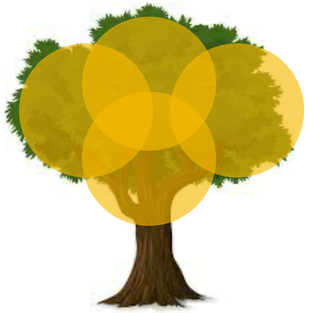

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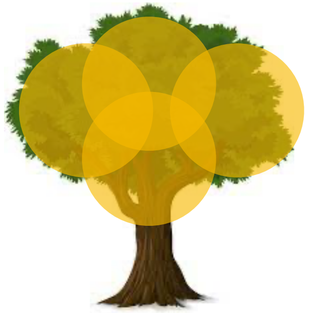

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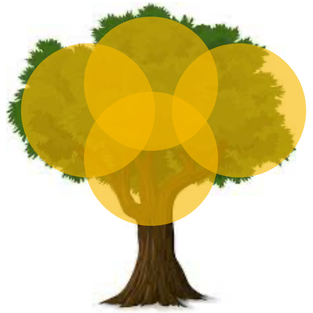
S[0]=

5	1	7	2	7	9	2	6	5



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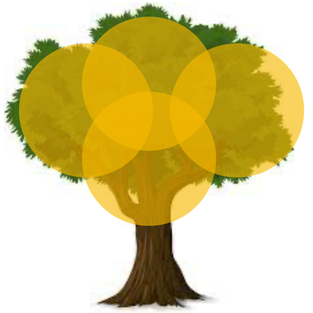
S[1]=	9	4	7	1	2	8	9	7	6
S[2]=	0	8	2	0	9	7	7	0	1
	...								
S[*N*]=	1	2	3	4	5	6	7	8	9



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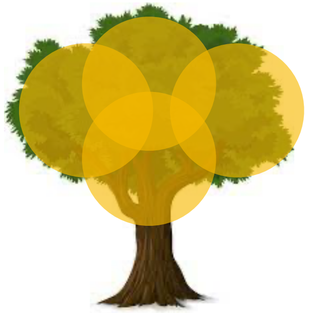

Training: for every S, build a distinct classifier C using the same learning algorithm

L. Breiman, *Bagging Predictors,* in *Machine* Learning, Springer, 1996

Bootstrap Aggregating (Bagging)

A weighted sum of weak classifiers creates a single strong classifier

Useful when a small change to training set causes large change in the output classifier ("learner is unstable")

training set *D* with *m* examples

Create *N* bootstrap samples S drawing *m* random examples from *D* *with replacement*

D=	1	2	3	4	5	6	7	8	9
S[0]=	5	1	7	2	7	9	2	6	5
S[1]=	9	4	7	1	2	8	9	7	6
S[2]=	0	8	2	0	9	7	7	0	1
	...								
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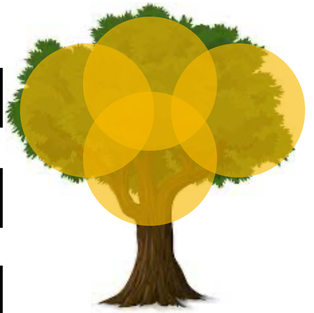
→C[0] →C[1] →C[2] →C[*N*]



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Random Forests (RF)

- **Data bagging**: creates *N* decision trees trained on bagged data

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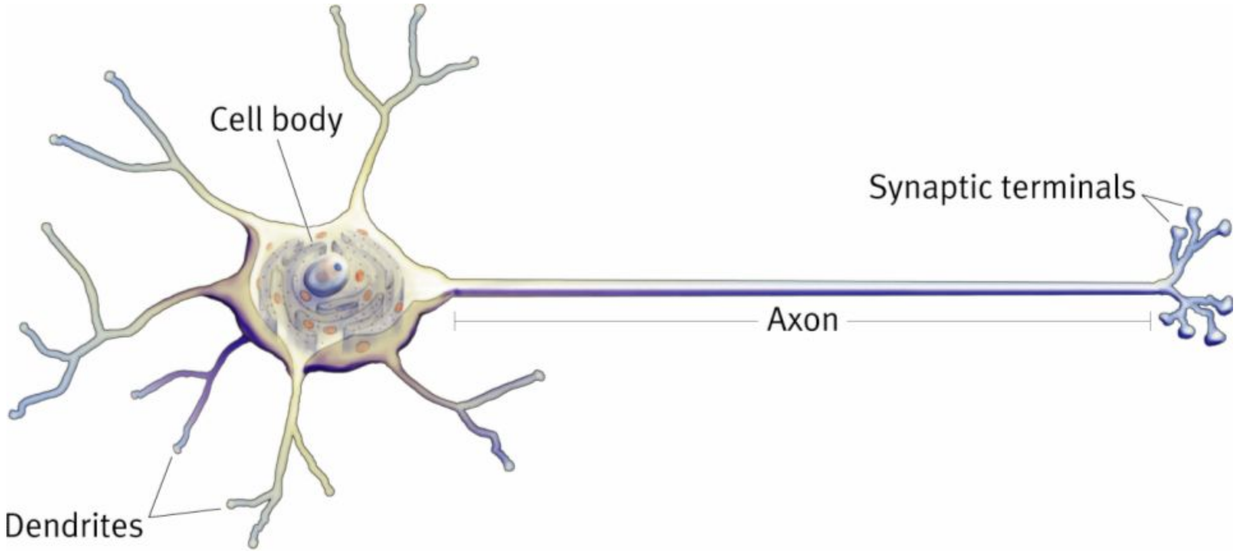
Advantages:

- does *not* overfit
- Can handle thousands of features
- estimates what variables are important for classification

