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Introduction to machine learning

Associated notebook: https://github.com/keeeto/reading-ml-chemistry/blob/master/01_classification_decision_tree.ipynb

Course overview

- Intro to machine learning
- Classical Machine Learning
- Deep Machine Learning
- Notebooks to work through the lectures

What you (don't) need

- Don't need
  - Strong mathematical background
  - Any particular computer programming experience
- Do need
  - A google account
  - Curiosity about the content

Overview Today(ish)

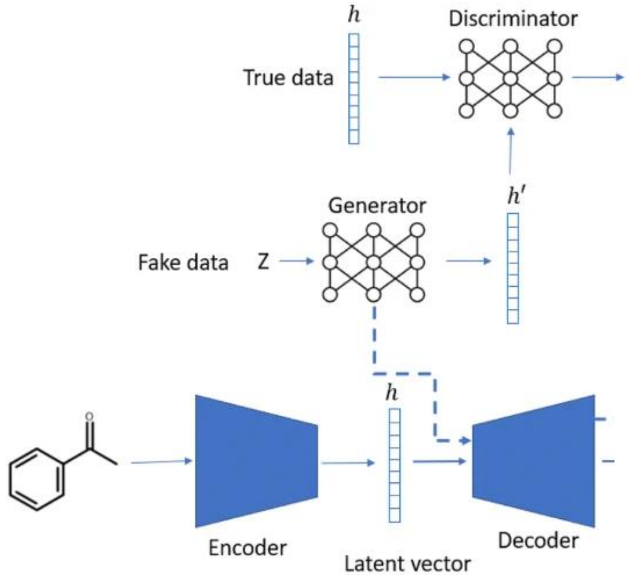
- Define ML
- Types of ML
- Parameters and hyperparameters
- Features
- Decision trees

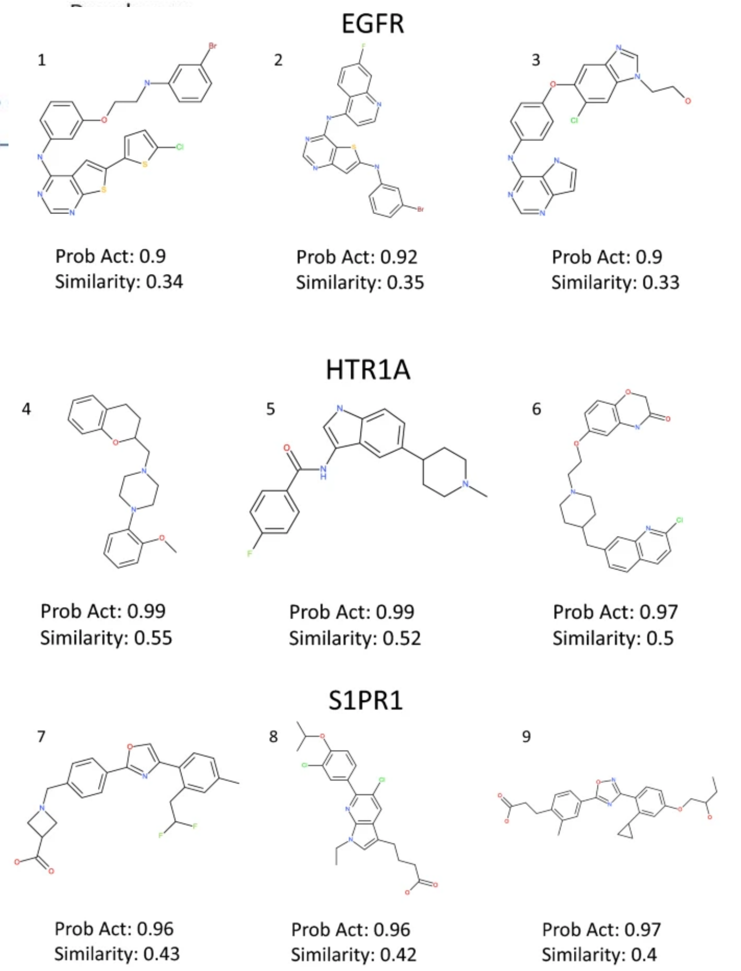
Setting up a notebook

- You will need a Google account to do this
- Go to https://colab.research.google.com/
- Search for https://github.com/keeeto/reading-ml-chemistry

