# Machine Learning:

# A new toolbox for Theoretical Physics

**Juan Rojo**

VU Amsterdam & Theory group, Nikhef

***D-ITP Advanced Topics in Theoretical Physics***

***18/11/2019***

# Course Overview

# Schedule

- **Four lectures**, each taking place **between 11am and 1pm** at room **H331** of Nikhef
- In the corresponding afternoons: hands-on tutorials, divided between **H331** and **H320**

☑ Monday **18th of November** 2019: Lecture (11am to 1pm) and Tutorial (2pm to 5pm).

☑ Monday **25th of November** 2019: Lecture (11am to 1pm) and Tutorial (2pm to 5pm).

☑ Monday **2nd of December** 2019: Lecture (11am to 1pm) and Tutorial (2pm to 5pm).

☑ Monday **9th of December** 2019: Lecture (11am to 1pm) and Tutorial (2pm to 5pm).

The course is at **full capacity**, to please make sure to be in the lecture and tutorial rooms in time to find place and to avoid disrupting the teaching

# Course evaluation

The **marking** of this module is composed by **two parts**

- Writing of a **short report** (4 pages) about a specific **application of Machine Learning algorithms** to a physics problem that you find interesting or relevant for your research. This report can be written individually or in groups of at most 3 students. Including possible **code examples** is encouraged but not required

  You need to send by email this report by **Friday 13th December**

- **Presentation** of the contents of this report on **Monday 16th:** 10 min + discussion

Only students that write and present their report will obtain a **pass** for the course, provided their **quality is deemed sufficient**

The examination is only required if you aim to obtain ECs from this course!

# References

the literature on **Machine Learning and their applications to physics** is vast.

When preparing these lectures the following resources have been used:

- ☑ *A high-bias, low-variance introduction to Machine Learning for physicists,* Pankaj Mehta, Ching-Hao Wang, Alexandre G. R. Day, and Clint Richardson, Phys. Rept. 810, 1 (2019), arXiv:1803.08823 [physics.comp-ph]]

  ***main reference, also for the tutorials. Most examples discussed in this lectures are taken from this report***

- ☑ *Machine learning and the physical sciences,* G. Carleo, I. Cirac, K. Cranmer, L. Daudet, M. Schuld, N. Tishby, L. Vogt-Maranto and L. Zdeborová, arXiv:1903.10563 [physics.comp-ph].

- ☑ *Lectures on Machine Learning,* S. Carrazza, Taller de Altas Energies 2018 (TAE18), *http://benasque.org/2018tae/*

- ☑ *Lectures on Artificial Intelligence, Deep Learning, Advanced Machine Learning, G*. Louppe, lecture materials and tutorials available from *https://github.com/glouppe/info8010-deep-learning*, *https://github.com/glouppe/info8004-advanced-machine-learning*

***plus many other ML resources online!***

# Tutorials

the hands-on tutorials will allow you to familiarise with the machine learning concepts presented in the lectures by means of **practical examples**

these tutorials, alongside with the rest of course materials, can be found in

***https://github.com/juanrojochacon/ml-ditp-attp/***

this **GitHub repository** will be updated as the course goes on, so make sure you pull frequently

the course tutorials will be based on **Python** (3.7) which hopefully most of you have experience with. These tutorials do not involve writing new code altogether but rather adapting existing programs and try new things

make sure you bring your laptop and have an **up-to-date Python installation** beforehand, e.g. from **Conda** or Homebrew. Test it with some of the example programs in the repo!

# Today's lecture

- Why Machine Learning? Basic concepts and terminology
- Supervised Learning: model fitting and polynomial regression
- The need for regularisation in ML (cross-validation)
- Optimisers in Supervised Learning: Gradient Descent and Genetic Algorithms

***Tutorial 1:***

***(a) Model fitting with polynomial regression***

***(b)Testing Gradient Descent strategies***

# Why Machine Learning?

**with input from *Lectures on Machine Learning,* S. Carrazza, TAE2018**

# Why this course?

Machine Learning rightly deserves to be part of the **toolbox of a theoretical physicist**

- Essential for building **modern models and algorithms** in various areas of physics

- Very **fast developments** both in algorithms and in computing platforms have significantly extended the breadth of problems that can be tackled with ML

- Deep **physical connections** with many problems in theoretical physics, *e.g.* quantum computation, condensed matter systems

- Applied to problems even in very **formal fields,** *e.g.* string theory

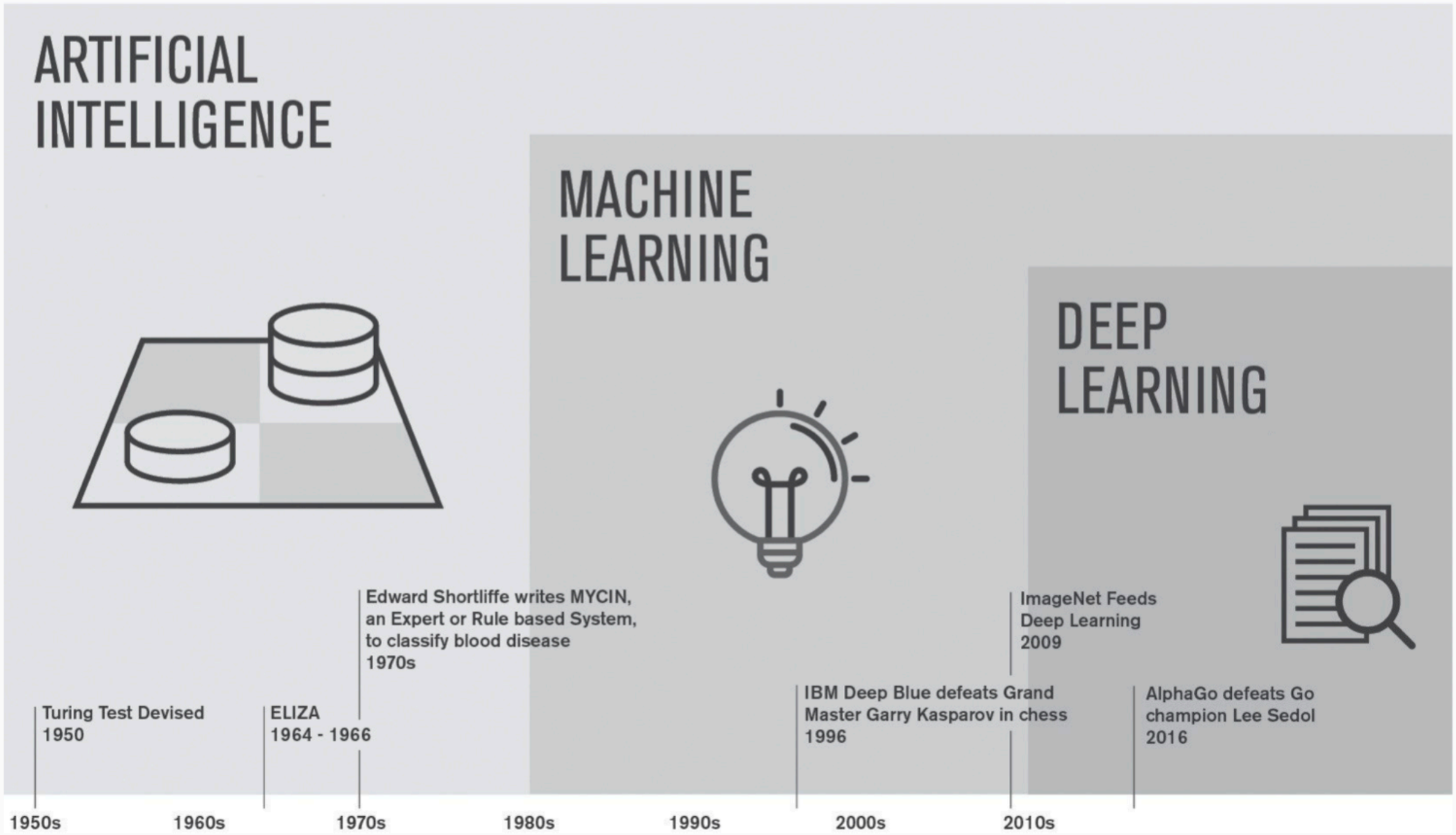
- Large interested in the community, **societal implications** (AI hype)

Furthermore, **expertise in ML/AI** is powerful asset for also for careers outside academia

# AI vs ML

Machine Learning is part of the **Artificial Intelligence paradigm**

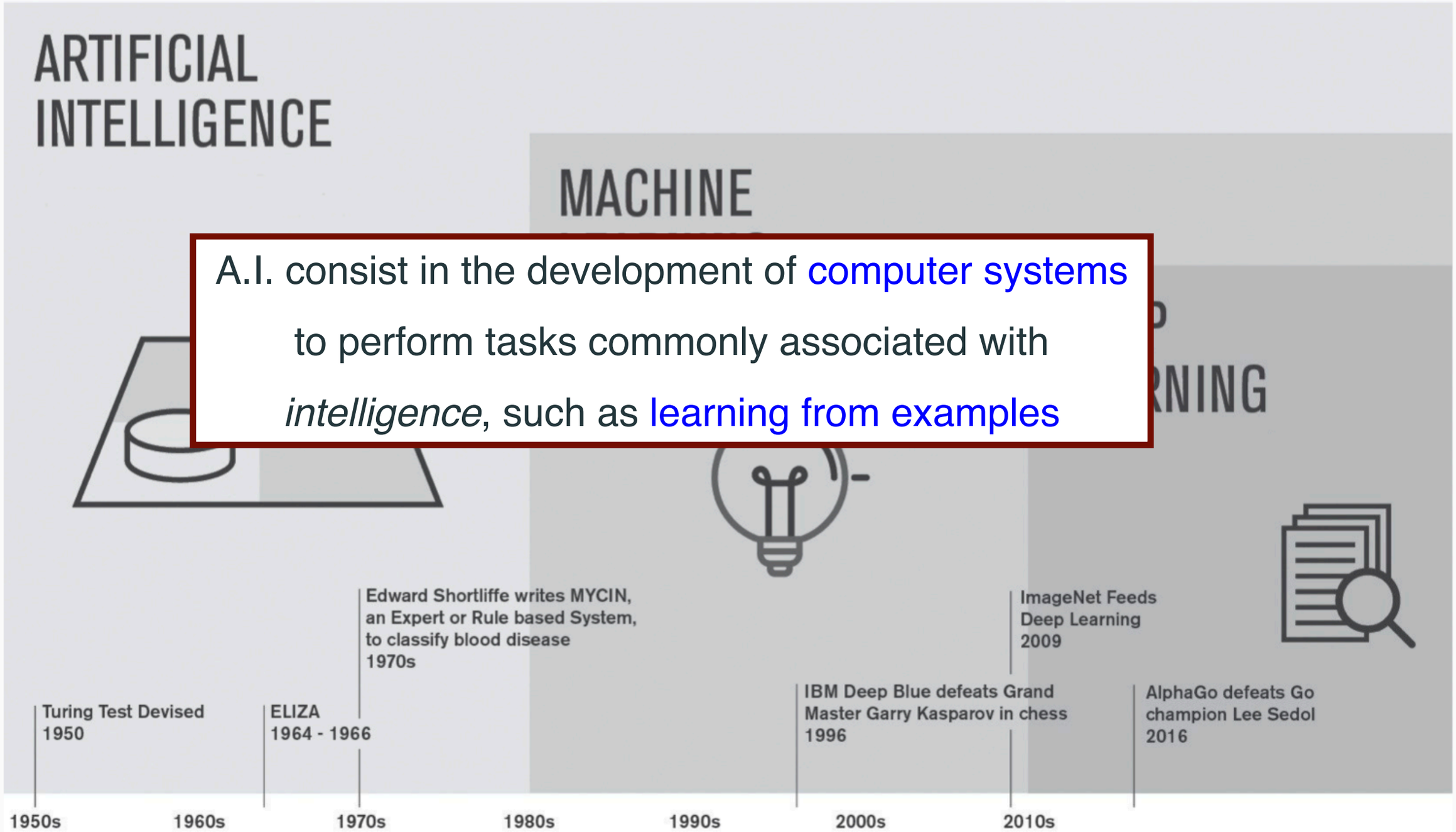
*AI is the science and engineering of making intelligent machines (McCarthy '56)*