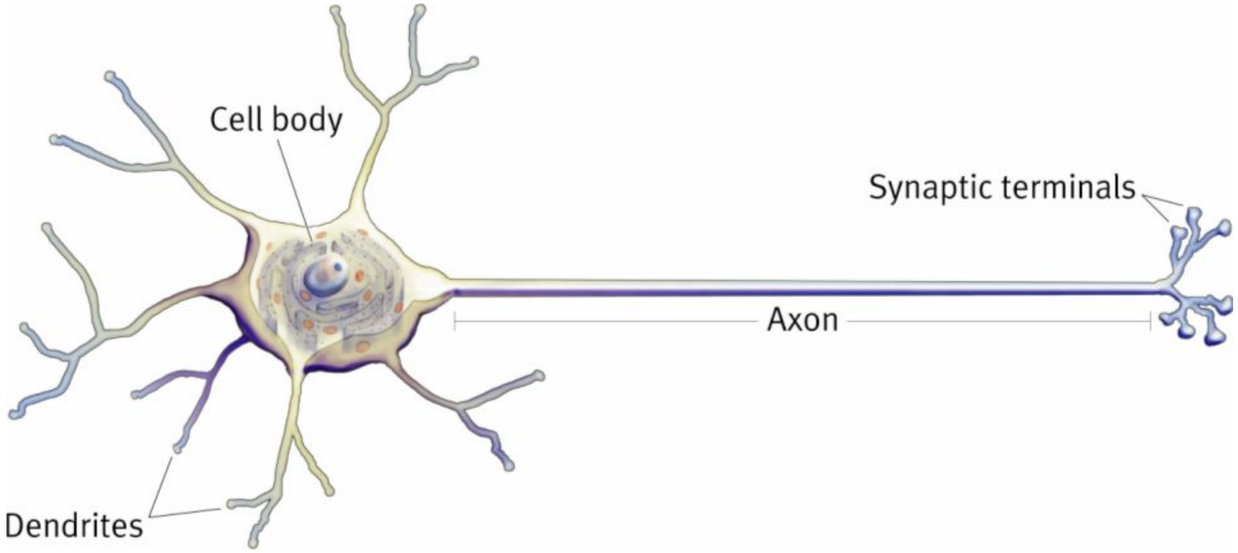
L. Breiman, *Random Forests*, Machine Learning, 2001

Artificial Neural Network



A **neuron** fires if input signal is above a threshold

Artificial Neural Network



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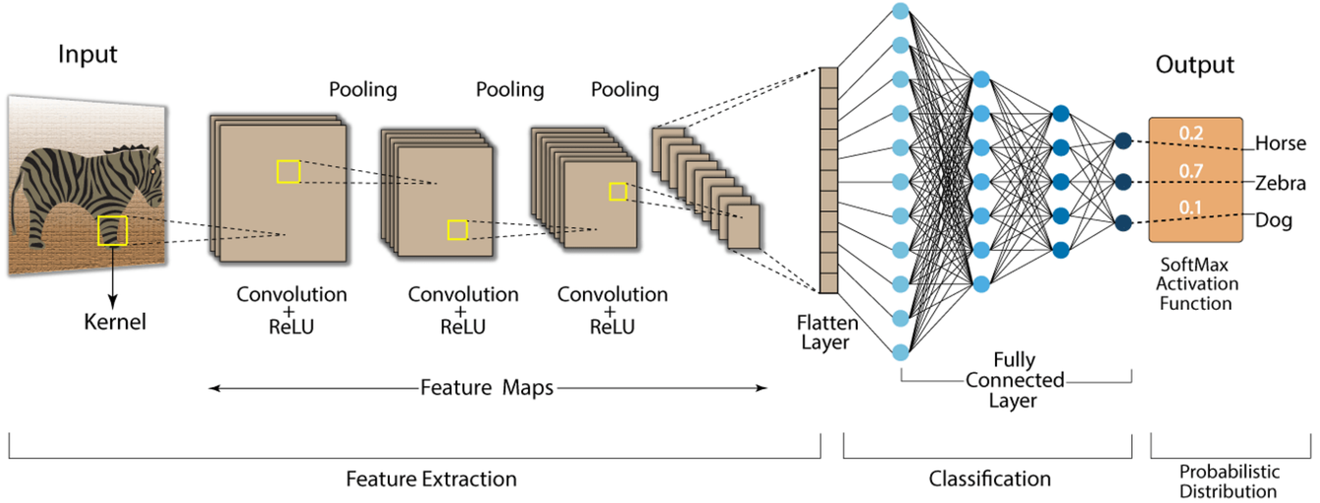
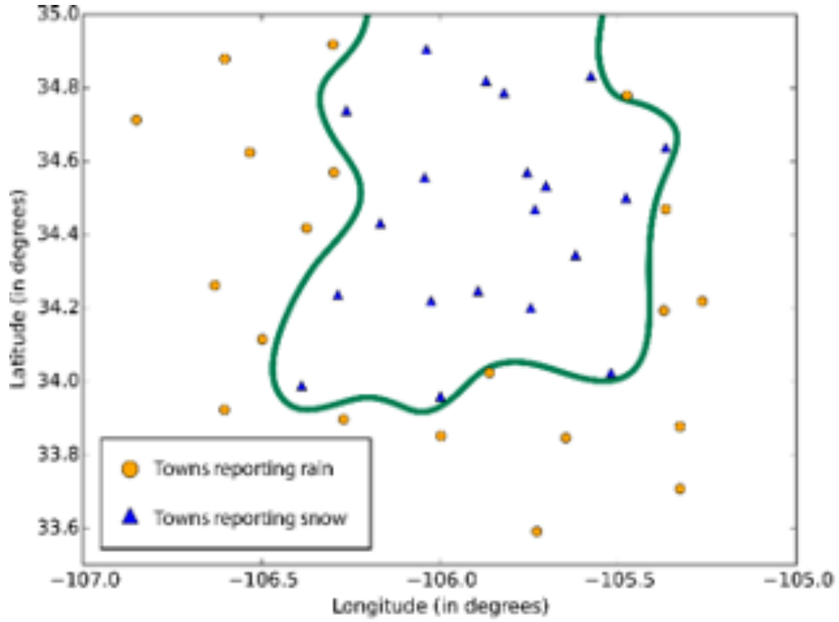
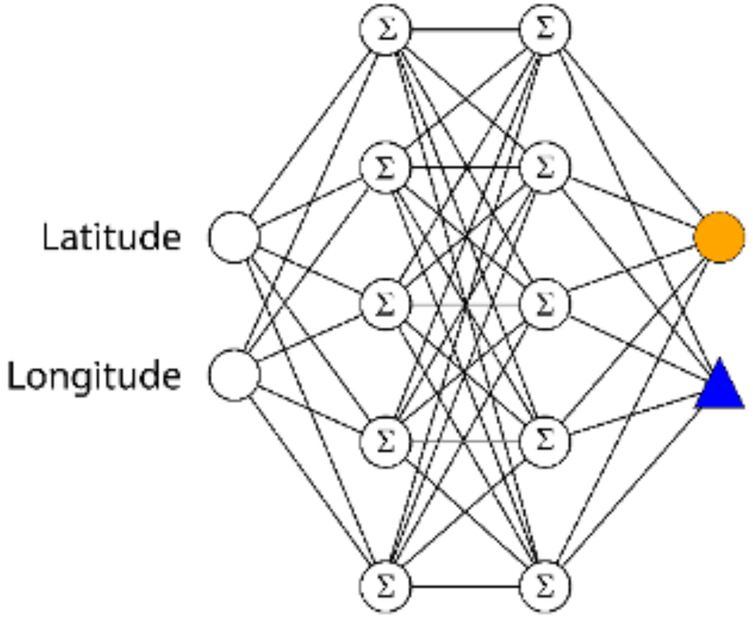
Many different complicated architectures are possible