Showcase

- A model is trained to generate new drug molecules from scratch
- Trained to design molecules which are drug-like but have not been tested before
- The method can develop previously un-explored molecules
- Probable activities are promising





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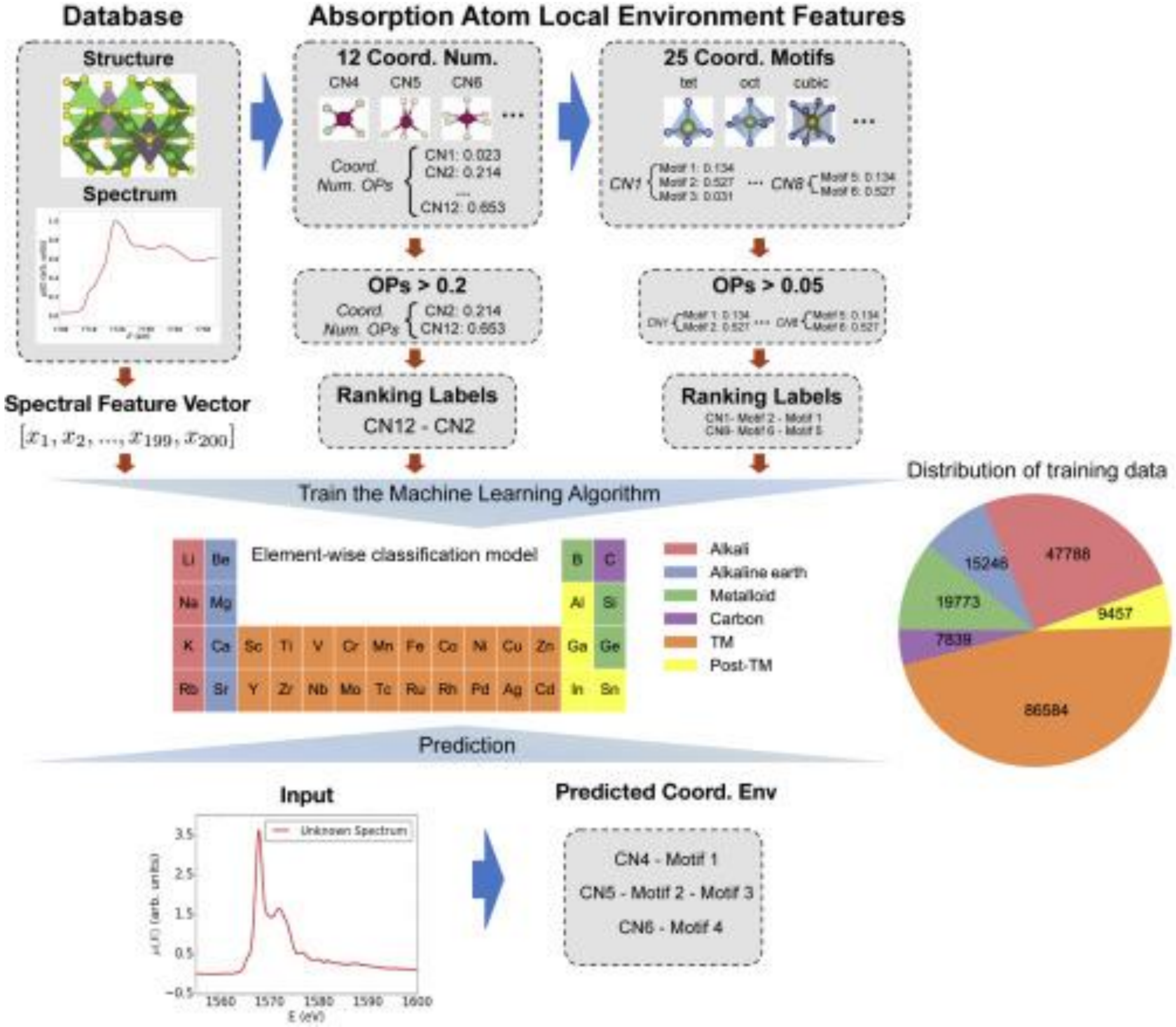
Journal of Cheminformatics **volume 11**, Article number: 74 (2019)

Showcase

- Directly predicts the atomic environment labels from the X-ray absorption near-edge structure
- Accuracy exceeding 80%
- Accelerated or even on-the-fly interpretation of spectra directly from experiments