# AI vs ML

Machine Learning is part of the **Artificial Intelligence paradigm**

*AI is the science and engineering of making intelligent machines (McCarthy '56)*

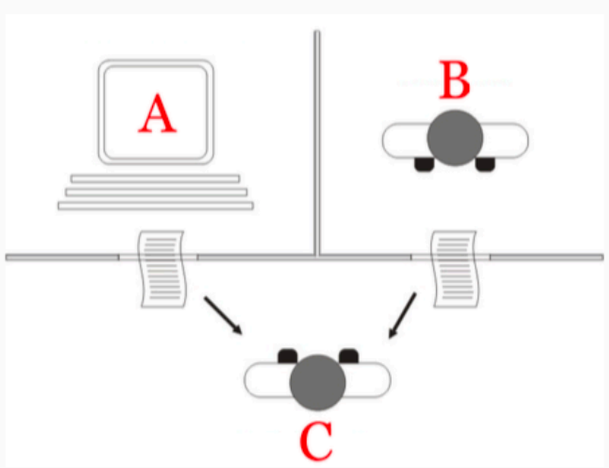


# Problems in AI

Most problems tackled with Artificial Intelligence fall in **two categories**

**(1)** abstract and formal: *easy for computers* but *difficult for humans*

**knowledge-based approach**





***e.g. chess (DeepBlue)***

***(chess is deterministic game with finite number of options )***

**(2)** intuitive, hard to formalize: *easy for humans* but *difficult for machines*

**concept capture and generalisation**

***e.g. pattern recognition***

# Problems in AI

Most problems tackled with Artificial Intelligence fall in **two categories**

**(1)** To excel in tasks which are intuitive to humans but difficult *s* to machines, an A.I. system needs to **acquire its own knowledge**: the Machine is Learning

Machine Learning algorithms allow computers the ability to **carry out a task without being explicitly programmed how to do it** by **learning from examples**

***chess (DeepBlue)***

**(2)** intuitive, hard to formalize: *easy for humans* but *difficult for machines*

**concept capture and generalisation**

***e.g. pattern recognition***

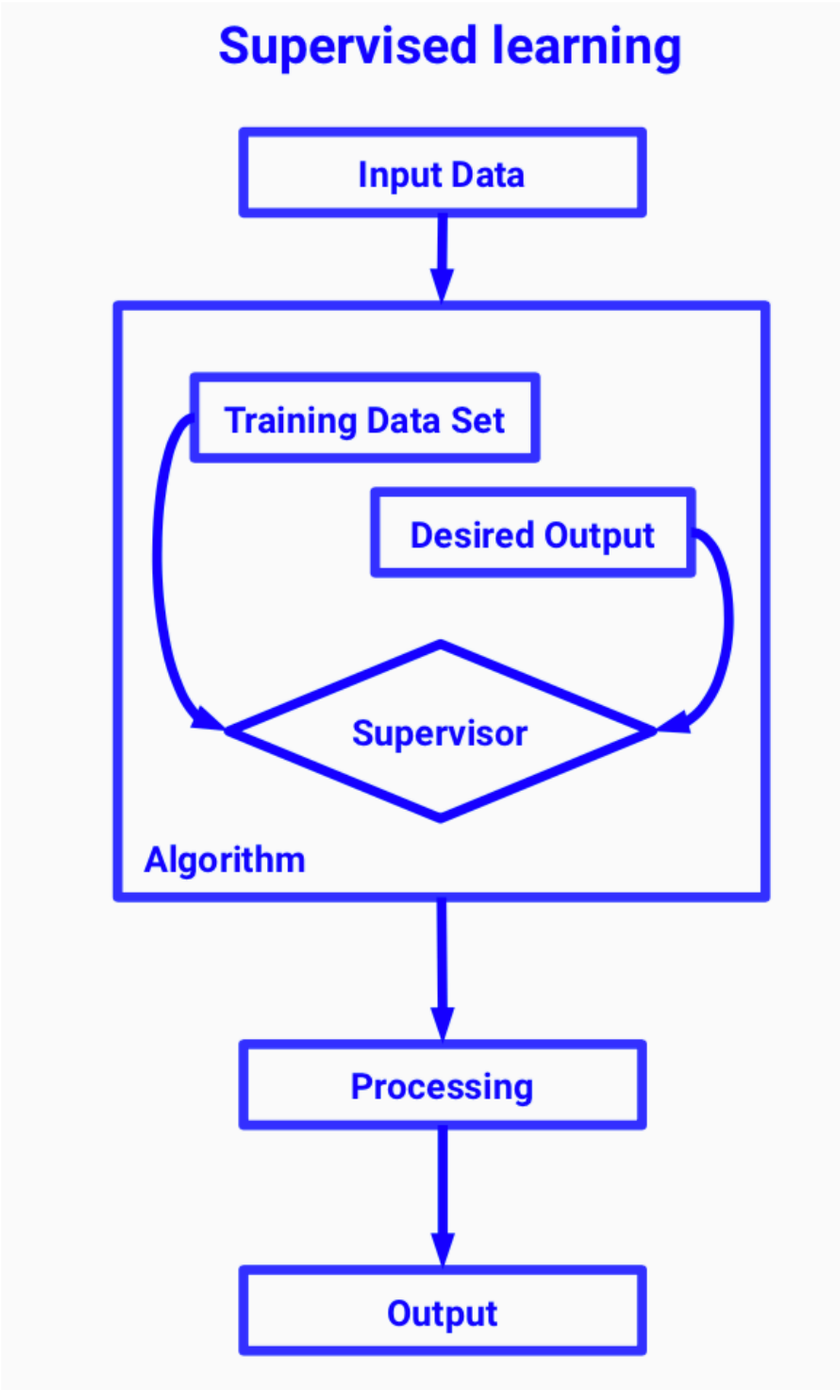
# ML is everywhere

- **Database mining:**
  - Search engines
  - Spam filters
  - Medical and biological records
- **Intuitive tasks for humans:**
  - Autonomous driving
  - Natural language processing
  - Robotics (reinforcement learning)
  - Game playing (DQN algorithms)
- **Human learning:**
  - Concept/human recognition
  - Computer vision
  - Product recommendation

# Learning to learn

**Machine Learning** algorithms can be divided into several classes, including

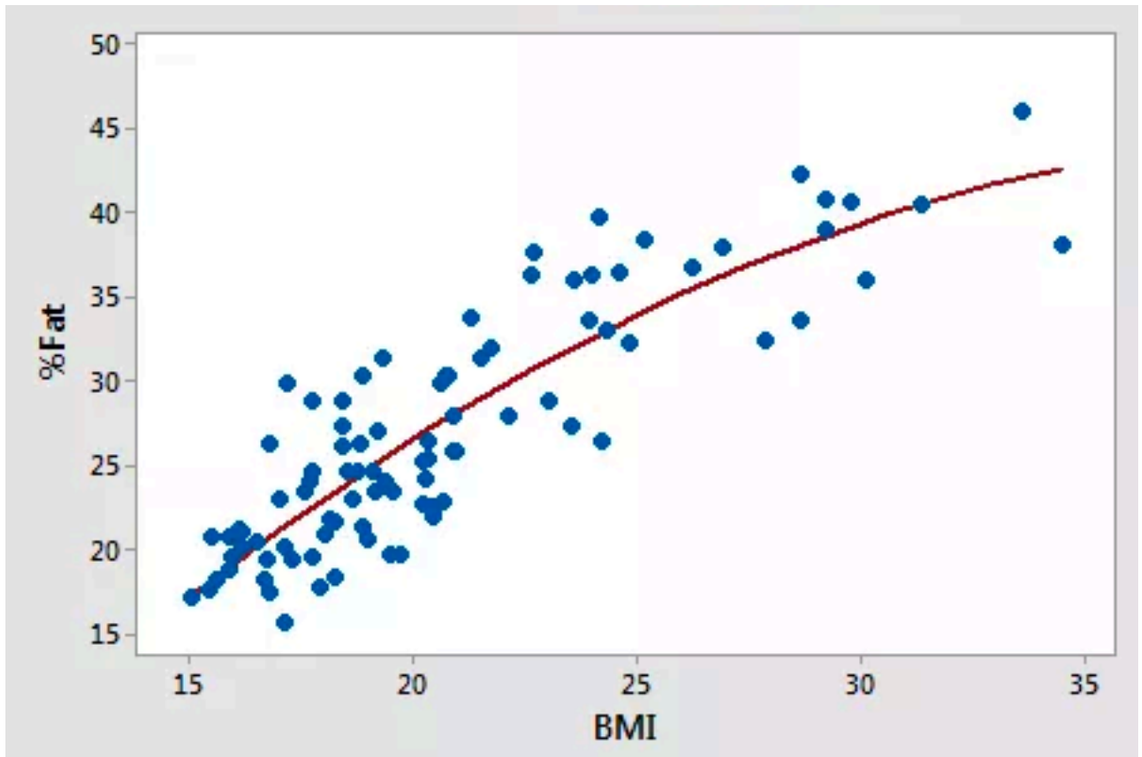
- **Supervised Learning**:
  regression, classification, …