Artificial Neural Network

Neurons can be arranged in **networks**
Hidden layers enable producing any complex boundary (in classification) or data fitting model (in regression)

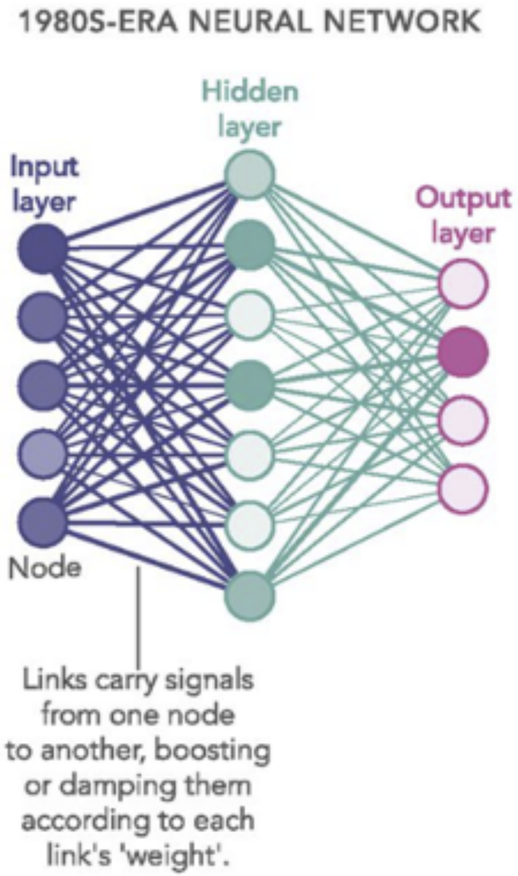


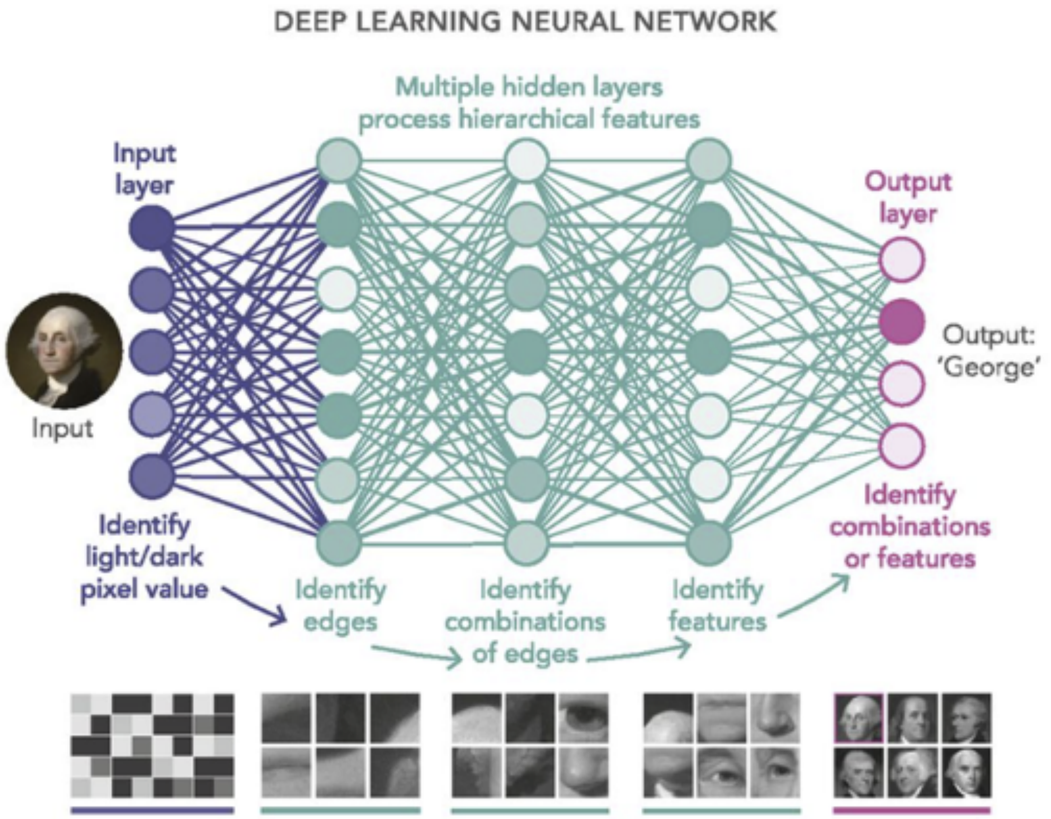


Training the ANN = finding synapses weights w_i minimizing error

ANN can fit any data, but are not easily interpretable

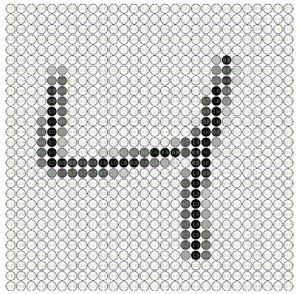
Multilayer perceptron





M.M. Waldrop, *News Feature: What are the limits of deep learning?*, ***PNAS***, 2019

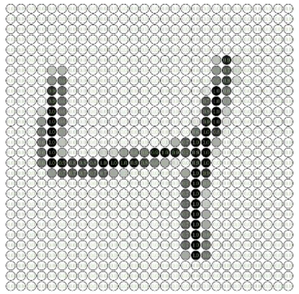
Multiple Output classification using a Multilayer Perceptron