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Patterns, 2020, 1, 100013

Showcase

- Interpreting electron diffraction crystallography using supervised ML
- Models trained on simulated diffraction patterns
- Can narrow down possible spacegroups to the top two with 95% confidence
- Even peaks in low signal-to-noise images can be potentially used

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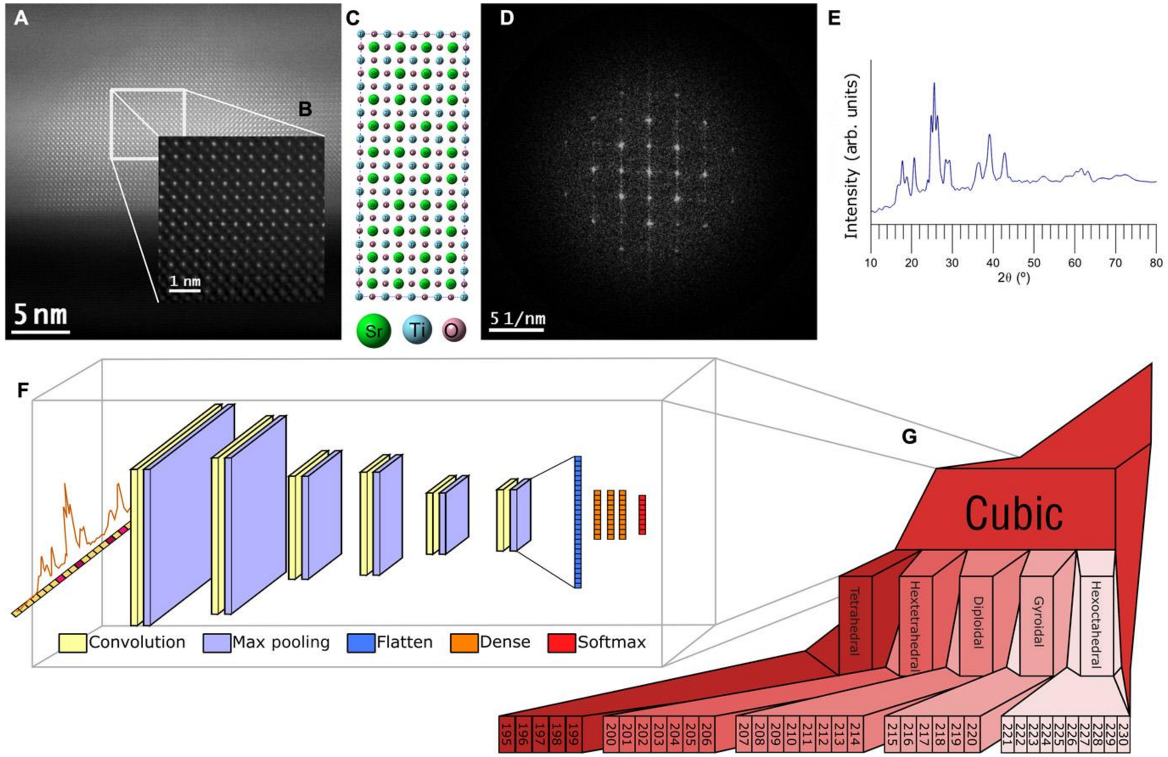
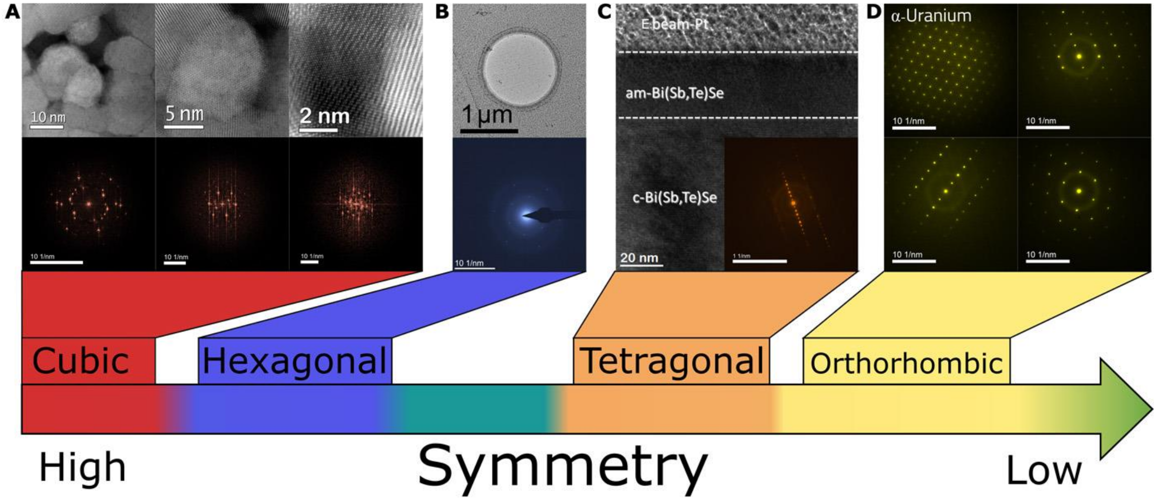
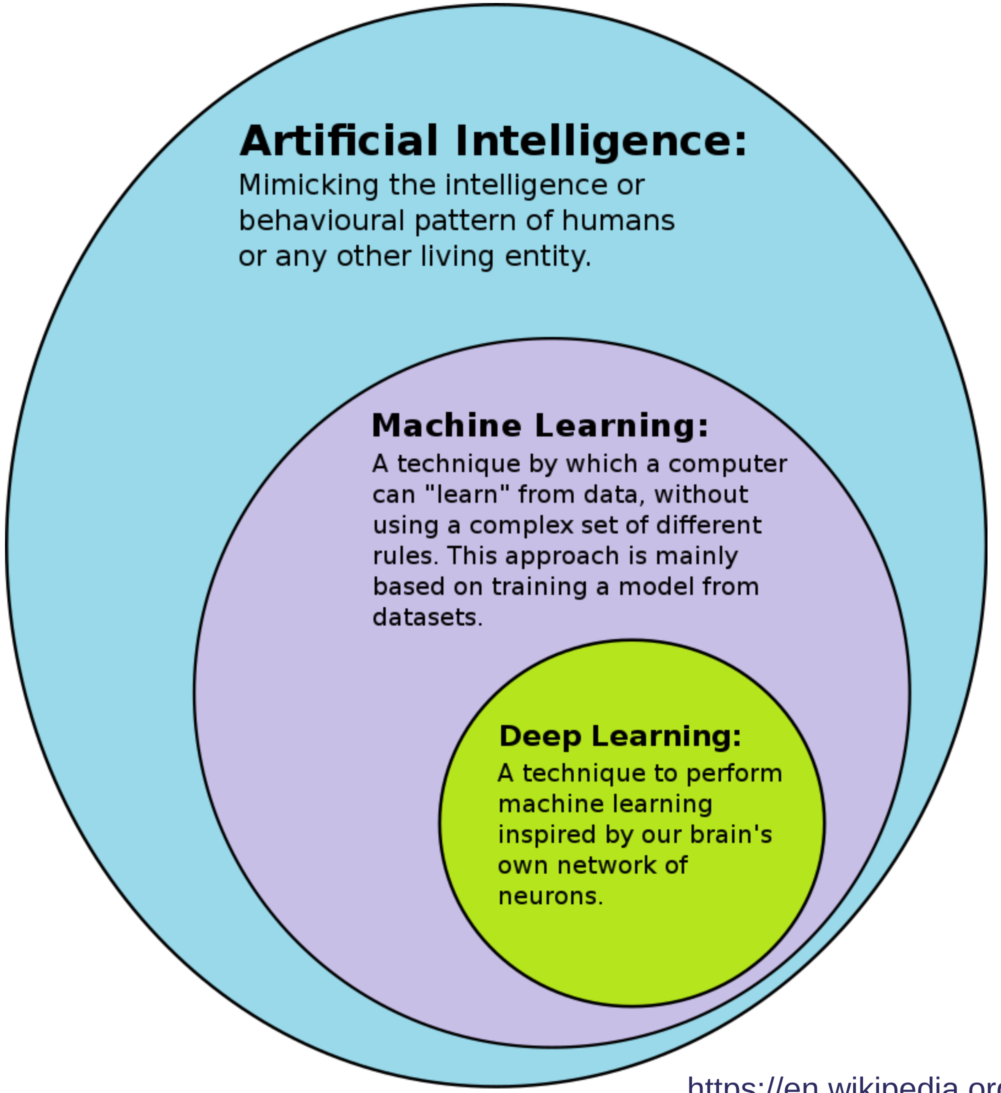




Science Advances 2019, 5, eaaw1949

What is machine learning?