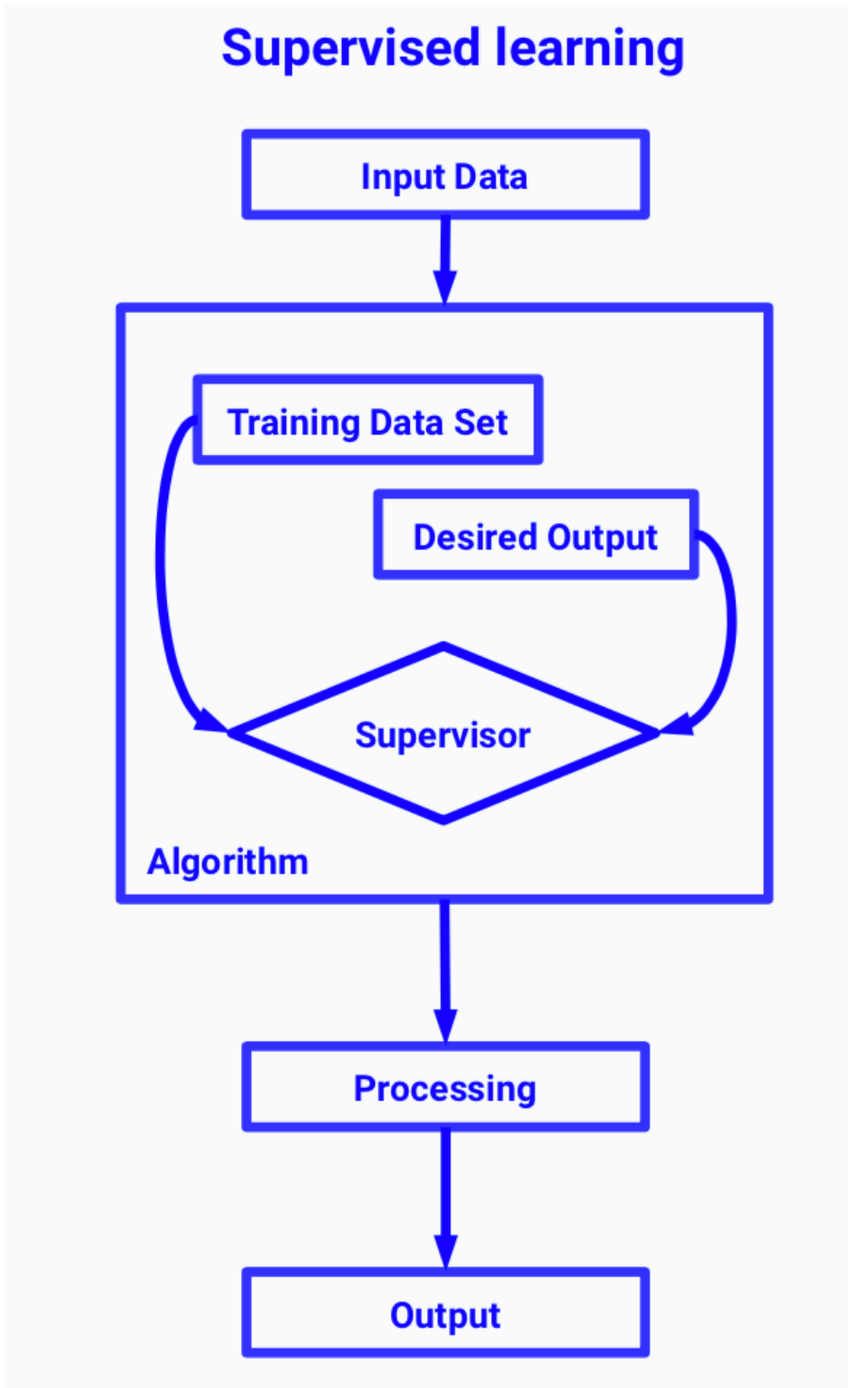


# Learning to learn

**Machine Learning** algorithms can be divided into several classes, including

- **Supervised Learning**:
  regression, classification, …



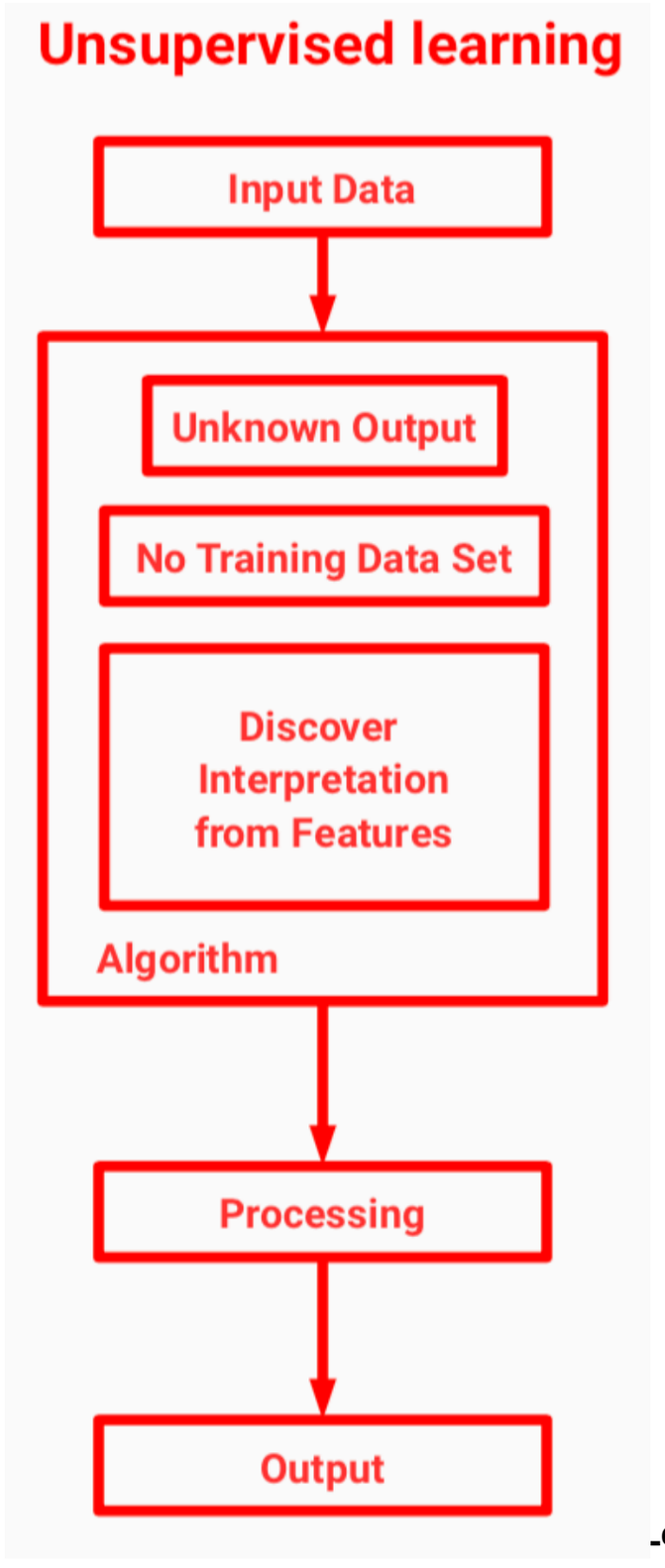



# Learning to learn

**Machine Learning** algorithms can be divided into several classes, including

- **Supervised Learning**:
  regression, classification, …

- **Unsupervised Learning**:
  clustering, data dimensional reduction, ….

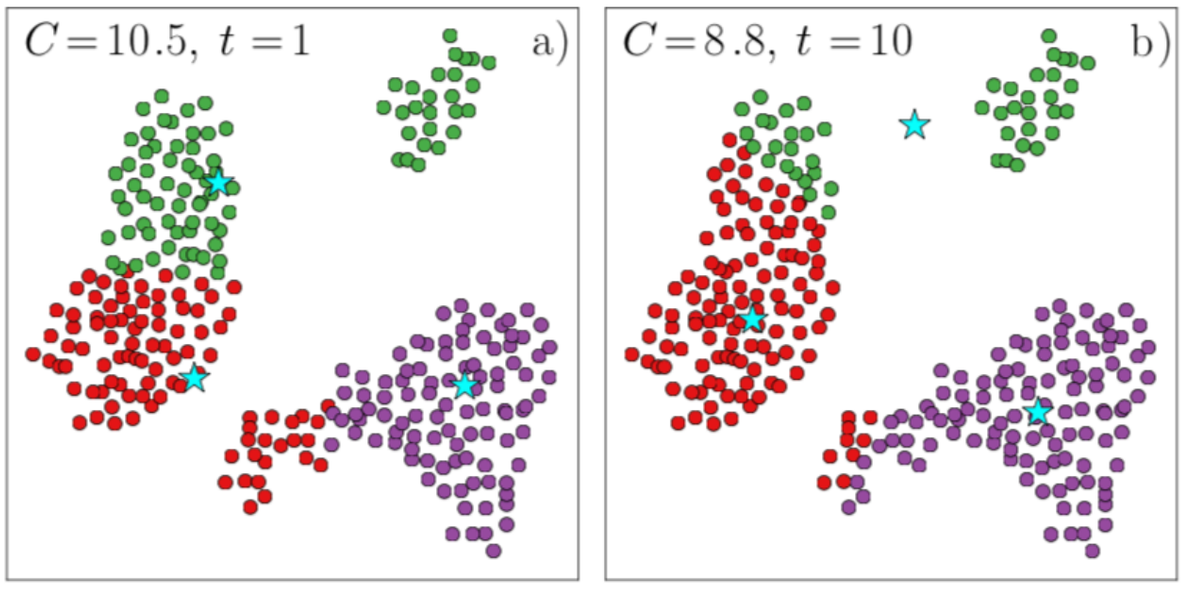


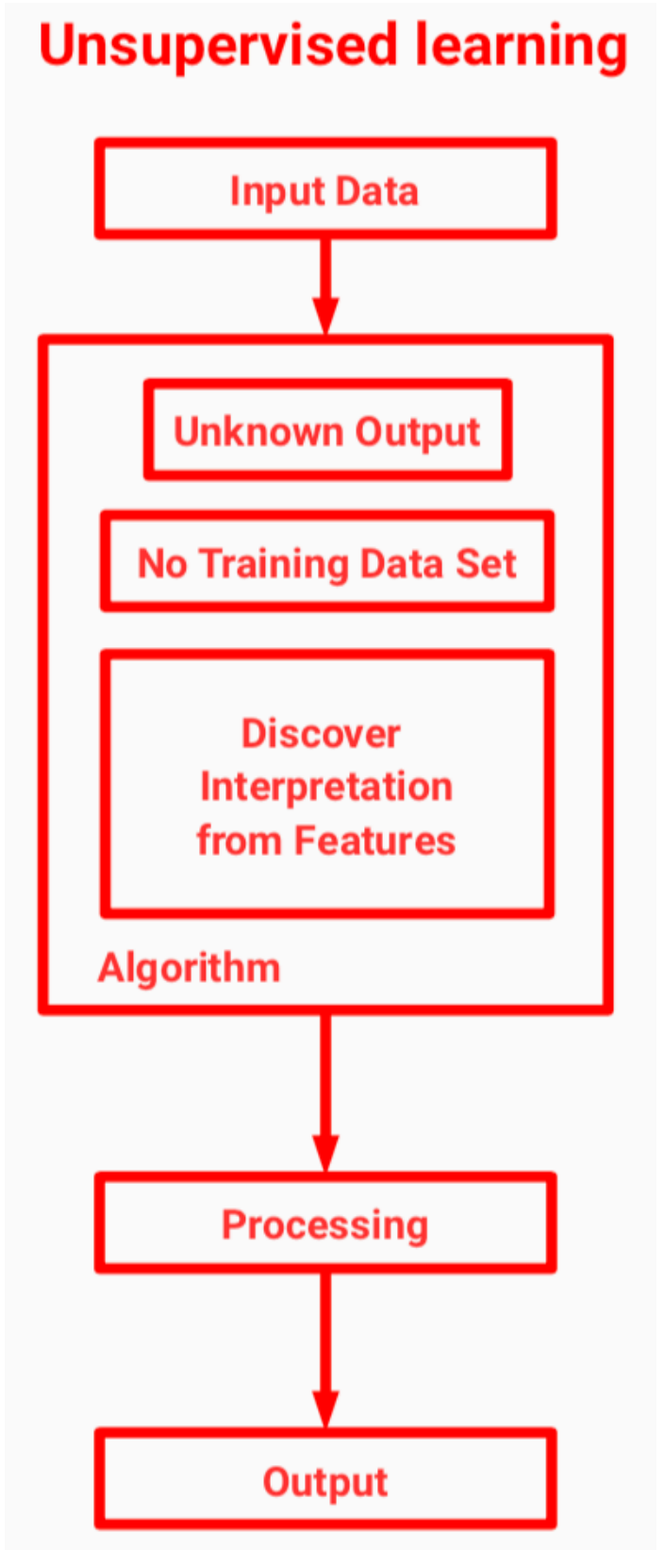
# Learning to learn

**Machine Learning** algorithms can be divided into several classes, including

- **Supervised Learning**:
  regression, classification, …

- **Unsupervised Learning**:
  clustering, data dimensional reduction, ….