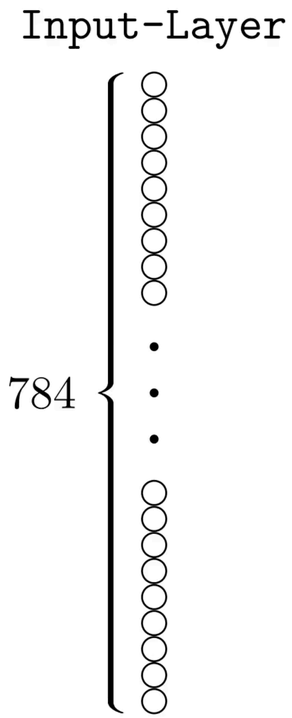


Artificial Neural Network (ANN)

4

Multiple Output classification using a Multilayer Perceptron





4

https://www.i-am.ai

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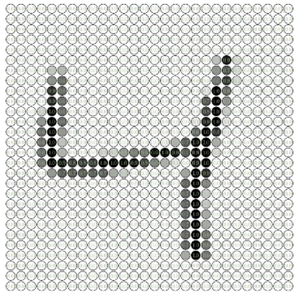

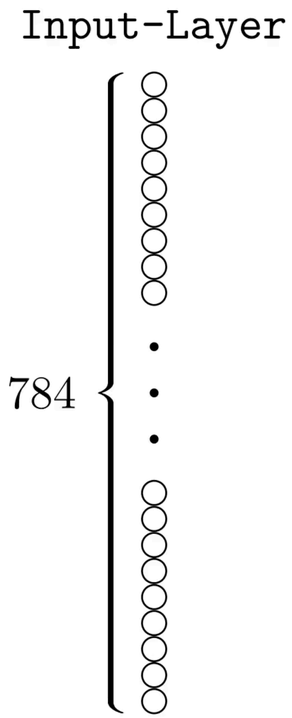

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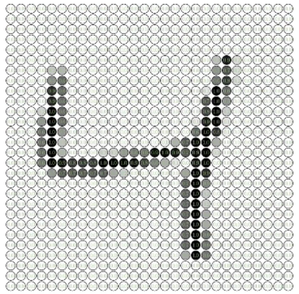

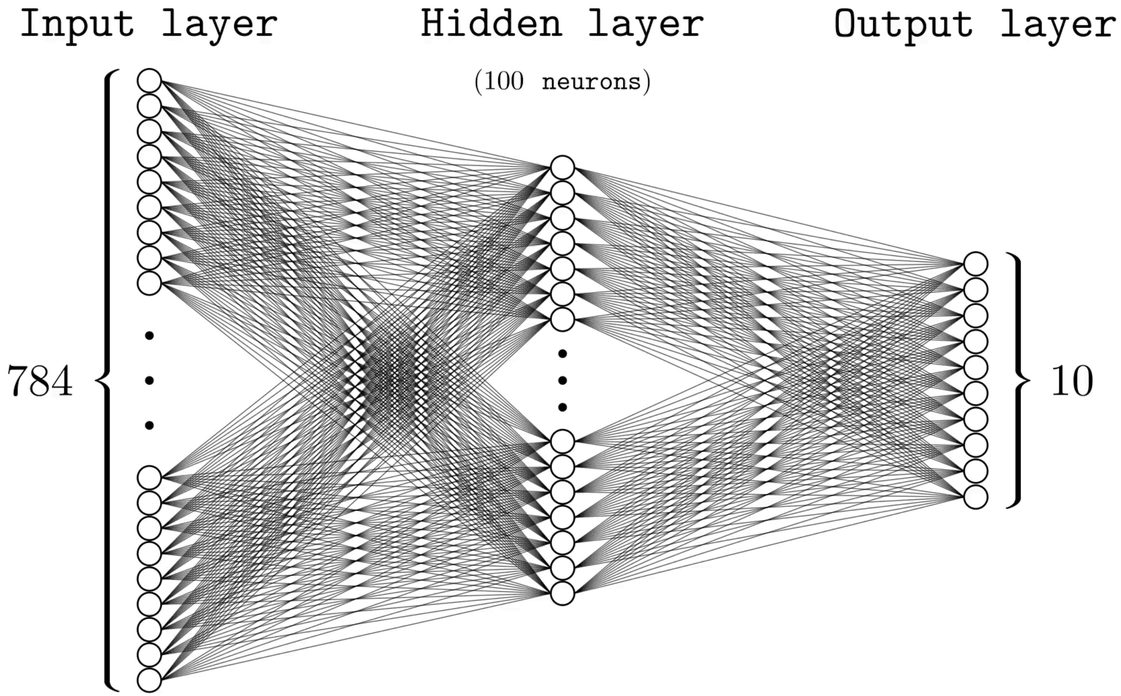

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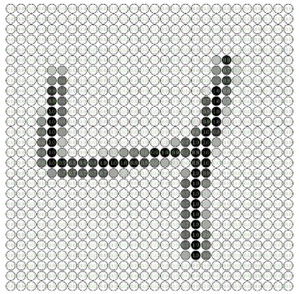

