

IMPERIAL

Machine Learning for Neuroscience

ML4NS

## Introduction to Machine Learning

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**Leia: Yaté. Yaté. Yotó.**

(SUBTITLE: "I have come for the bounty on this Wookiee.")

C-3PO relays this message and Jabba says he'll offer 25,000 for Chewie.

**Leia: Yotó. Yotó.** (SUBTITLE: "50,000, no less.")

C-3PO relays this message and Jabba asks why he should pay so much.

**Leia: Eí yótó.**

The above isn't subtitled, but Leia pulls out a bomb and activates it.

C-3PO : Because he's holding a thermal detonator!  
Jabba is impressed by this and offers 35,000.



**Leia: Yató cha.**

The above isn't subtitled, but Leia deactivates the bomb and puts it away.

C-3PO : He agrees.  
Order is restored.



Adapted from: The Art of Language Invention: From Horse-Lords to Dark Elves, The Words Behind World-Building, by David J. Peterson, Penguin, 2015.

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**IMPERIAL** $\forall \rightarrow \mathbf{Yotó} :$ if :  $f([\mathbf{Yotó}]) == 1 \rightarrow \mathbf{Yotó} \propto \text{"thisWookiee"}$ if :  $f([\mathbf{Yotó}]) == 2 \rightarrow \mathbf{Yotó} \propto \text{"50,000"}$ if :  $f([\mathbf{Yotó}]) == 3 \rightarrow \mathbf{Yotó} \propto \text{"noless"}$ if :  $(f([\mathbf{Yotó}]) == 3 \& \text{SeasonOnEarth}() == \text{"Spring"}) \rightarrow \mathbf{Yotó} \propto \text{"Welcome!"}$ 

...

...

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## However, don't underestimate the human brain

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- For example, in German:
  - you must distinguish between “the” and “a” articles
  - and then each one has **four case forms**
  - **three genders**
  - and **singular and plural forms**
  - and then the **adjectives have to agree**
  - and then there are verbs!
  - or take this as an example:



(biáng)

Adapted from: The Art of Language Invention: From Horse-Lords to Dark Elves, The Words Behind World-Building, by David J. Peterson.

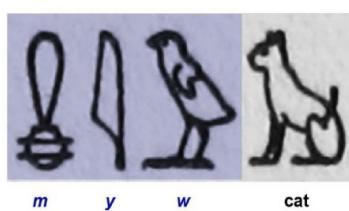
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### "Cat" in Ancient Egyptian

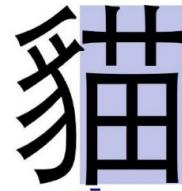
function: phonetic component determinative



m      y      w      cat

### "Cat" in Chinese Hanzi

function: radical phonetic component



legendary beast ( <i>zhi</i> )	sprouts growing in field (implies fertility) ( <i>miào</i> )
--------------------------------------	--

Source: <https://www.originofalphabet.com/meow-is-just-another-name-for-cat-2/>

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Source: <https://cdn.sinauer.com/wolfe4e/wa07.05.html#Movie1>

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Patterns and generalisation

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## Attention

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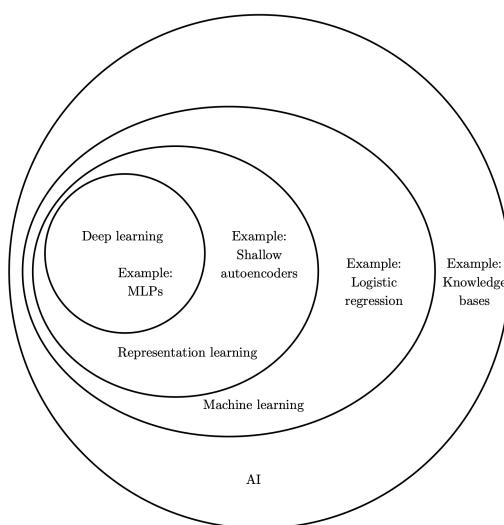
Source: <https://www.youtube.com/watch?v=xNSgmm9FX2s>  
Via: <https://www.youtube.com/watch?v=48gBPL7aHJY&t=0s>

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## AI and Machine Learning

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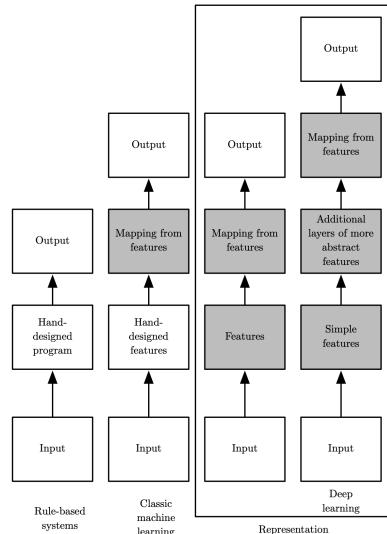
Source: Deep Learning, Ian Goodfellow et al., MIT Press.