# Learning to learn

**Machine Learning** algorithms can be divided into several classes, including

- **Supervised Learning**:
  regression, classification, …

- **Unsupervised Learning**:
  clustering, data dimensional reduction, ….

- **Reinforcement learning**:
  efficiently react to changing environment

# Learning to learn

**Machine Learning** algorithms can be divided into several classes, including

- **Reinforcement learning**: efficiently react to changing environment

# The Machine Learning Galaxy I


*In this course we will have time to cover only subset of ML algorithms and applications!*

# The Machine Learning Galaxy II

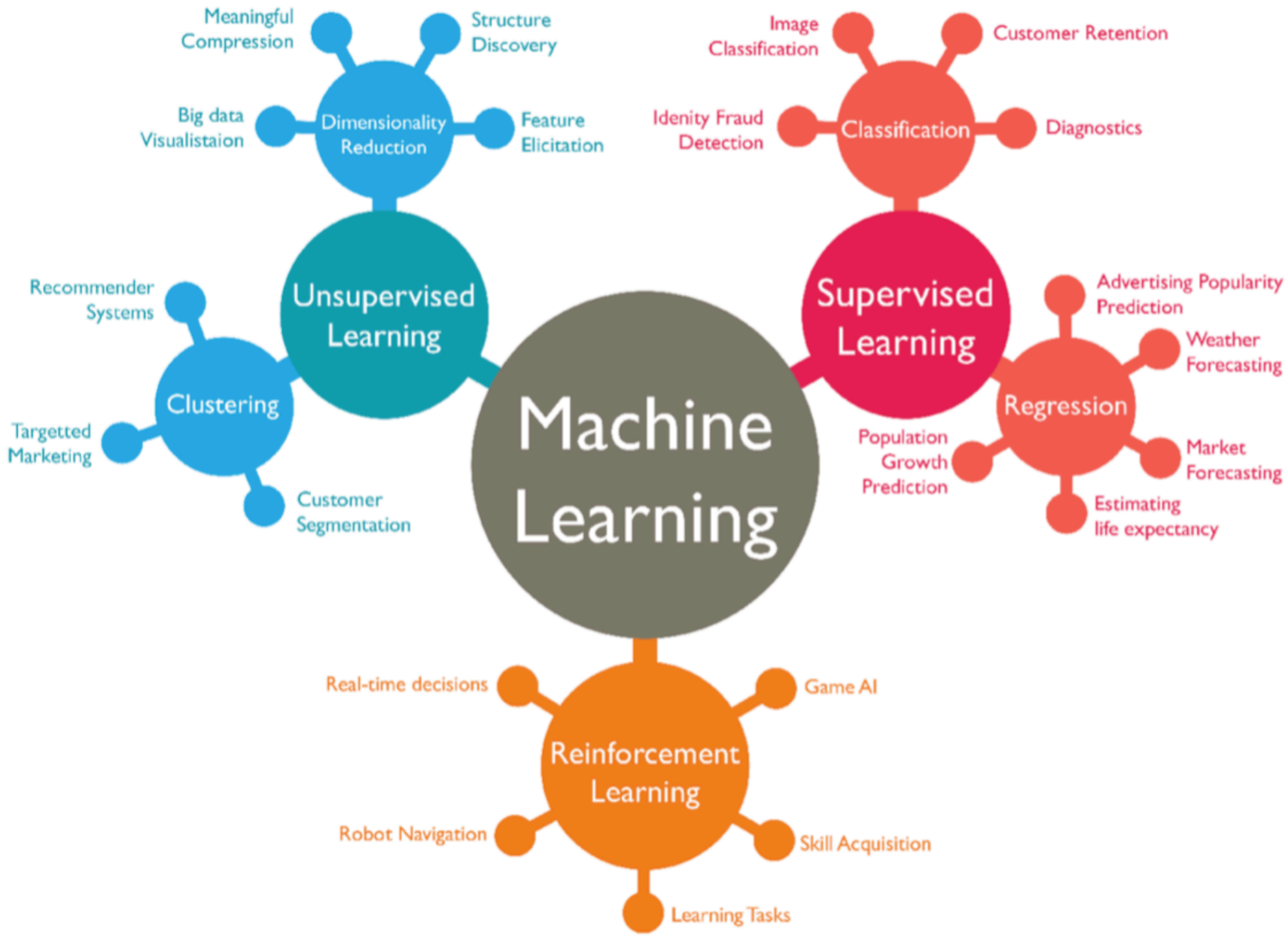



*Image via Abdul Rahid*

*In this course we will have time to cover only subset of ML algorithms and applications!*

# Supervised Learning:

# Model Fitting and Regression

# Supervised learning

We denote as **supervised learning** the ML task of **learning a function** that maps a **vector of inputs** to a **vector of outputs** from a finite set of training example

note that some assumptions will be needed: a function is an **infinite-dimensional object** but learning takes place from a **finite number of examples**

main property of supervised learning: the **training samples are labeled**

# Supervised learning

We denote as **supervised learning** the ML task of **learning a function** that maps a **vector of inputs** to a **vector of outputs** from a finite set of training example

note that some assumptions will be needed: a function is an **infinite-dimensional object** but learning takes place from a **finite number of examples**

main property of supervised learning: the **training samples are labeled**

$$\boldsymbol{x}_i = \left( x_{i,1}, x_{i,2}, \ldots, x_{i,p} \right) \quad \rightarrow \quad y_i$$

***data point (p features)*** ***label***

the label can be **discrete** (signal/noise, cat/dog) or **continuous** (output of function )

# Supervised learning

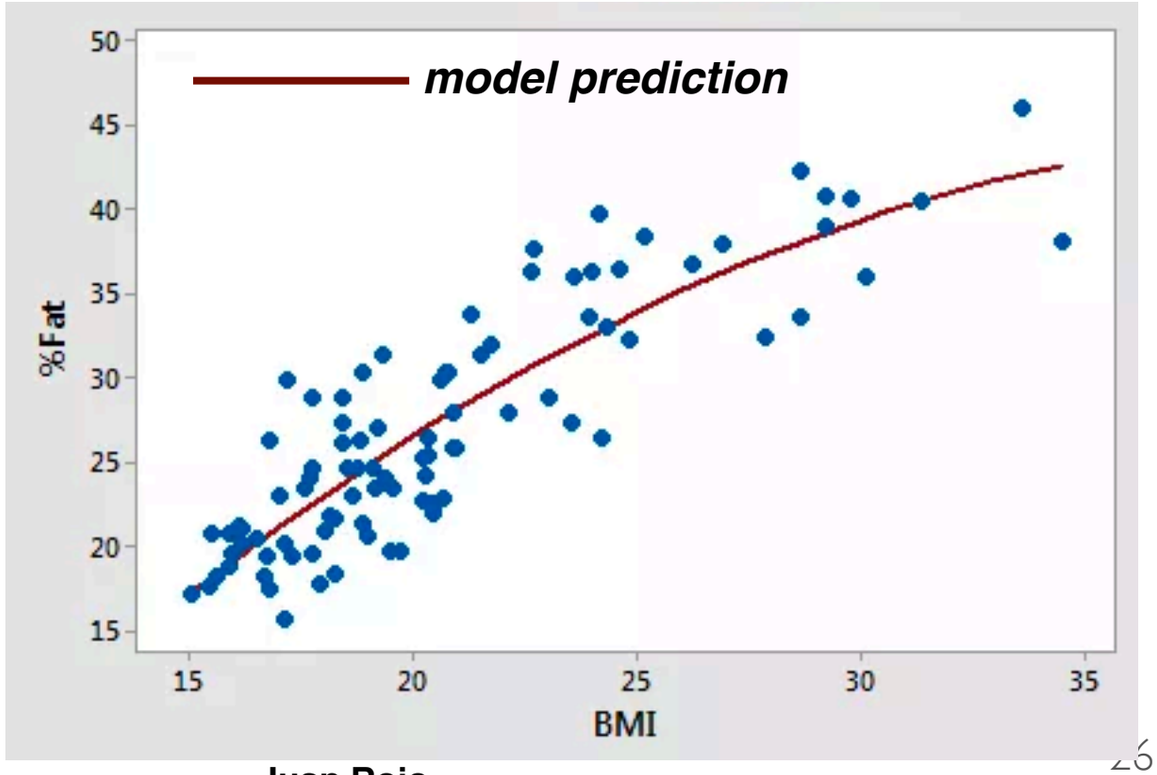
We denote as **supervised learning** the ML task of **learning a function** that maps a **vector of inputs** to a **vector of outputs** from a finite set of training example

note that some assumptions will be needed: a function is an **infinite-dimensional object** but learning takes place from a **finite number of examples**