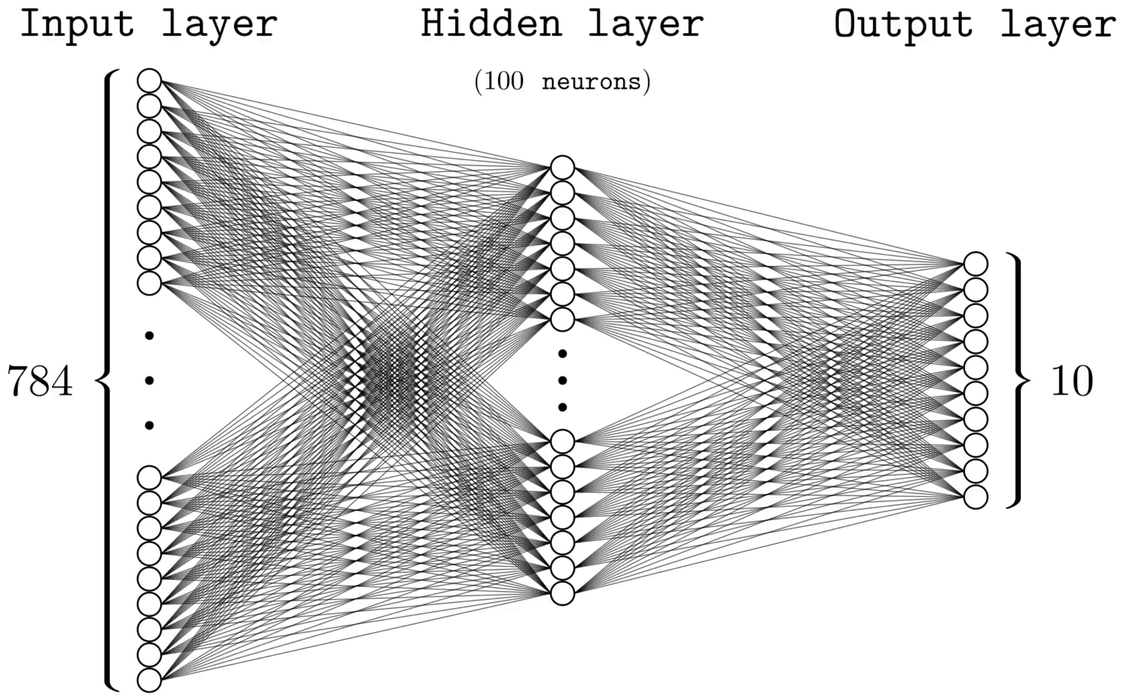

4

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Multilayer perceptron: the maths

Weighted input/output Weighted matrix input Bias

$$z^{(1)} = W^{(0)} a^{(0)} + b^{(1)}$$

$$a^{(l)} = \varphi^{(l)}(z^{(l)}) = \varphi^{(l)}\left(W^{(l-1)} a^{(l-1)} + b^{(l)}\right).$$

Activation function

Activation functions:

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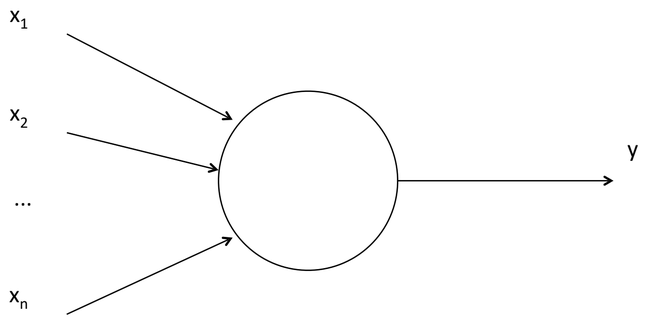

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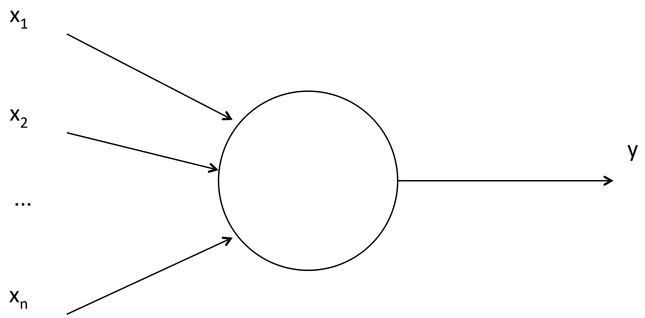

$f(a_1w_1 + a_2w_2 + ... + a_nw_n+b) = z$

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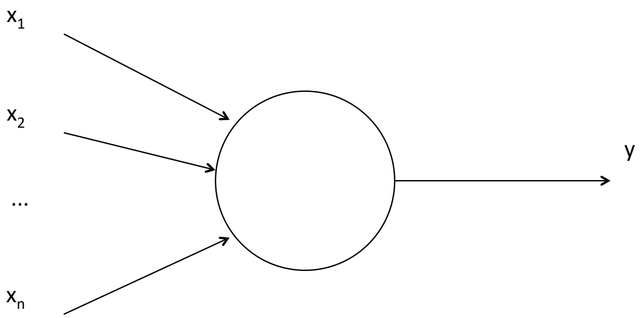

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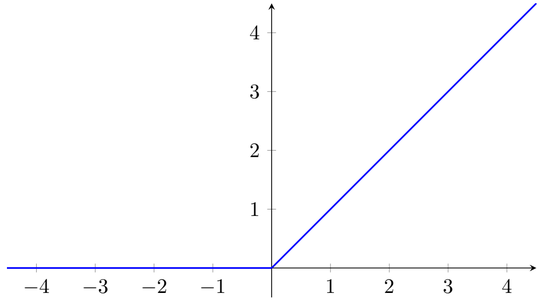
Activation functions:

ReLu:

$$\mathrm{ReLU}(z) = \begin{cases} 0, & z \leq 0 \\ z, & z > 0 \end{cases}$$



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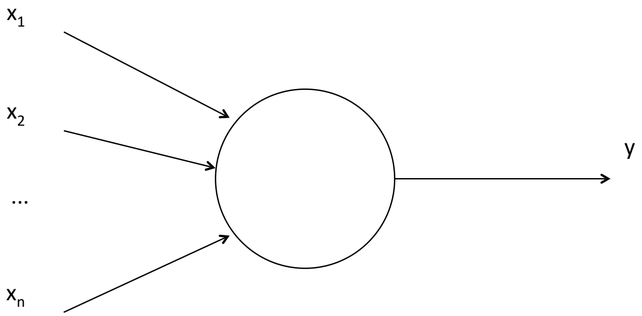

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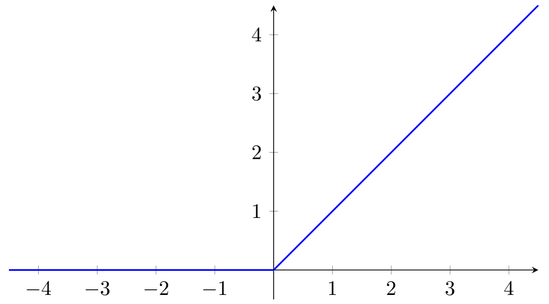
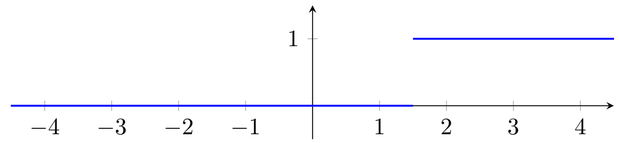


Binary Threshold:

$$s_t(z) = \begin{cases} 0, & z \leq t \\ 1, & z > t \end{cases}$$



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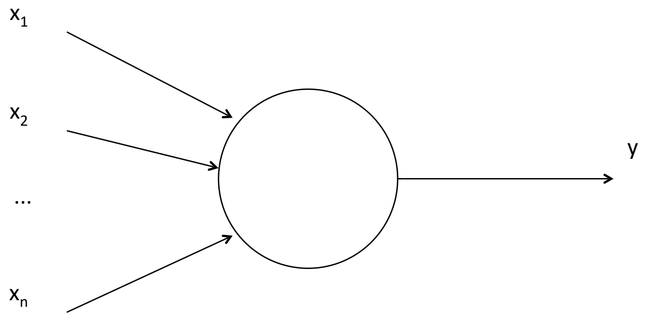