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## Categories of learning and intelligent systems

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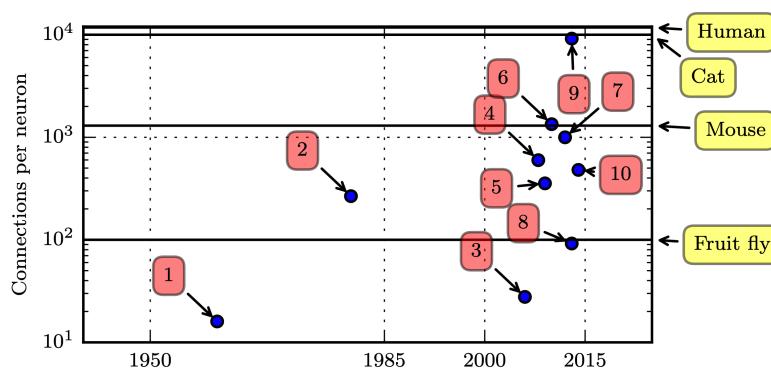
Source: Deep Learning, Ian Goodfellow et al., MIT Press.

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## Connections per neuron

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1. Adaptive linear element (Widrow and Hoff, 1960)

...

8. Multi-GPU convolutional network (Krizhevsky et al., 2012)

9. COTS HPC unsupervised convolutional network (Coates et al., 2013)

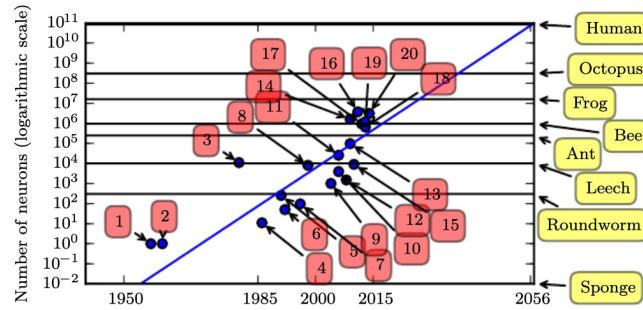
Source: Deep Learning, Ian Goodfellow et al., MIT Press.

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- 17. Distributed autoencoder (Le et al., 2012)
  - 18. Multi-GPU convolutional network (Krizhevsky et al., 2012)
  - 19. COTS HPC unsupervised convolutional network (Coates et al., 2013)
  - 20. GoogLeNet (Szegedy et al., 2014a)

- The human brain has approximately 86 billion neurons
  - The GPT-4 model has approximately 1.8 trillion parameters.
  - However, the artificial neurons are not equal to biological neurons

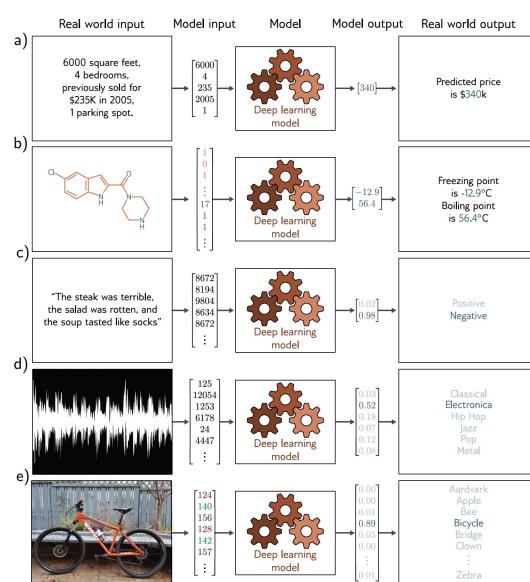
Source: Deep Learning, Ian Goodfellow et al., MIT Press

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## Machine learning models

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Source: Understanding Deep Learning, Simon I.D. Prince, MIT Press

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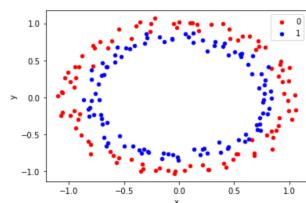
## Machine Learning (ML)

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- Most of machine learning methods are designed as a learning process to learn a function  $f^*$  for which:

$$f^*(x) \approx f^*(x + \varepsilon)$$

- In other words, this means if we know the answer for a training sample  $x$ , then that answer is *probably* good in the neighbourhood of  $x$ .