main property of supervised learning: the **training samples are labeled**

***continuous outputs:***

***regression***




***data point: BMI***

***label: % Fat***

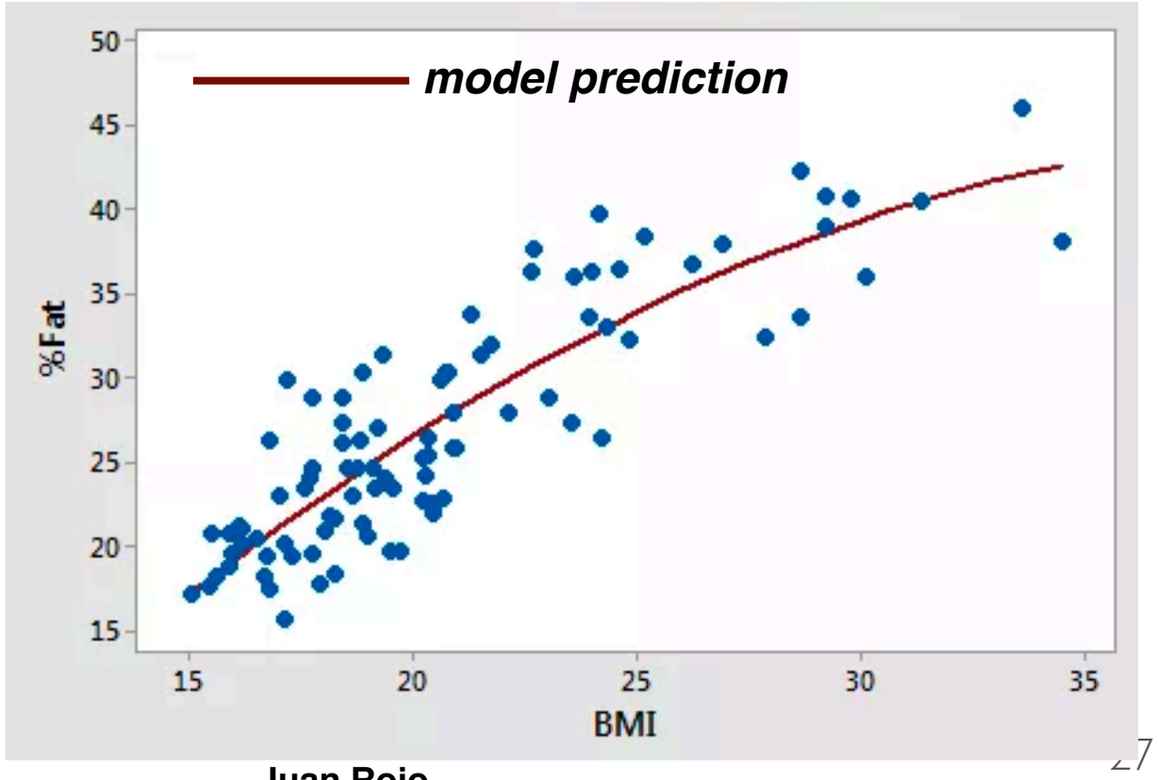
# Supervised learning

We denote as **supervised learning** the ML task of **learning a function** that maps a **vector of inputs** to a **vector of outputs** from a finite set of training example

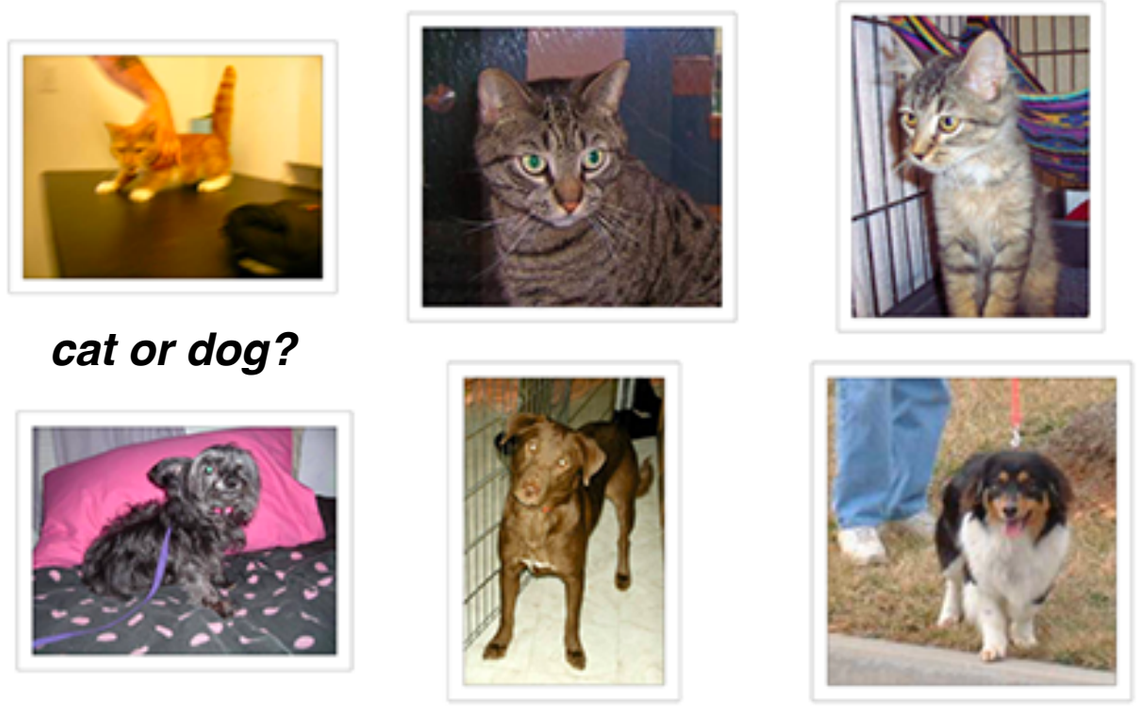
note that some assumptions will be needed: a function is an **infinite-dimensional object** but learning takes place from a **finite number of examples**

main property of supervised learning: the **training samples are labeled**

***continuous outputs: regression***




***discrete outputs: classification***



# Supervised learning

We denote as **supervised learning** the ML task of **learning a function** that maps a **vector of inputs** to a **vector of outputs** from a finite set of training example

note that some assumptions will be needed: a function is an **infinite-dimensional object** but learning takes place from a **finite number of examples**

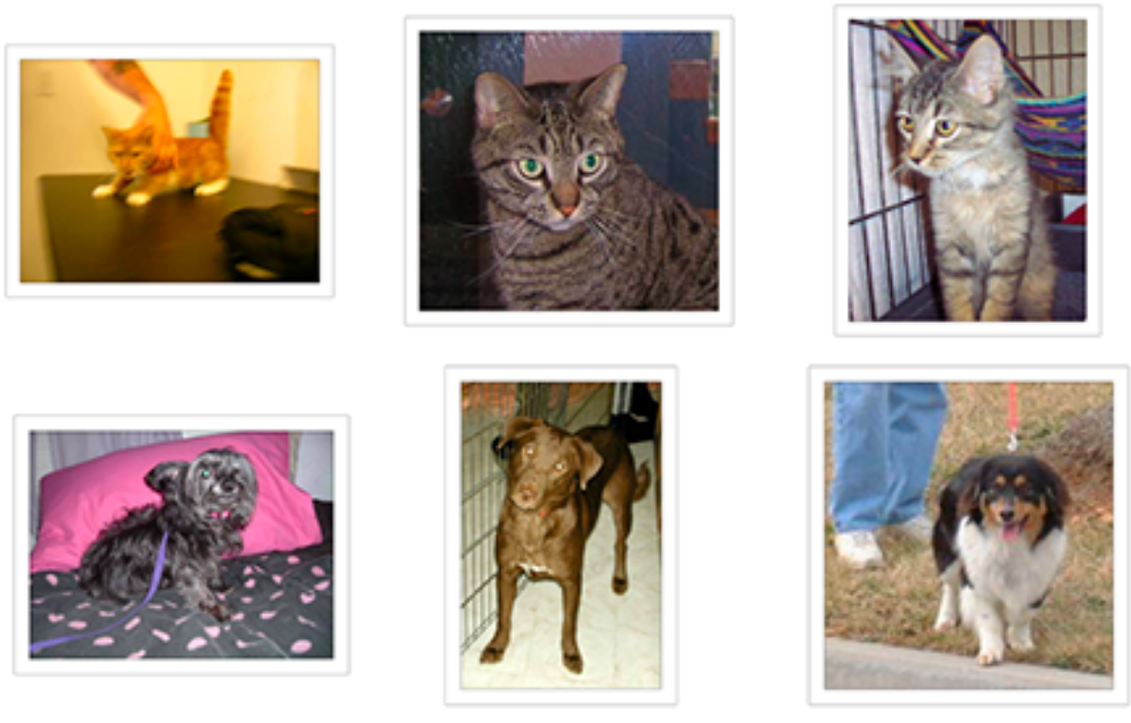
main property of supervised learning: the **training samples are labeled**

***data point: RGB values of each pixel***

***label: car or dog***

***discrete outputs:***

***classification***



# Setting up the problem

problems in **Supervised Machine Learning** are defined by the following ingredients:

***(1) Input dataset:*** $\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$

*array of **independent** variables*

*array of **dependent** variables*

$$\boldsymbol{X} = \left(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\right) \qquad \boldsymbol{Y} = \left(y_1, y_2, \ldots, y_N\right)$$

$$\boldsymbol{x}_i = \left(x_{i,1}, x_{i,2}, \ldots, x_{i,p}\right)$$

***each independent variable contains p features***

# Setting up the problem

problems in **Supervised Machine Learning** are defined by the following ingredients:

***(1) Input dataset:*** $\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$

*array of **independent** variables*

$$\boldsymbol{X} = \left(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\right)$$

*array of **dependent** variables*

$$\boldsymbol{Y} = \left(y_1, y_2, \ldots, y_n\right)$$

$$\boldsymbol{x}_i = \left(x_{i,1}, x_{i,2}, \ldots, x_{i,p}\right)$$

***each independent variable contains p features***

***(2) Model:*** $f\left(\boldsymbol{X}, \boldsymbol{\theta}\right)$

*mapping between dependent and independent variables*

$$f : \boldsymbol{X} \rightarrow \boldsymbol{Y}$$

*model parameters*

$$\boldsymbol{\theta} = \left(\theta_1, \theta_2, \ldots, \theta_m\right)$$

# Setting up the problem

problems in **Supervised Machine Learning** are defined by the following ingredients:

***(1) Input dataset:*** $\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$

***(2) Model:*** $f\left(\boldsymbol{X}, \boldsymbol{\theta}\right)$

***(3) Cost function:*** $C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right)$

The cost function measures how well the model (for a specific choice of its parameters) is able to **describe the input dataset**

***example of cost function for single dependent variable: sum of residuals squared***

$$C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right) = \chi^2 = \frac{1}{n}\sum\left(y_i - f(\boldsymbol{x}_i, \boldsymbol{\theta})\right)^2$$

# Setting up the problem

problems in **Supervised Machine Learning** are defined by the following ingredients:

***(1) Input dataset:*** $\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$

***(2) Model:*** $f\left(\boldsymbol{X}, \boldsymbol{\theta}\right)$

***(3) Cost function:*** $C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right)$

The cost function measures how well the model (for a specific choice of its parameters) is able to describe the input dataset

Fitting the model means determining the values of its parameters which **minimise the cost function**

$$\left.\frac{\partial C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right)}{\partial \theta_i}\right|_{\theta=\theta_{\text{opt}}} = 0$$

# Model fitting

before dealing with more sophisticated samples of Machine Learning, let's illustrate the main aspects of model fitting with a simple example: **polynomial regression in 1D**

First of all we can generate data following a **known underlying law** and then adding **stochastic noise**, to emulate a realistic situation

$$y_i = f(x_i) + \eta_i\,, \qquad i = 1,\ldots,n$$

***dependent*** *variable*

*the **physical law** (might be known)*

***independent*** *variable*

*uncorrelated Gaussian variable*

$$\langle \eta_i \rangle = 0$$

$$\langle \eta_i \eta_j \rangle = \sigma^2 \delta_{ij}$$

*noise strength*

The larger the value of the **noise *σ*** compared to the variations of the **law *f,*** the noisier the data

# Model fitting

in the real world we would have only the information about the ``measurements''

$$\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$$

and our goal is to extract the **underlying physical law** from this data

We need to define **classes of models** that might provide a good description of the data, in a way that its parameters encode the main features of the physical law

$$f_\alpha(x;\, \boldsymbol{\theta}_\alpha)$$

*model prediction* — *label of model class* — *parameters of model class α*

we want to compare the performance of models with **different complexities:** different functional forms, number of parameters, intrinsic flexibility, ….