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https://en.wikipedia.org/wiki/Deep_learning#/media/File:AI-ML-DL.svg

A working definition

ML = Representation + Evaluation + Optimisation

DOI:10.1145/2347736.2347755

Tapping into the "folk knowledge" needed to advance machine learning applications.

BY PEDRO DOMINGOS

A Few Useful Things to Know About Machine Learning

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"A Few Useful Things to Know About Machine Learning" by Pedro Domingos

A working definition

ML = Representation + Evaluation + Optimisation

- Representation
    - How we represent the knowledge.
    - What type of model do you use.
    - What data do you use in what format
    - Hypothesis space.
    - Eg. Neural network, decision tree …

A working definition

ML = Representation + Evaluation + Optimisation

- Evaluation
  - Objective function or scoring function.
  - Distinguish good from bad models.

A working definition

ML = Representation + Evaluation + Optimisation

- Optimisation
  - Searches between models.
  - Updates the parameters of a model to improve performance.
  - Identifies the highest-scoring one.
  - Determines the efficiency of a learner.

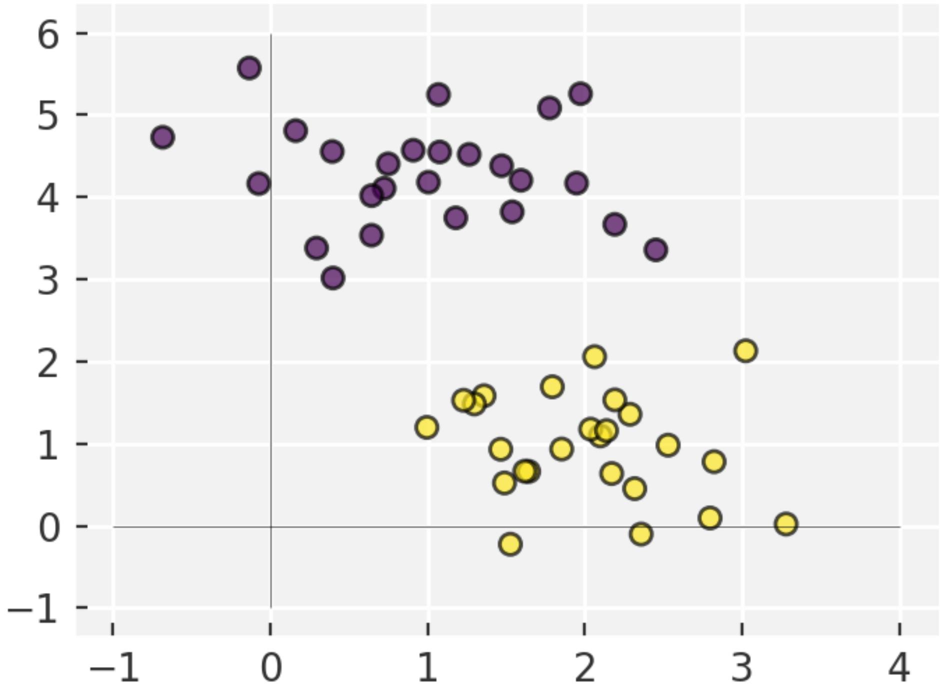
A working definition

ML = Representation + Evaluation + Optimisation

- Representation
  - Choice of model
  - Choice of hyper-parameters
  - Choice of features

Supervised ML

- Data plus labels
- **Learning** a function that maps an input to an output based on example input-output pairs.