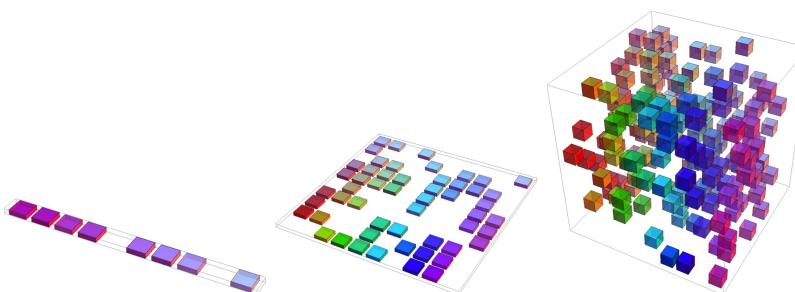


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## Curse of dimensionality

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Overall, for  $d$  dimensions with  $v$  values we need  $O(v^d)$  regions and examples

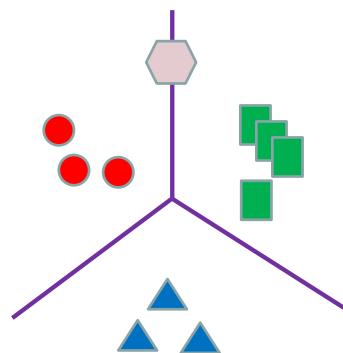
Source: Deep Learning, Ian Goodfellow et al., MIT Press.

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## K-nearest neighborhood

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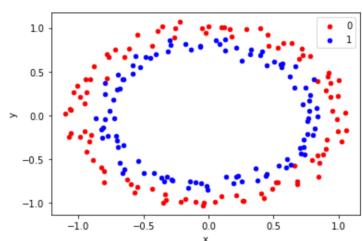


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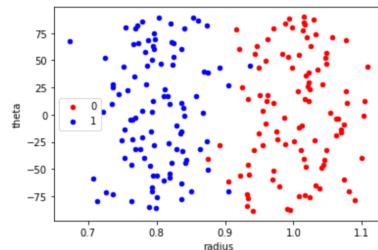
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## Data/sample representation

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$(x, y)$



$$r = \sqrt{x^2 + y^2}$$

$$\theta = \tan^{-1} \left( \frac{y}{x} \right).$$

[Code](#)



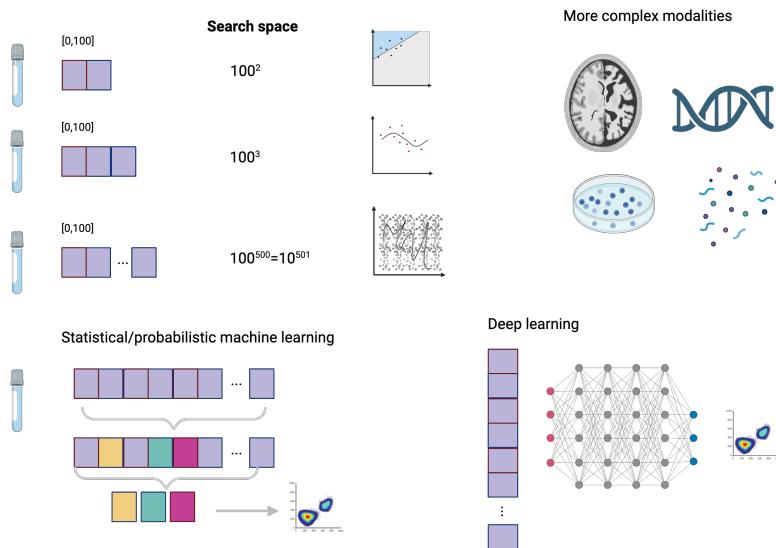
<https://github.com/PBarnaghi/Basic-ML-Code/>

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## Machine Learning: looking back, looking forward

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## What you are going to learn in this module

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- Principles of machine learning models and designing ML models for applications in neuroscience and medicine.
- Hands-on skills on how to:
  - Decide and choose suitable models
  - Design machine learning tasks/experiments
  - Choose and apply suitable metrics to evaluate the models
  - Identify and resolve common issues such as overfitting/underfitting

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## By the end of this module

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- You should be able to:
  - Construct machine learning experiments
  - Create and run different probabilistic/statistical learning and deep learning models
  - Read and interpret existing works and assess their applicability/validity [to different use cases]
  - Be familiar with common concepts such as training/test, cross-validation, performance evaluation metrics
  - Learn common issues and pitfalls in developing ML models
  - Obtain practical experience in developing ML models and running (simple) experiments.