# Model fitting

The simplest possible model is a polynomial: **polynomial regression**

$$f_\alpha(x;\boldsymbol{\theta}_\alpha) = \sum_{j=0}^{N_\alpha} \theta_{\alpha,j} x^j$$

for example the model class that contains all possible cubic polynomials is

$$f_3(x;\boldsymbol{\theta}_3) = \sum_{j=0}^{3} \theta_{3,j} x^j$$

a more complex model does not necessarily imply a more predictive one: the appropriate amount of complexity depends on the **features of the data sample** (*e.g.* size, variability)

in polynomial regression the model parameter are given by **least-squares method**

$$\hat{\theta} = \arg\ \min_\theta \left\{ \sum_{i=1}^{n} \left( y_i - f_\alpha(x_i;\boldsymbol{\theta}_\alpha) \right)^2 \right\}$$

***minimise sum of residuals squared***

# Model fitting

Simples case: **least-squares method** for order-one polynomials

$$f_q(x;\boldsymbol{\theta}_1) = \sum_{j=0}^{1} \theta_{\alpha,j} x^j = \theta_{1,0} + \theta_{1,1} x$$

which is nothing but the **linear regression** taught in first-year statistics

$$\hat{\theta} = \arg\min_{\theta} \left\{ \sum_{i=1}^{n} \left( y_i - \theta_{1,0} - \theta_{1,1} x \right)^2 \right\}$$

where you can compute analytically the best-fit values of the coefficients

# Model fitting

Simples case: **least-squares method** for order-one polynomials

$$\left.\frac{\partial}{\partial\theta_0}\sum_{i=1}^{n}\left(y_i-\theta_0-\theta_1 x_i\right)^2\right|_{\widehat{\theta_0}}=0$$

$$\left.\frac{\partial}{\partial\theta_1}\sum_{i=1}^{n}\left(y_i-\theta_0-\theta_1 x_i\right)^2\right|_{\widehat{\theta_1}}=0$$

and by solving this linear system of equations one obtains the **model parameters**

$$\widehat{\theta_1}=\frac{\langle xy\rangle-\langle x\rangle\langle y\rangle}{\langle x^2\rangle-\langle x\rangle^2}$$

$$\widehat{\theta_0}=\langle y\rangle-\widehat{\theta_1}\,\langle x\rangle$$

***averages computed ever the n elements of the data sample***

# Best-fit model

What is the best strategy to **determine the model parameters**?

Seems a silly question, surely those are simply **minimum of cost function?**

$$\hat{\theta} = \arg\min_{\theta}\left\{ \sum_{i=1}^{n} \left(y_i - f_\alpha(x_i; \boldsymbol{\theta}_\alpha)\right)^2 \right\}$$

However this is in general **not the case**, because:

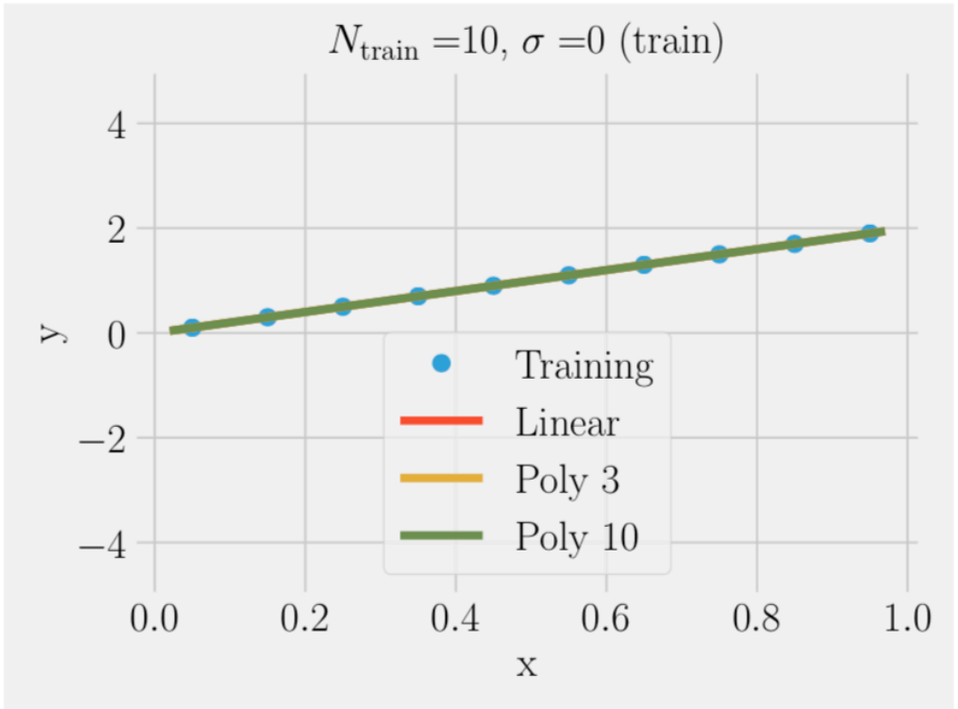
- Real world data is **noisy**: we want to **learn the underlying law**, not the statistical fluctuations

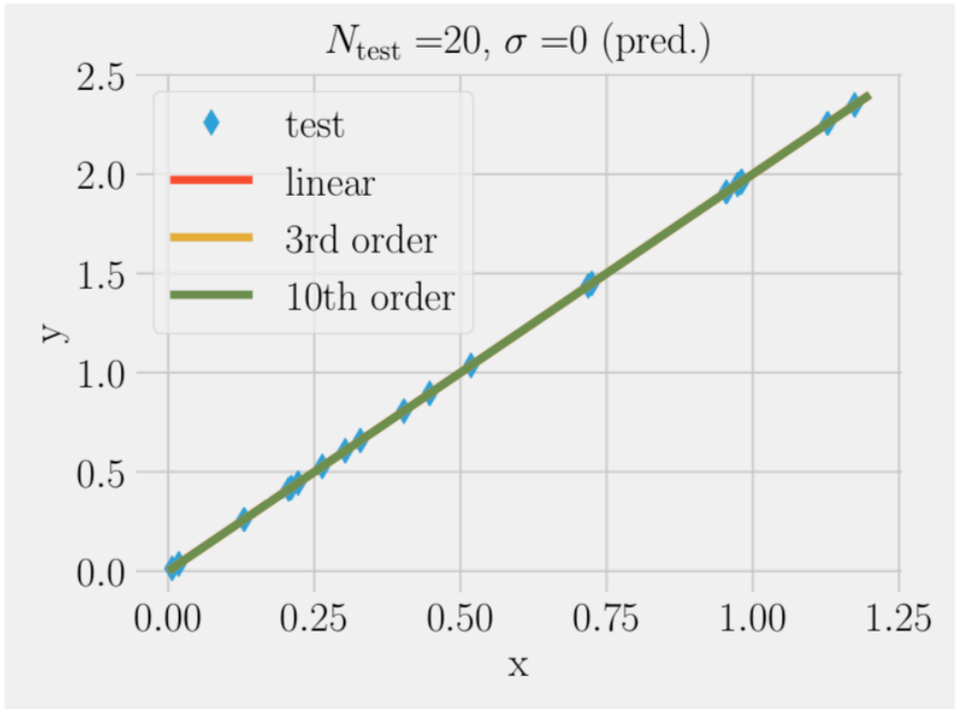
- More than fitting the data, our real goal is to create a model that **predicts future/ different data:** we need figures of merit outside the training dataset!

- To ensure that our model describes the underlying law (and thus one can safely generalise) rather than the noise, a **regularisation procedure** needs to be used