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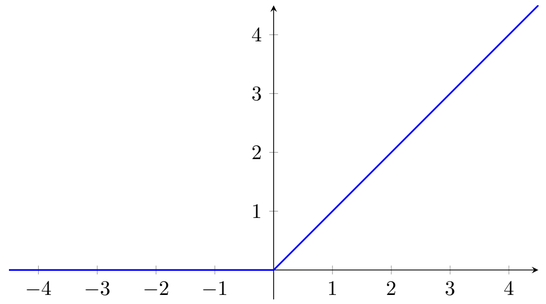

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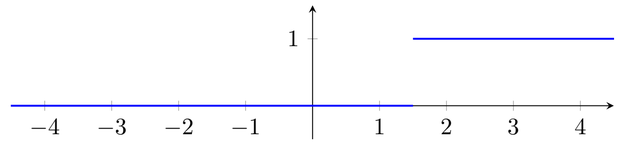
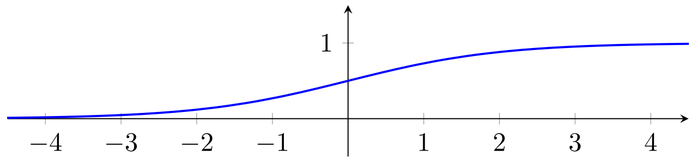


Sigmoid:

$$\mathrm{sig}(z) = \frac{1}{1 + e^{-z}}$$



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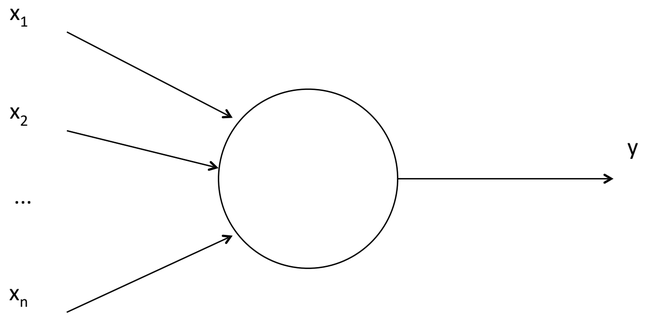

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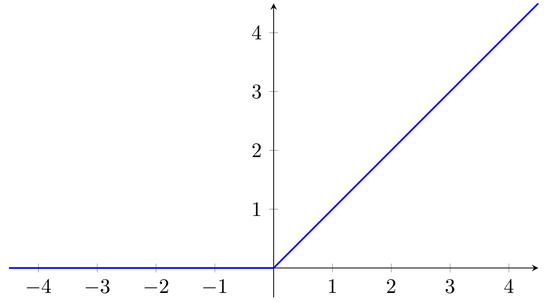

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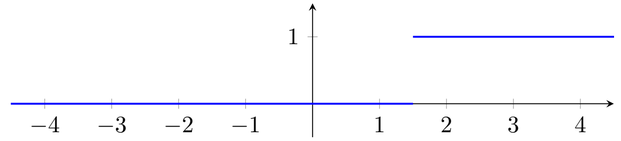

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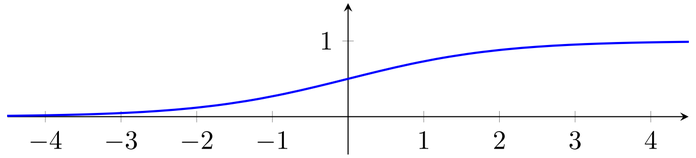


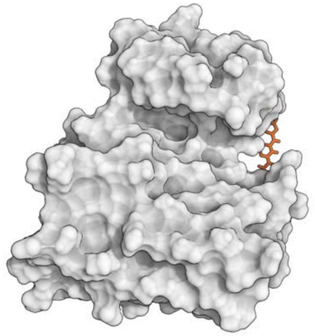
Softmax:

$$\sigma(z) = \frac{1}{\sum_{j=0}^{k-1} e^{z_j}} \begin{pmatrix} e^{z_0} \\ e^{z_1} \\ \vdots \\ e^{z_{k-1}} \end{pmatrix}$$

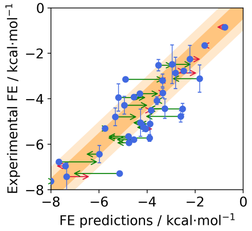
Predicting binding affinities from simulation and experimental data

Jenke Scheen

$$\Delta G_{\mathrm{bind},L} = -k_B T \ln \frac{k_{\mathrm{on}}}{k_{\mathrm{off}}}$$



Learning binding affinity corrections



Scheen *et al. J. Chem. Inf. Model. 60, 11, 5331–5339 (2020)*

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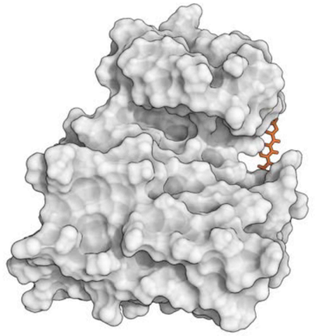

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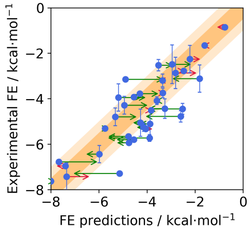