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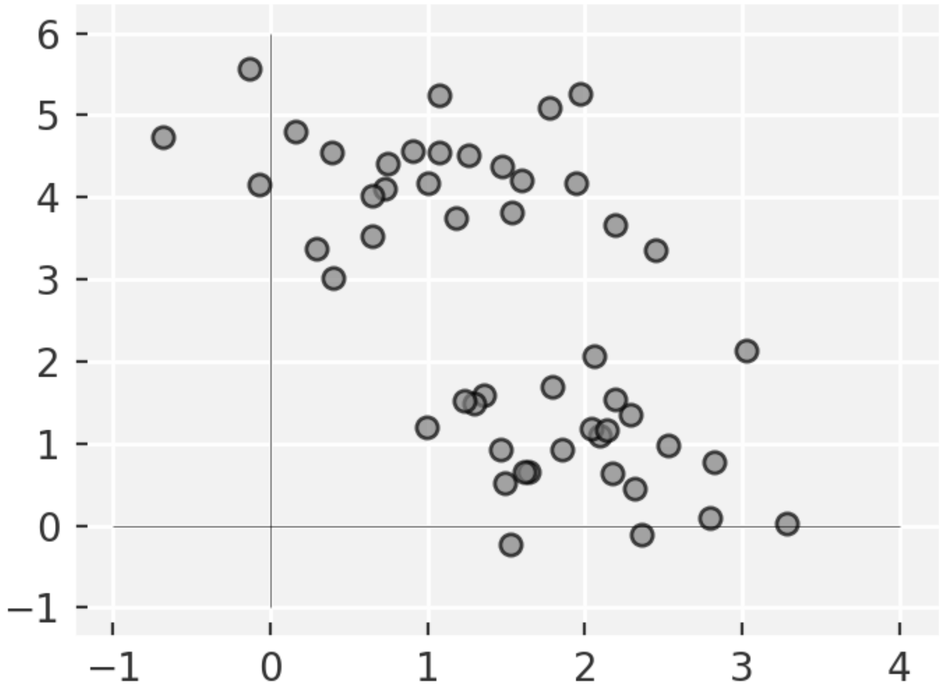
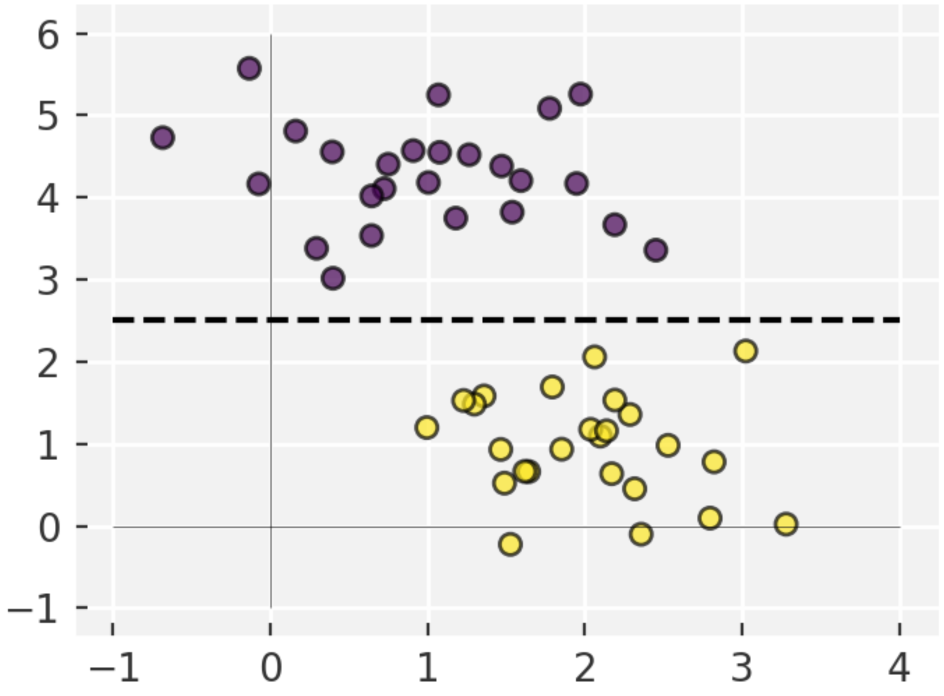
Unsupervised ML

- Data do not have labels
- Identifying trends in unlabelled datasets
- E.g. cluster analysis, is used for exploratory data analysis to find hidden patterns or grouping in data



Classification

- Identifying to which of a set of categories a new sample belongs, on the basis of a training set
- E.g. spam filter or which crystal structure gives a certain pattern