# Model fitting

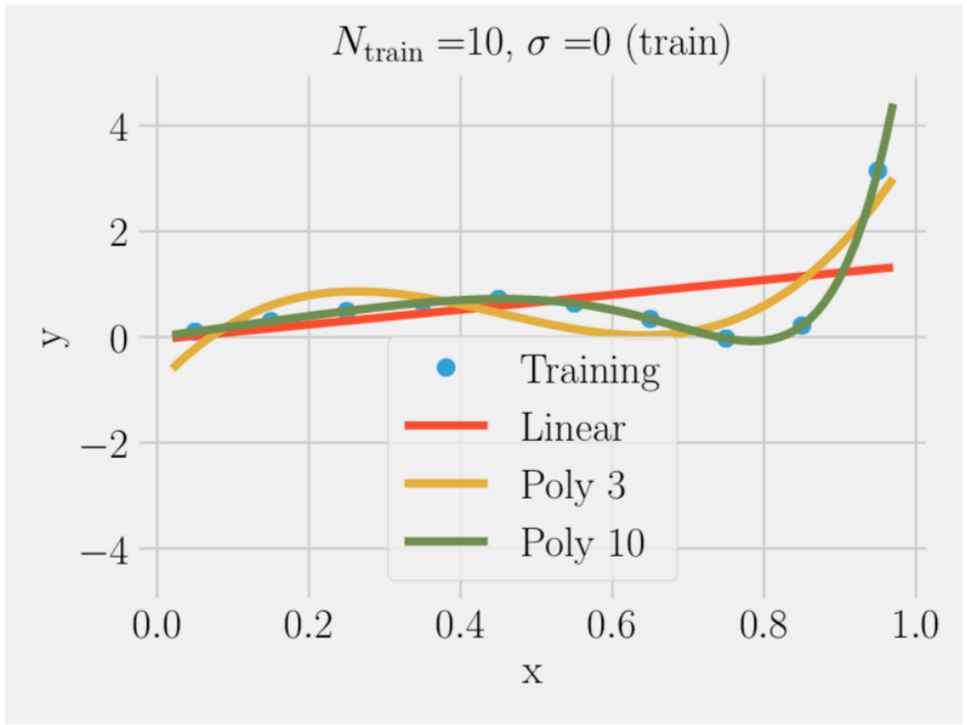
$f(x) = 2x\,, \quad x \in [0,1]$

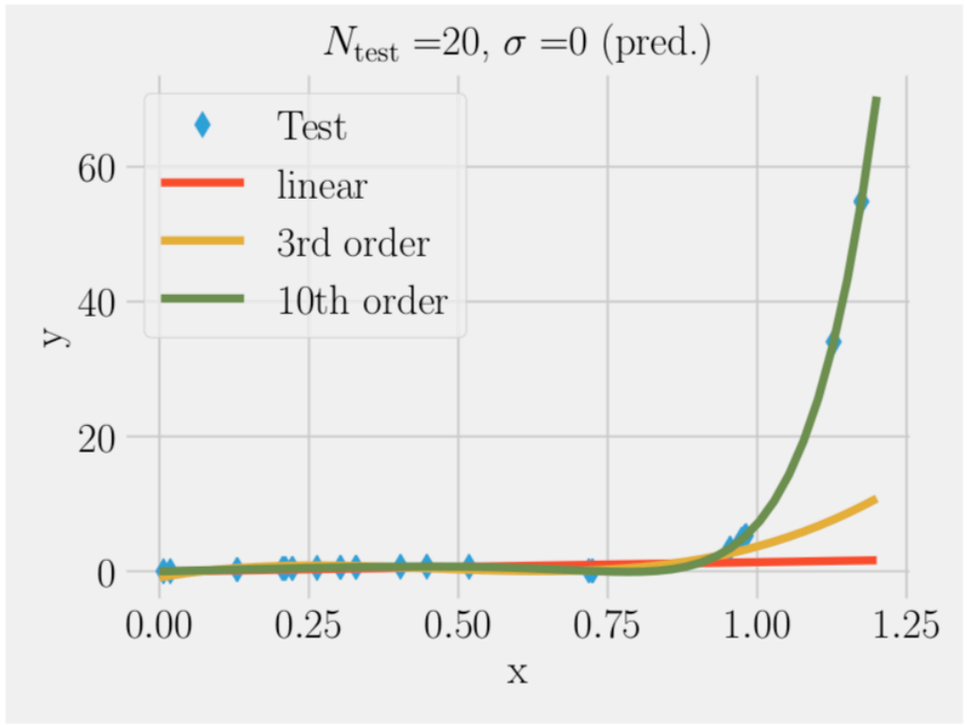



$f(x) = 2x - 10x^5 + 15x^{10}\,, \quad x \in [0,1]$

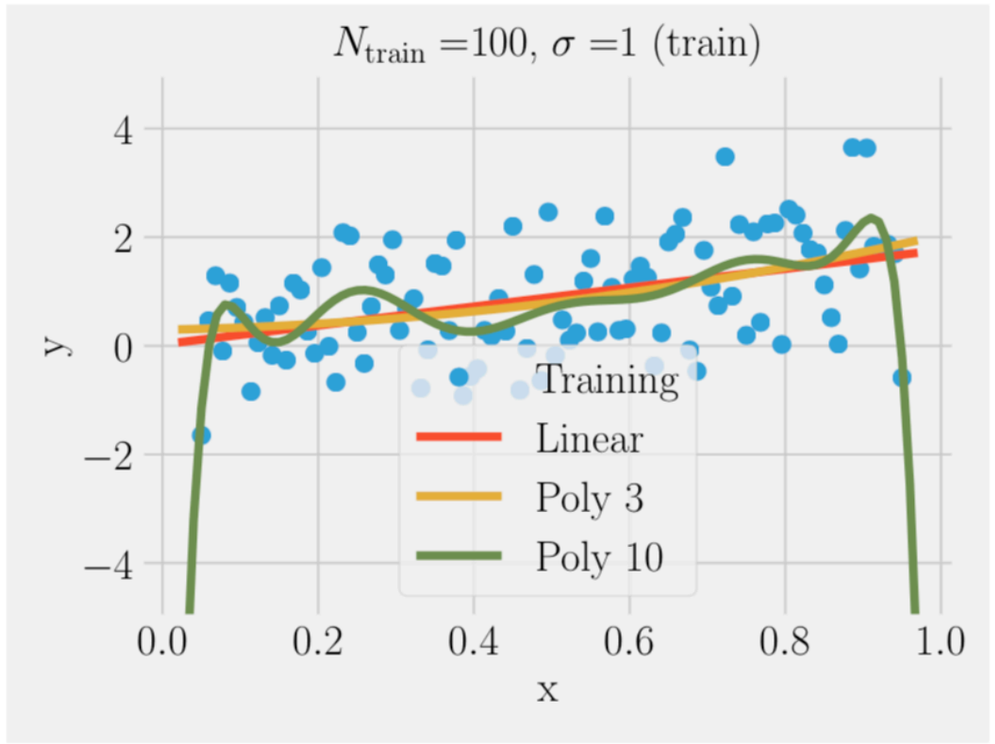
***in the absence of noise, fitting and predicting are identical, provided model has enough flexibility***

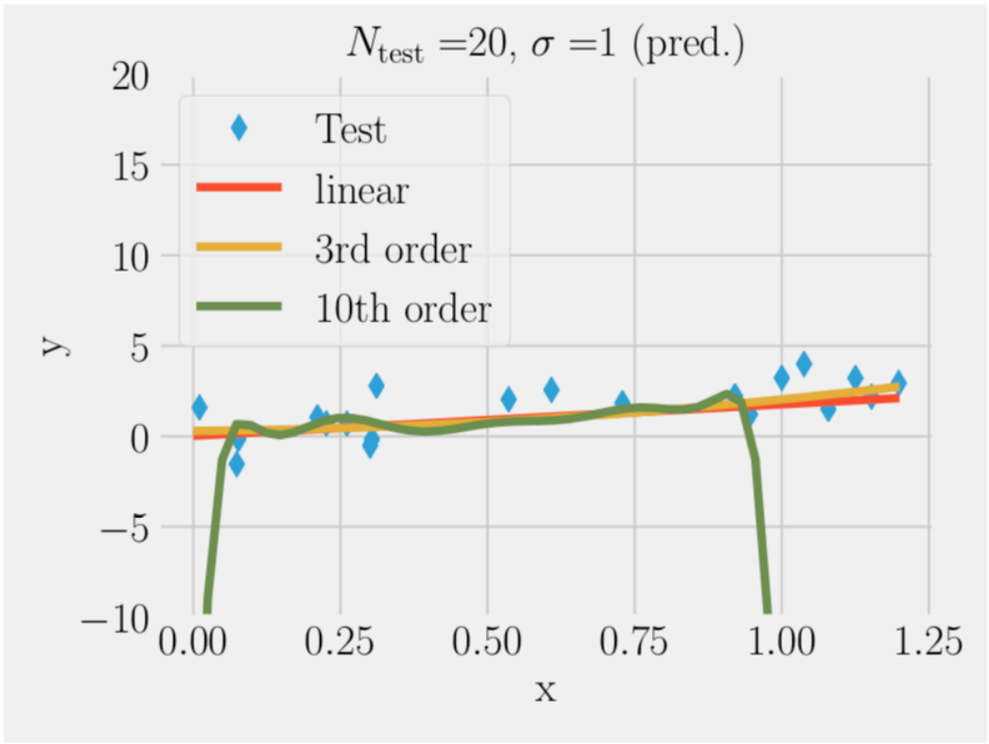


# Model fitting

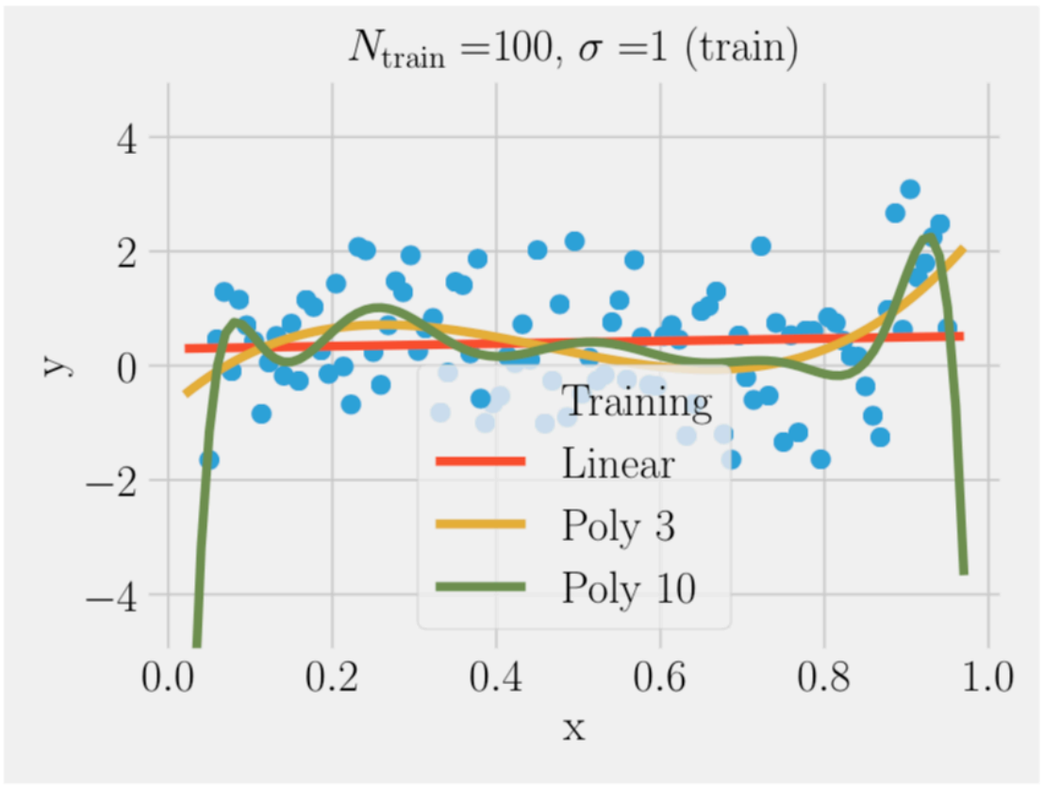
$f(x) = 2x\,, \quad x \in [0,1]$

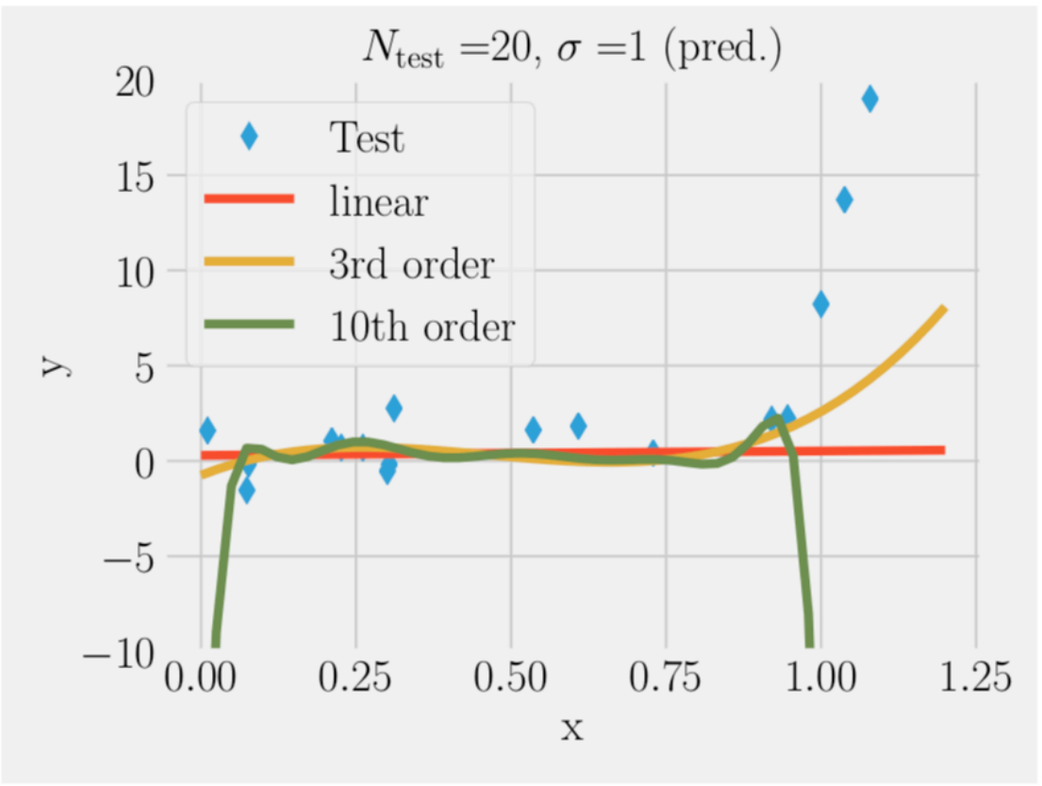



$f(x) = 2x - 10x^5 + 15x^{10}\,, \quad x \in [0,1]$

***in the presence of noise, models with less complexity can exhibit improved predictive power***



# Cross-validation (regularisation)

What is the best strategy to determine the model parameters?