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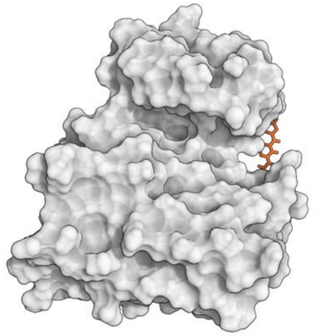
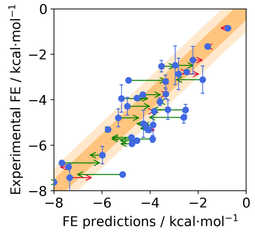
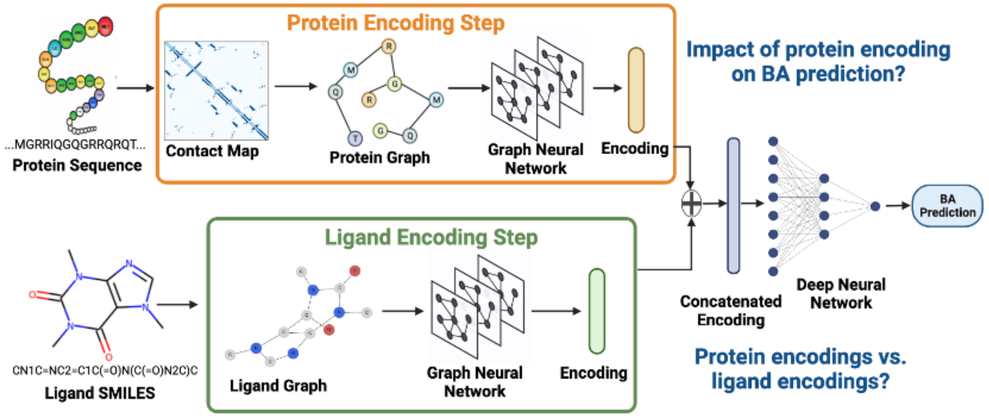


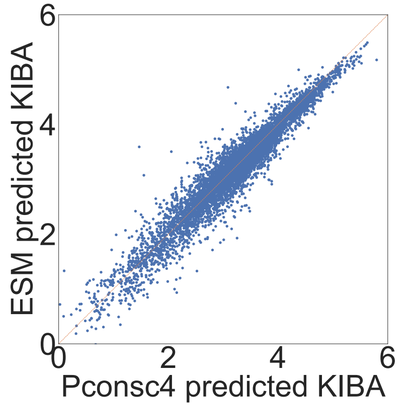
Learning binding affinity corrections



Scheen *et al. J. Chem. Inf. Model. 60, 11, 5331–5339 (2020)*

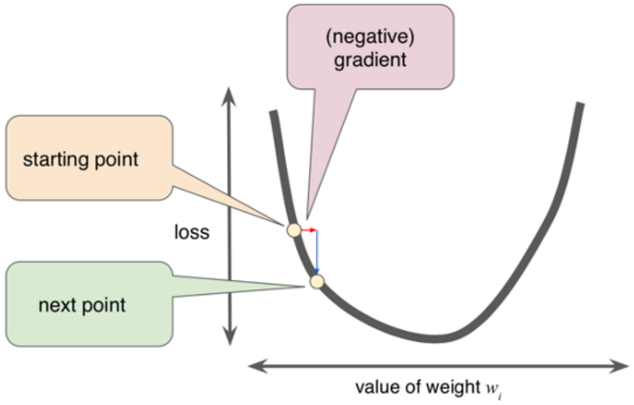
Rohan Gorantla





From mathematical concepts to applications in peptides

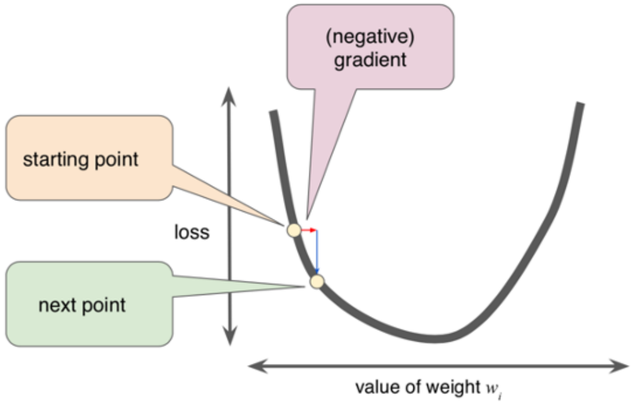
Katarina Karoni



Katerina works on Continual learning problems.
She developed a new optimiser for Multirate learning and proved its convergence.

From mathematical concepts to applications in peptides

Katarina Karoni



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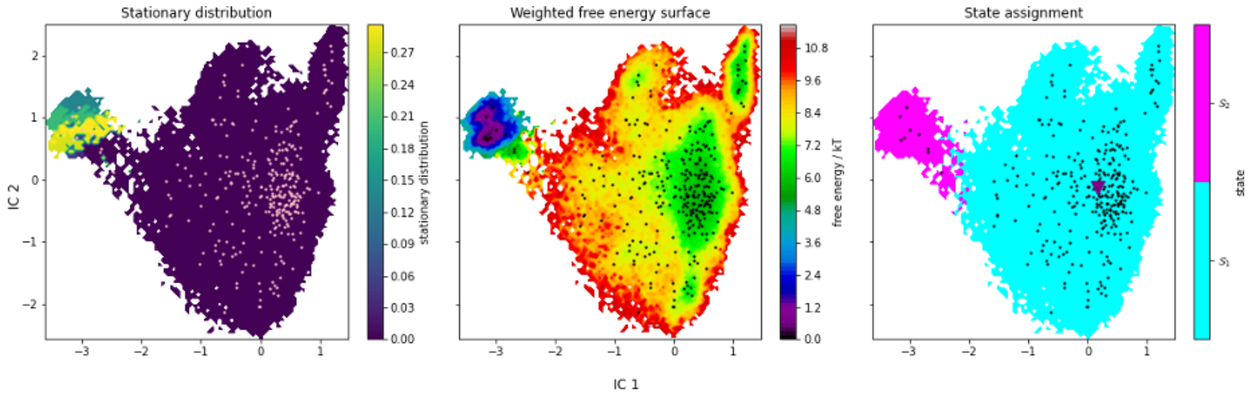
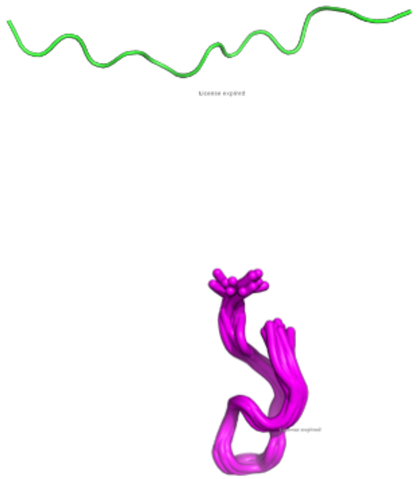
How can we find good transition paths between conformations?