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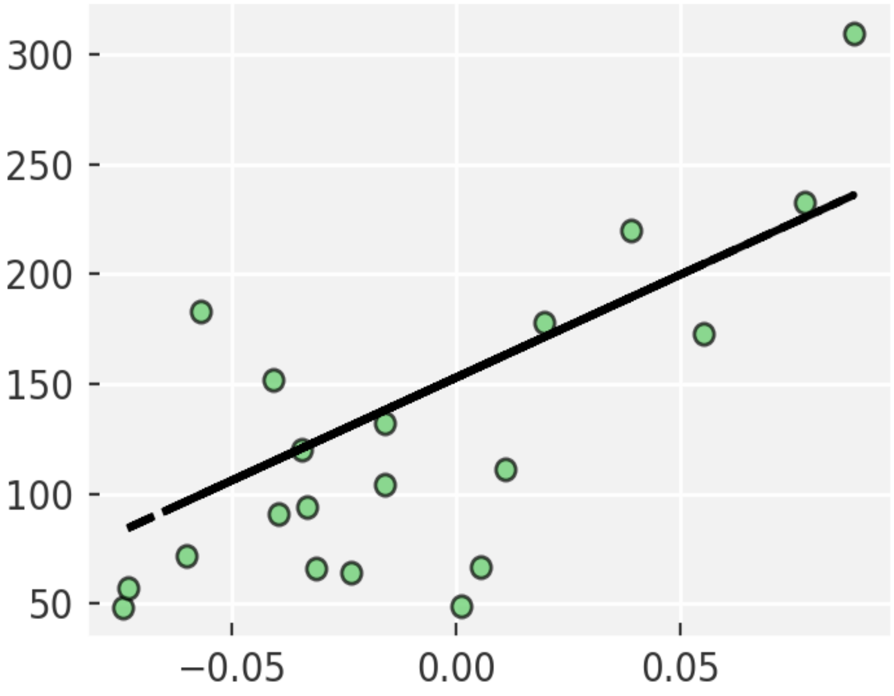
Regression

- Models a target prediction value based on independent variables



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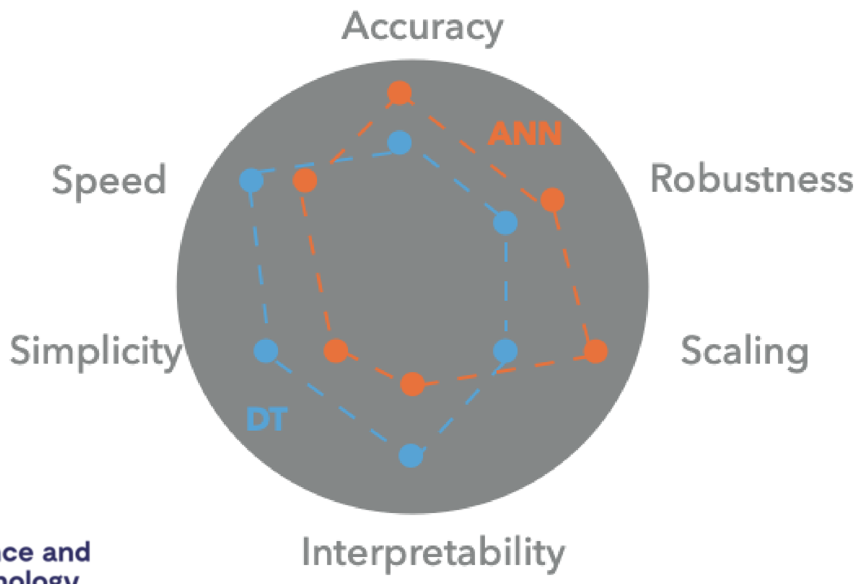
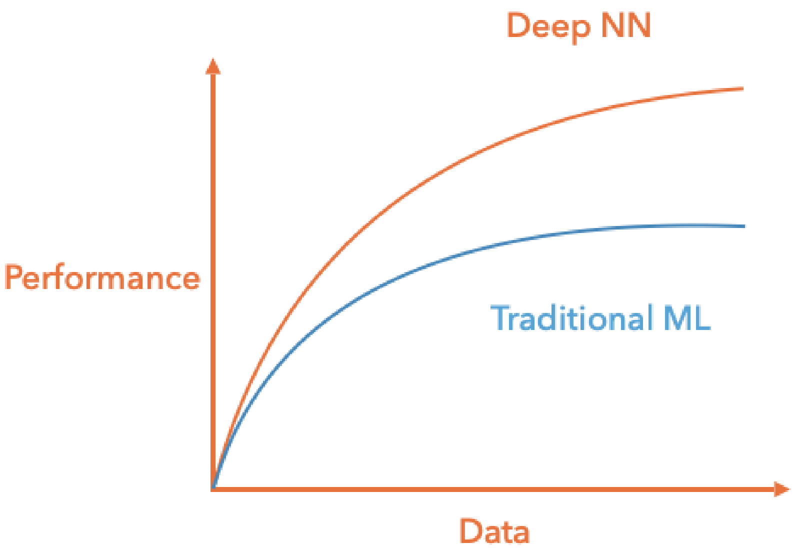
Classical/deep methods

- Classical: linear regression, trees etc..
- Deep: neural network type models





Parameters and hyper-parameters

- Parameters – properties of the model that are modified during training
- Hyperparameters – set of values that define the model and how it trains. Do not update during training
  - E.g. loss function, learning rate, number of parameters

Features

- In ML approaches the data will typically consist of several or more features
- Features are simply the input variables for the model – x in f(x) = y

> "…some machine learning projects succeed and some fail. What makes the difference? Easily the most important factor is the features used."