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## Key topics covered

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- Introduction to machine learning
- Regression models and linear prediction
- Probability and information theory
- Bayesian models and maximum likelihood estimation
- Linear models, ensemble models and kernel functions
- Artificial Neural Networks (ANNs) and Multilayer Perceptron (MLP) models
- Deep Neural Networks (DNN) and Deep Learning (DL)
- Convolutional Neural Networks (CNNs)
- Responsible machine learning and ethical considerations
- Applications in neuroscience and neuroscience-inspired machine learning
- Ethical AI/ML: Principles and Practices

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## Module delivery

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- 10 teaching sessions

- Primary tutorials and workshops (primary programming and data handling/visualisation skills)
- 2 hours lectures (Mon-Fri; 10-12:00) for two weeks in January 2024.
- 3 hours lab experiments (supported by TAs)
- 1 final project (modelling and machine learning experiment on a small dataset)

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## Datasets

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- Syntenic data and programmatical generated data to demonstrate the concepts.
- In-home monitoring data in a dementia cohort study from the UK DRI Minder/TIHM Study (movement, sleep, physiology, and associated healthcare events) will be in the form of numerical time-series data (Final Project).
- Common benchmark imaging data (non-medical) such as CIFAR-10.
- Publicly available clinical/experimental datasets
  - e.g. Physionet.org

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## Tools and languages

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- Python and common machine learning libraries in Python including *Scikit – learn* and *PyTorch*



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## Development/learning framework

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```
In [1]: import numpy as np
import matplotlib.pyplot as plt
import matplotlib
matplotlib.use('TkAgg')
%matplotlib inline

Number of sample
```

```
In [2]: n= 50
```

```
In [4]: n +5
```

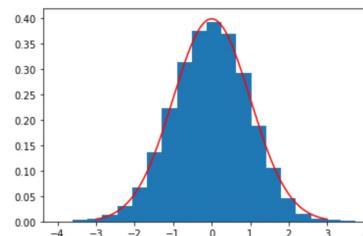
```
Out[4]: 55
```

```
In [9]: mu, sigma = 0,1
dist = gaussian_mcmc(100_000,mu=mu,sigma=sigma)
lines = np.linspace(-3,3,10_000)
normal_curve = [normal(x=i,mu=mu,sigma=sigma) for i in lines]
```

```
In [11]: plt.hist(dist,bins=20,density=True)
plt.plot(lines,normal_curve, color='red')
```