Ryan Zhu

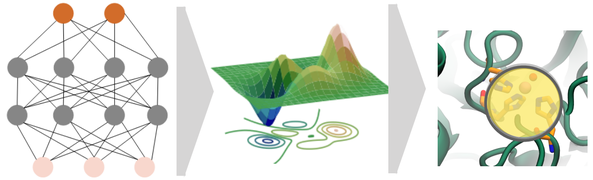


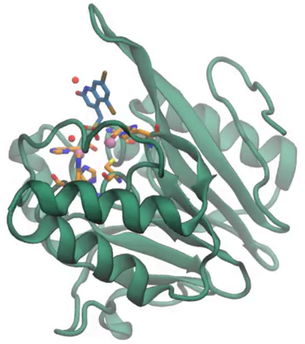


Understanding layers of complexity with ML models

Jasmin Güven

Neural Network potentials for metalloproteins





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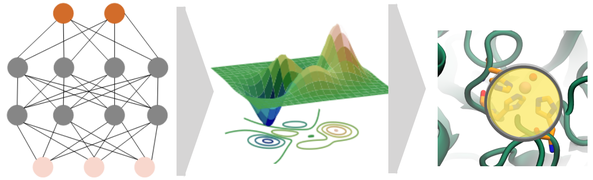

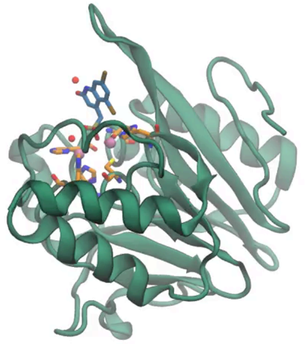

Understanding layers of complexity with ML models

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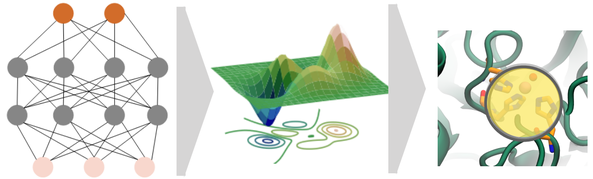
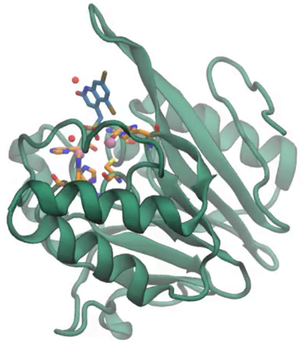
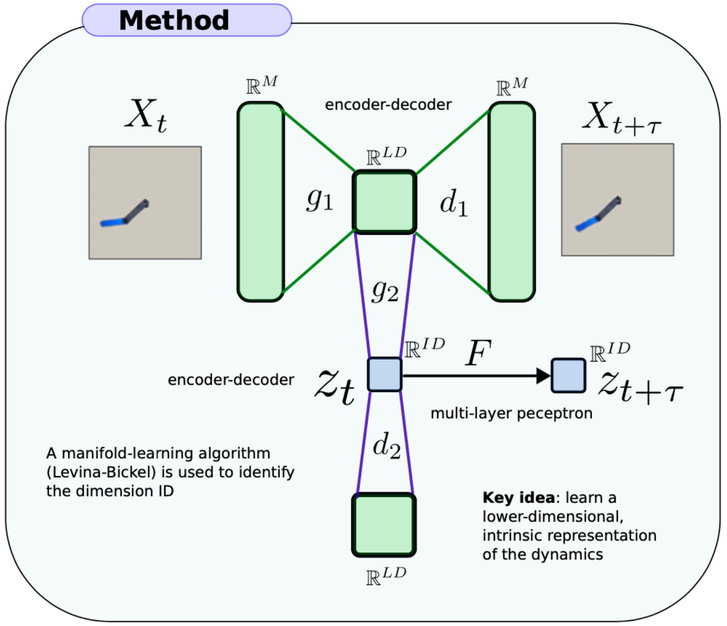


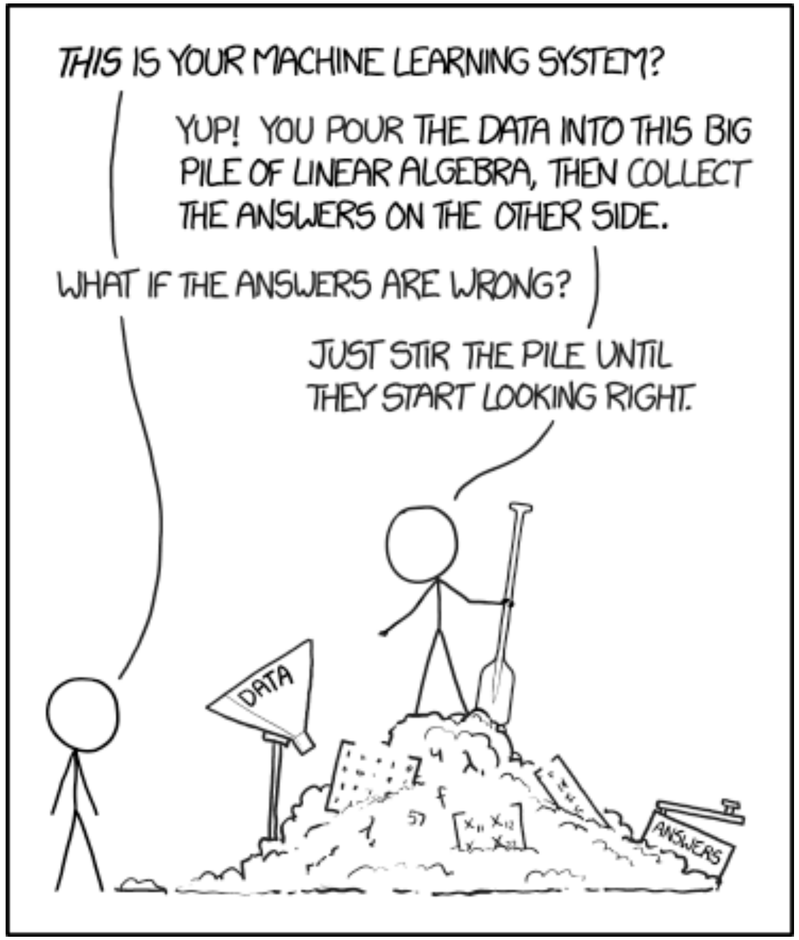


Dominic Philips

Automated Discovery of Fundamental Variables in Experiments and or Simulation



Valuable lessons on machine learning



https://xkcd.com/1838/

Something you liked 😎👍

Something you think could be improved 😬👎