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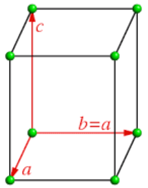
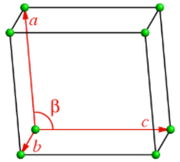
"A Few Useful Things to Know About Machine Learning" by Pedro Domingos

Feature engineering

- Transforming raw data into features that better represent the underlying problem
- Make inputs into things that an algorithm can understand
- E.g. Convert a date-time stamp into something more useful 2014-09-20T20:45:40Z -> Day: Tuesday; Year: 2014; Month: Sept
- Note that ‘Tuesday’ and ‘Sept’ are not particularly algorithm ready – how can we convert them to something more useful?

One hot encoding

- Classification problems
- Vector of length = number of categories
- Each element is the probability that the data represents a given class

Material	Ortho	Rhomb
	1	0
	0	1

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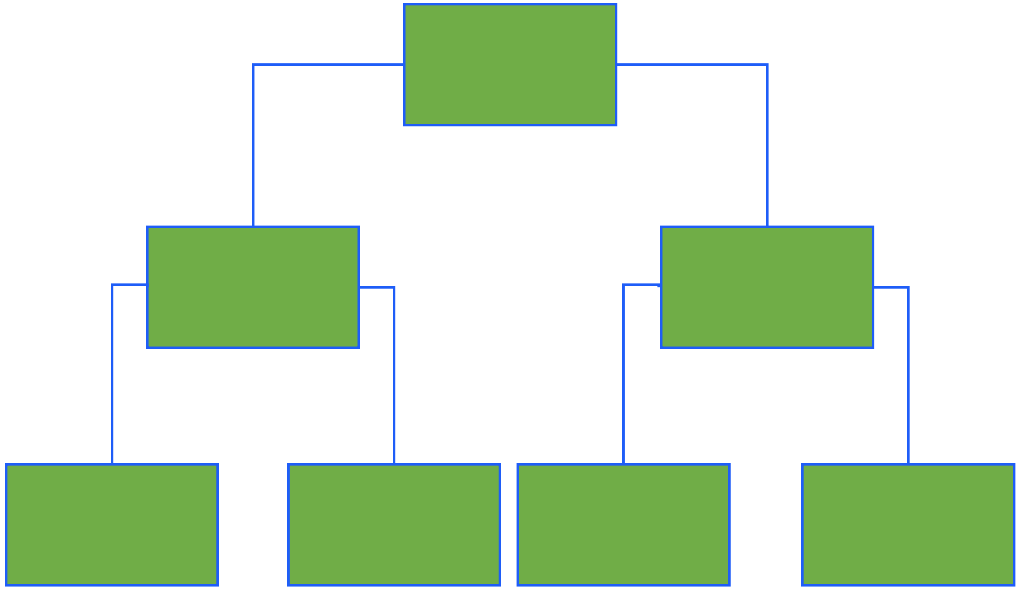
Decision trees



Data is split by features. E.g. brightness of a pixel
Splits are arranged such that the data splits as evenly as possible at each point.

Decision trees

$$Q_{left}(\theta) = (x, y) | x_f \leq t_j$$
$$Q_{right}(\theta) = Q \setminus Q_{left}(\theta)$$

Data is split according to a threshold value tj.

$$C(Q, \theta) = \frac{n_{left}}{N_j} H(Q_{left}(\theta)) + \frac{n_{right}}{N_j} H(Q_{right}(\theta))$$

The cost of the split is calculated based on some impurity function H() e.g. RMSD of the data.

$$\theta^* = \underset{\theta}{\operatorname{argmin}} C(Q, \theta)$$

The splitting parameters are chosen to minimise C at each split.

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Go to notebook

Concept checklist

- Supervised/unsupervised machine learning
- Classical machine learning/deep learning
- Parameters/hyperparameters
- Features and feature engineering
- Decision trees