```
Out[11]: [

```



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## Teaching team

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Nan Fletcher-Lloyd



Alex Capstick



Yu Chen



Marirena Bafaloukou



Anastasia Ilina



Anastasia Gailly  
De Taurines



Antigone Fogel



Iona Biggart



Payam Barnaghi

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## Our Aim

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- We aim to encourage neuroscientists and clinical scientists to enjoy developing robust and reliable AI/ML models for practical applications. We hope this will help to prosper the practice of medicine and discovery science.
- We hope this module will remove some of the fears naturally felt when starting a career in computational neuroscience and computational modelling in medicine and bioscience, thereby allowing the practitioners to focus on solving unmet health and care needs and advancing knowledge and practice of neuroscience and medicine.

The text is inspired by the preface of the Oxford Handbook of Clinical Medicine by I. Wilkinson *et al.*

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## "Patients" and "Patient data"

**I M P E R I A L**

- The terms "patient" and "patient data" will appear throughout this module in the slides and presentation. Please note that we do not take this lightly. Every single piece of data displayed or used from anonymised patient information throughout this module is donated to science by individuals.
- We are grateful for their contributions, which support scientific discovery to enhance existing procedures and to design and develop new treatments and practices. Privacy and the ethical use of data and modelling must be essential elements for any AI/ML design.

Inspired by the Oxford Handbook of Clinical Medicine by I. Wilkinson *et al.* and a talk given by Junaid Bajwa, Flagship Pioneering.

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## Frequently Asked Questions (I)

**I M P E R I A L**

- I don't know Python. Can I take this module?
  - Yes, we have provided an introductory lecture/workshop on Python (at the level that is required for this module).
- I haven't done any programming before. Can I still take this module?
  - Yes, but you should be prepared to learn scripting/programming and get familiar with the concepts quickly. We will provide examples/templates to follow and there are plenty of online material but there would be a steep learning curve.

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## Frequently Asked Questions (II)

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- Machine learning seems to involve a lot of mathematics, especially statistics and probability. Do I need to know all these before taking this module?
  - You need to be familiar with the basic concepts of statistics and probability- but we have provided a brief refresher online tutorial. The lecture content/concepts will not be mathematically focused but when needed the underlying mathematical concepts will be described/shown to elaborate the concepts.
  - Learning mathematical concepts in a group is often easier.
  - We will focus on concepts and skills that won't be easy to find/learn by watching a series of online videos.

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## Concepts that will not be covered in this module

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- Image processing and machine learning for medical imaging,
- Natural language processing and text analysis,
- Advanced machine learning and deep learning concepts such as transfer learning, generative models (some of these will be covered in an optional series after the module),
- Signal processing and feature engineering for specific modalities/data such as EEG, ECG, and Brain imaging.

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## What will I learn in this module?

**I M P E R I A L**

- Primary concepts and foundations of machine learning (statistical/probabilistic learning and deep learning models).
- Some of the basic/key models to design and develop supervised and unsupervised machine learning.
- Cross-validation, hyperparameter tuning, evaluation metrics
- Hands-on skills and working with real-world data and designing/evaluating models with different real-world datasets.
  
- Ultimately, this module (hopefully) will help you learn fundamental concepts on how ML models are constructed and applied to real-world problems.

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## Module assessment

**I M P E R I A L**

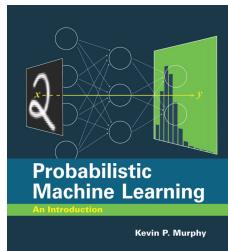
- 3 Marked Lab assignments (40%)
  - Lab 5 (Friday)
  - Lab 6 (Monday)
  - Lab 8 (Wednesday) – this will be a one-page report on a use-case that will be given to review/evaluate.
- Final project (60%)
  - In the 2<sup>nd</sup> week, we will give you a dataset and ask you to:
    - Conduct a set of exploratory data analysis
    - Develop a simple ML model and evaluate it
    - Submissions on 31<sup>st</sup> of January 2024 (5:00 pm)
    - Code with markdown in Jupyter Notebook will be sufficient.

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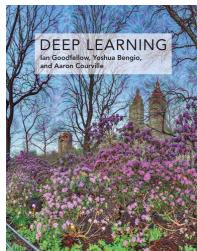
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## Reference and sources

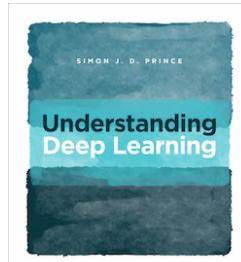
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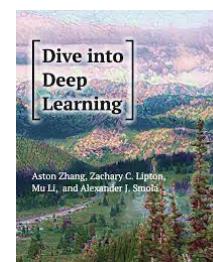
Probabilistic Machine Learning  
Kevin P. Murphy, MIT Press



Deep Learning  
Goodfellow et al., MIT Press



Understanding Deep Learning,  
Simon J.D. Prince, MIT Press



Dive into Deep Learning  
Aston Zhang et al.

### Links to Preprints (PDFs/online versions):

- Probabilistic Machine Learning: An Introduction, <https://probml.github.io/pml-book/book1.html>
- Deep learning: <https://www.deeplearningbook.org>
- Understanding Deep Learning, <https://udlbook.github.io/udlbook/>
- Dive into deep learning, <https://d2l.ai/index.html>

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## Some other online sources

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- Andrew Ng lecture notes:  
[https://cs229.stanford.edu/lectures-spring2022/main\\_notes.pdf](https://cs229.stanford.edu/lectures-spring2022/main_notes.pdf)
- <https://towardsdatascience.com/machine-learning/>
- Good online sources for questions/troubleshooting
  - <https://stackoverflow.com>
  - <https://stackexchange.com>

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## MS Teams Link

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- Module 5 Machine Learning in Neuroscience 24-25 - WB

- [https://teams.microsoft.com/l/team/19%3AbRaMz8hbk\\_nnjBm25c22A4bThQaIh2oMxAB6EMU8kIQ1%40thread.tacv2/conversations?groupId=6e99abc2-8eef-493b-970c-4cd6e25a1e13&tenantId=2b897507-ee8c-4575-830b-4f8267c3d307](https://teams.microsoft.com/l/team/19%3AbRaMz8hbk_nnjBm25c22A4bThQaIh2oMxAB6EMU8kIQ1%40thread.tacv2/conversations?groupId=6e99abc2-8eef-493b-970c-4cd6e25a1e13&tenantId=2b897507-ee8c-4575-830b-4f8267c3d307)

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## Typical machine learning approaches

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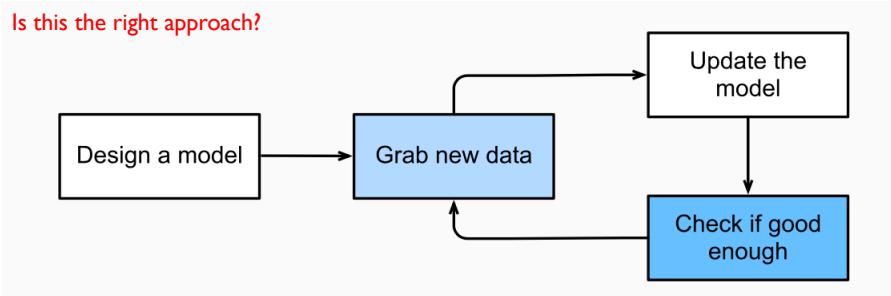
- Supervised learning
- Unsupervised learning
- Reinforcement learning

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## Machine learning development

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Source: Dive into Deep Learning, Aston Zhang et al.

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## Key components of ML development

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- The *data* that we can learn from.
- A *model* of how to transform the data.
- An *objective function* that quantifies how well (or badly) the model is doing.
- An *algorithm* to adjust the model’s parameters to optimise the objective function.

Source: Dive into Deep Learning, Aston Zhang et al.

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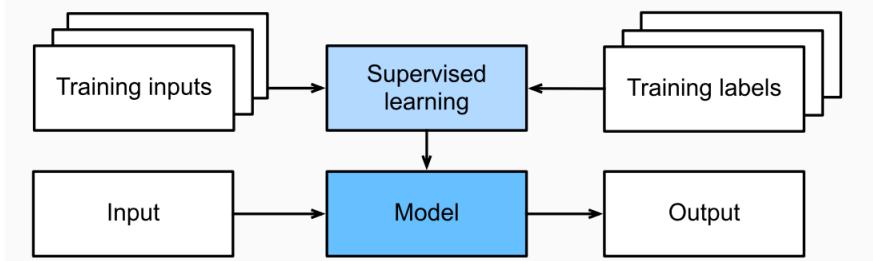
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## Supervised learning

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- In supervised learning the data comes with additional attributes (i.e. labels) that we want to predict.



Source: Dive into Deep Learning, Aston Zhang et al.

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## Classification

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- Samples belong to two or more classes, and we want to learn from **already labelled data** how to **predict the class of unlabelled data**.
- An example of a classification problem would be the activity recognition example, in which the aim is to assign each input vector to one of a finite number of discrete categories.
- Another way to think of classification is as a discrete (as opposed to continuous) form of supervised learning where one has a limited number of categories, and for each of the ***n*** samples provided, one is to try to label them with the correct category or class.

Source: Scikit learn documentation

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## Regression

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- The task is called regression if the desired output consists of one or more continuous variables.
- An example of regression problems:
  - How long will it take for an Alzheimer's Disease AD patient to decline to an MMSE\* score of  $x$ ? (judging by previously seen data)
  - How long will it take for a patient to decline from one stage to another stage (in a neurodegenerative condition)?
  - Predicting the length of hospital stay for a patient

\*MMSE: The Mini-Mental State Examination (MMSE)

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## Unsupervised learning

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- In unsupervised learning the training data consists of a set of input **vectors  $x$**  without any corresponding target values.
- The goal in such problems may be to **discover groups of similar** examples within the data, where it is called clustering, or to **determine the distribution of data** within the input space, known as density estimation, or to **project the data from a high-dimensional space** down to two or three dimensions for the purpose of visualisation

Source: Dive into Deep Learning, Aston Zhang et al.

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## Training set and testing set

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- Machine learning is about learning some properties of a data set and applying them to new data.
- This is why a common practice in machine learning to evaluate an algorithm is to split the data at hand into two sets, one that we call the training set on which we learn data properties and one that we call the testing set on which we test these properties.

Source: Dive into Deep Learning, Aston Zhang et al.

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## Dataset

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### 7.1.3. Diabetes dataset

Ten baseline variables, age, sex, body mass index, average blood pressure, and six blood serum measurements were obtained for each of  $n = 442$  diabetes patients, as well as the response of interest, a quantitative measure of disease progression one year after baseline.

**Data Set Characteristics:**

<b>Number of Instances::</b>	442
------------------------------	-----

<b>Number of Attributes::</b>	First 10 columns are numeric predictive values
-------------------------------	--

<b>Target::</b>	Column 11 is a quantitative measure of disease progression one year after baseline
-----------------	--

<b>Attribute Information::</b>	<ul style="list-style-type: none"> <li>• age age in years</li> <li>• sex</li> <li>• bmi body mass index</li> <li>• bp average blood pressure</li> <li>• s1 tc, total serum cholesterol</li> <li>• s2 ldl, low-density lipoproteins</li> <li>• s3 hdl, high-density lipoproteins</li> <li>• s4 tch, total cholesterol / HDL</li> <li>• s5 ltg, possibly log of serum triglycerides level</li> <li>• s6 glu, blood sugar level</li> </ul>
--------------------------------	---

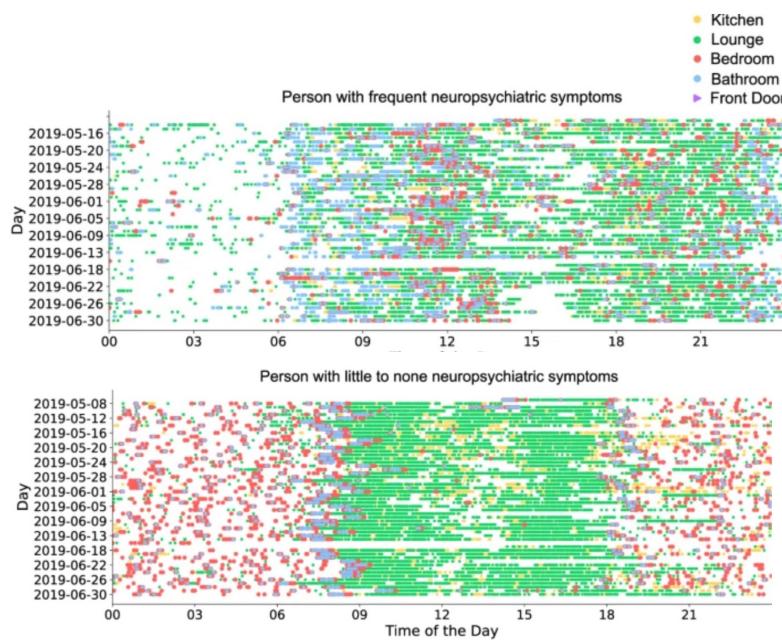
<https://www4.stat.ncsu.edu/~boos/var.select/diabetes.html>

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## Datasets

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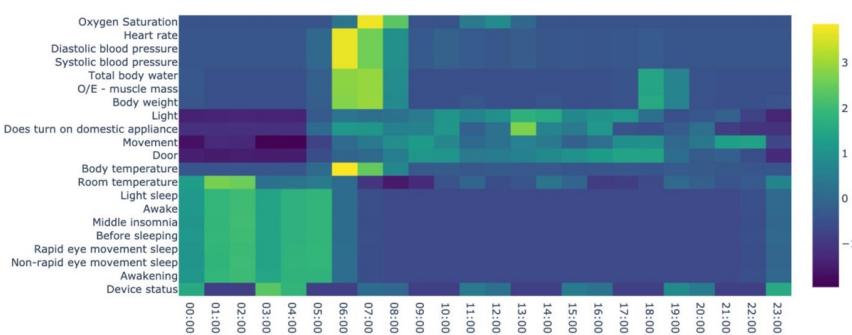
Palermo, F., Chen, Y., Capstick, A., et al. TIHM: An open dataset for remote healthcare monitoring in dementia. *Sci Data*, 10, 606 (2023).

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## A sample data for in-home activity

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## Dataset in the code/programming environment

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```
from sklearn import datasets
diabetes_X, diabetes_y = datasets.load_diabetes(return_X_y=True)
✓ 0.4s
```

```
diabetes_X
✓ 0.6s
array([[ 0.03807591,  0.05068012,  0.06169621, ..., -0.00259226,
       0.01990842, -0.01764613],
      [-0.00188202, -0.04464164, -0.05147406, ..., -0.03949338,
       -0.06832974, -0.09220405],
      [ 0.08529891,  0.05068012,  0.04445121, ..., -0.00259226,
       0.00286377, -0.02593034],
      ...,
      [ 0.04170844,  0.05068012, -0.01590626, ..., -0.01107952,
       -0.04687948,  0.01549073],
      [-0.04547248, -0.04464164,  0.03906215, ...,  0.02655962,
       0.04452837, -0.02593034],
      [-0.04547248, -0.04464164, -0.0730303 , ..., -0.03949338,
       -0.00421986,  0.00306441]])
```

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## Multivariate data

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- In general, a learning problem considers a set of *n* samples of data and then tries to predict the properties of previously unseen data.
- If each sample is more than a single number and, for instance, a *multi-dimensional* entry (aka multivariate data), it is said that the data has several attributes or features.

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## Feature vector

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## Training, Test and Validation

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- Training: is used to train the models and determine their parameters (e.g. weights in a neural network).
- Validating: Once you have a collection of algorithms, you need to pick one model. Sometimes, the model that performs best on the validation set is picked up.
- Testing: We use a test set once a model is chosen, but we don't know its performance on unseen data yet. We can apply the chosen model to a test set to see its performance on unseen data.
- How to divide the data? e.g. 60%, 20%, 20%; or 70%, 20%, 10% (need to make sure/check about potential bias and balance/imbalance- more on this later during this module).

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## Unsupervised learning

t-SNE with cluster labels

labels: 0, 1, 2, 3, 4

Length of stay (log scale)

Rate of emergency surgeries

Image source: J. Li et al., BMC Medical Informatics and Decision Making, 2024.

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## Clustering

- The problem that needs to be solved in clustering:
- For example, given a dataset, if we knew that there were 3 groups of data but did not have access to a taxonomy (i.e. labels) to directly identify them, we could try a clustering task.
- This means splitting the data into well-separated group called clusters.

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## K-means clustering

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- The *KMeans* algorithm clusters data by trying to separate samples in *n groups of equal variance*, minimising a criterion known as the inertia or within-cluster sum-of-squares.
- This algorithm requires the number of clusters to be specified. It scales well to a large number of samples and has been used across a large range of application areas in many different fields.
- The k-means algorithm divides a set of  $N$  samples  $X$  into  $K$  disjoint clusters  $C$ , each described by the mean  $\mu_j$  of the samples in the cluster.

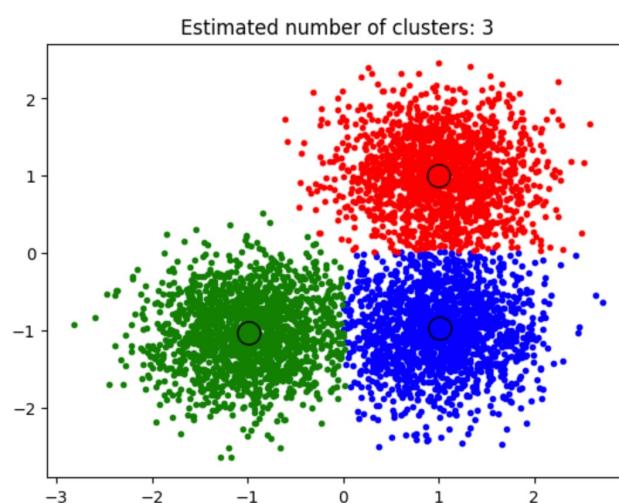
Source: Scikit learn documentation

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## K-means

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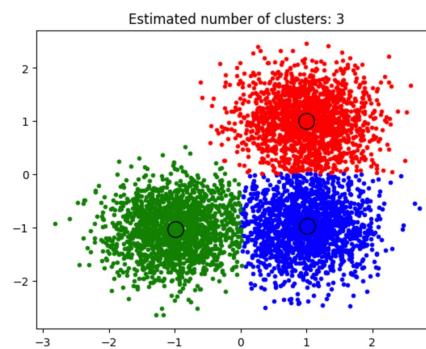
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## K-Means

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- The means are commonly called the cluster “centroids”; note that they are not, in general, points from  $X$ , although they live in the same space.
- The K-means algorithm aims to choose centroids that minimise the inertia, or within-cluster sum of squared criterion:

$$\sum_{i=0}^n \min_{\mu_j \in C} (\|\mu_j - \mu_i\|^2)$$



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## How K-means works

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- K-means has three steps.
- The first step chooses the initial centroids, with the most basic method being to choose  $k$  samples from the dataset  $X$ .
- After *initialisation*, K-means consists of looping between the two other steps.
- The first step assigns each sample to its nearest centroid. The second step creates new centroids by taking the mean value of all the samples assigned to each previous centroid.
- The difference between the old and the new centroids are computed and the algorithm repeats these last two steps until this value is less than a threshold. In other words, it repeats until the centroids do not move significantly.

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## K-Means Algorithm

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- First, the initial cluster for each of the points is calculated using the current centroids.
- Secondly, the centroids are **updated to the mean of each segment**.
- The algorithm then repeats this until a **stopping criterion** is fulfilled (e.g. error rate below a certain threshold).
- Or, for example, iteration stops when centroids move less than a threshold.

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## Convergence in K-means

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- Performing enough iterations, K-means will converge ; however, this may be to a local minimum. This is highly dependent on the initialisation of the centroids.
- As a result, the computation is often done several times, with different initialisations of the centroids.
- **Generally, repats are very important in developing robust machine learning models** (more on this in the coming days).

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## Convergence in K-means

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- One method to help address this issue is the “k-means++” initialisation scheme, which has been implemented in scikit-learn (use the `init='kmeans++'` parameter).
- This initialises the centroids to be (generally) distant from each other, leading to provably better results than random initialisation, as shown in the reference.

Source: Scikit learn documentation

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## K-means Example

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- Before you need to install sci-kit learn
- In Mac OS
  - `sudo easy_install pip`
  - `pip install -U numpy scipy scikit-learn`
- In Linux
  - `sudo apt-get install build-essential python-dev python-setuptools \python-numpy python-scipy \libatlas-dev libatlas3gf-base`

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## Practice questions

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## Practice questions

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- In a machine learning experiment, we have 1000 samples. We divide the data into training, validation and test sets as below:
  - Training samples: 300
  - Validation samples: 200
  - Test samples: 500
- Is this a good split?
- Please go to [menti.com](https://menti.com) and add your response (code will be given)

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## Hospital stay

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- In a machine learning experiment, you have been asked to design a model that can predict hospital stays for people who are admitted to a neurology ward.
- What type of model will you use to design your model?

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## If you have any questions

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- Please feel free to arrange a meeting or email ([p.barnaghi@imperial.ac.uk](mailto:p.barnaghi@imperial.ac.uk)).
- My office: 928, Sir Michael Uren Research Hub, White City Campus.

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