first of all, divide input dataset into **two disjoint sets**

$$\mathscr{D} = \mathscr{D}_{\text{tr}} + \mathscr{D}_{\text{val}}$$

***training dataset:***

*used to extract model parameters*

***validation dataset:***

*used to monitor generalisation power*

the model parameters are determined using information from training dataset

$$\widehat{\theta} = \arg\ \min_{\boldsymbol{\theta}} \{ C\left( \boldsymbol{Y}_{\text{th}}, f(\boldsymbol{X}_{\text{tr}}; \boldsymbol{\theta}) \right) \}$$

while the **performance of the model** (generalisation, extrapolation) is evaluated by computing the cost function on the validation dataset

$$C\left( \boldsymbol{Y}_{\text{val}}, f(\boldsymbol{X}_{\text{val}}; \widehat{\theta}) \right)$$

# Cross-validation (regularisation)

*In-sample (training) error* ⟶ $$E_{\text{tr}} \equiv C\left(\boldsymbol{Y}_{\text{tr}}, f(\boldsymbol{X}_{\text{tr}}; \hat{\boldsymbol{\theta}})\right)$$

*Out-of-sample (validation) error* ⟶ $$E_{\text{val}} \equiv C\left(\boldsymbol{Y}_{\text{val}}, f(\boldsymbol{X}_{\text{val}}; \hat{\boldsymbol{\theta}})\right)$$

Splitting the data into mutually exclusive training and validation sets provides an unbiased estimate for the **predictive performance of the model**

In ML problems one should select the model that **minimises** the out-of-sample error $\boldsymbol{E_{val,}}$ since this is the model that generalises in the most efficient way

***note that choices on how to partition the dataset will affect the conclusion about which is best model***

# Cross-validation (regularisation)

*In-sample (training) error* ⟶ $$E_{\text{tr}} \equiv C\left(\boldsymbol{Y}_{\text{tr}}, f(\boldsymbol{X}_{\text{tr}}; \hat{\boldsymbol{\theta}})\right)$$

*Out-of-sample (validation) error* ⟶ $$E_{\text{val}} \equiv C\left(\boldsymbol{Y}_{\text{val}}, f(\boldsymbol{X}_{\text{val}}; \hat{\boldsymbol{\theta}})\right)$$

Splitting the data into mutually exclusive training and validation sets provides an unbiased estimate for the **predictive performance of the model**

In ML problems one should select the model that **minimises** the out-of-sample error $\boldsymbol{E_{val,}}$ since this is the model that generalises in the most efficient way

***Fitting is not predicting:*** in general the model that describes better a given set of data will not be the one that generalises and predicts better related datasets

# Regularisation

In ML, the common goal of regularisation strategies is to modify the learning algorithms to **reduce its generalisation error without increasing its training error**

$$C(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(\boldsymbol{x}_i;\boldsymbol{\theta})\right)^2$$

*unregularised cost function*

$$C(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(\boldsymbol{x}_i;\boldsymbol{\theta})\right)^2 + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta}$$

*regularised cost function*

*regularisation hyperparameter, to be tuned*

*weight-decay regularisation: model parameters with smaller L2-norms are preferred*

# Regularisation

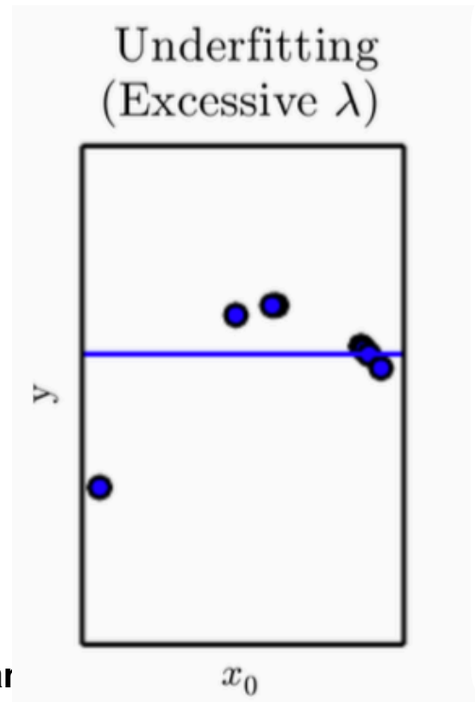
In ML, the common goal of regularisation strategies is to modify the learning algorithms to **reduce its generalisation error without increasing its training error**

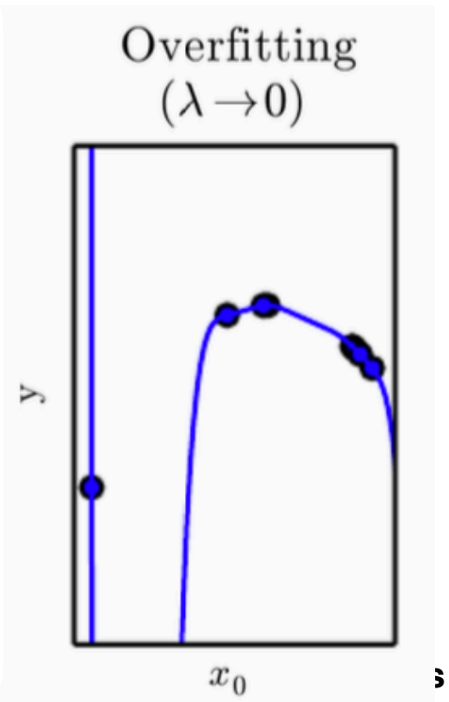
$$C(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(\boldsymbol{x}_i;\boldsymbol{\theta})\right)^2$$

*unregularised cost function*

$$C(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(\boldsymbol{x}_i;\boldsymbol{\theta})\right)^2 + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta}$$

*regularised cost function*




*no free lunch, careful tuning of regularisation required*

# Regularisation

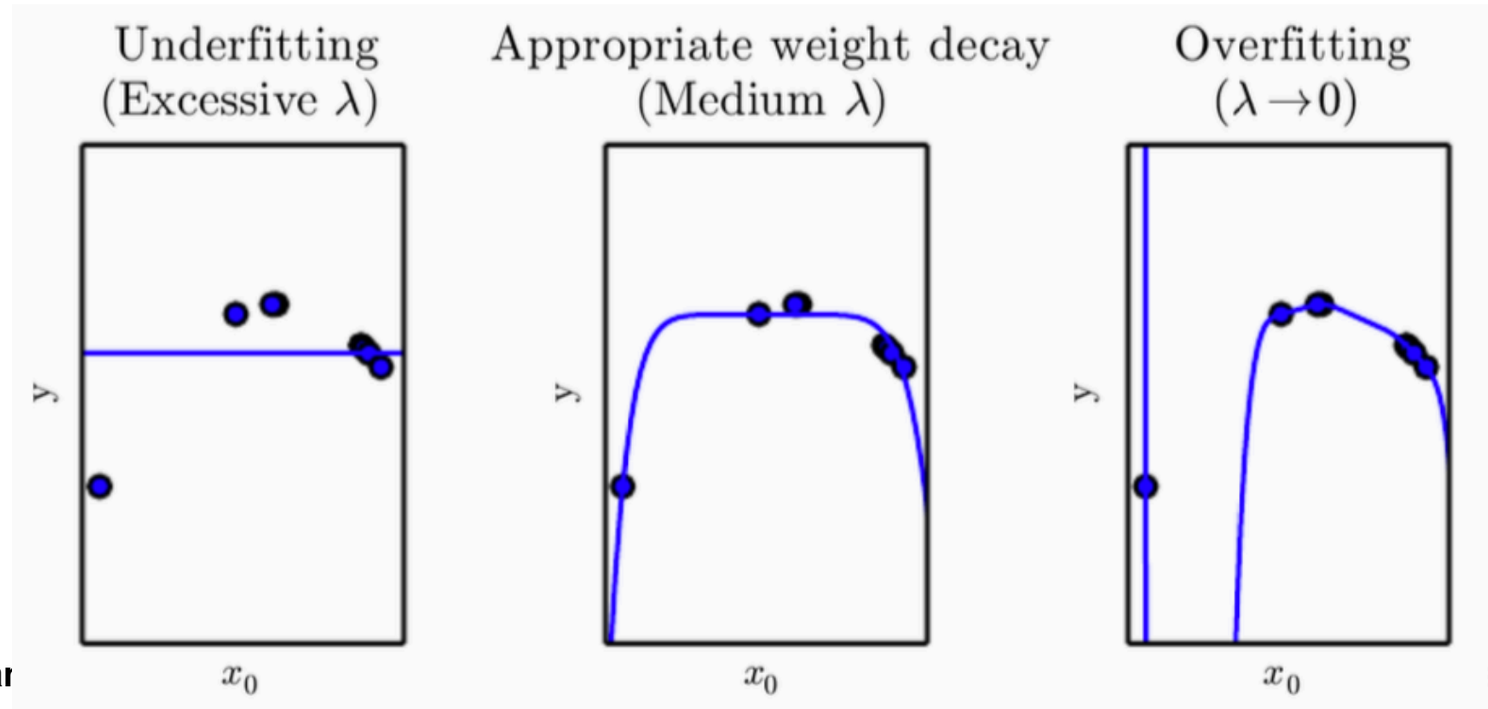
In ML, the common goal of regularisation strategies is to modify the learning algorithms to **reduce its generalisation error without increasing its training error**

$$C(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(\boldsymbol{x}_i;\boldsymbol{\theta})\right)^2$$

*unregularised cost function*

$$C(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f(\boldsymbol{x}_i;\boldsymbol{\theta})\right)^2 + \lambda\boldsymbol{\theta}^T\boldsymbol{\theta}$$

*regularised cost function*




*no free lunch, careful tuning of regularisation required*

# Tutorial 1 Exercise 1a

starting point is the **Python script** that you will find in

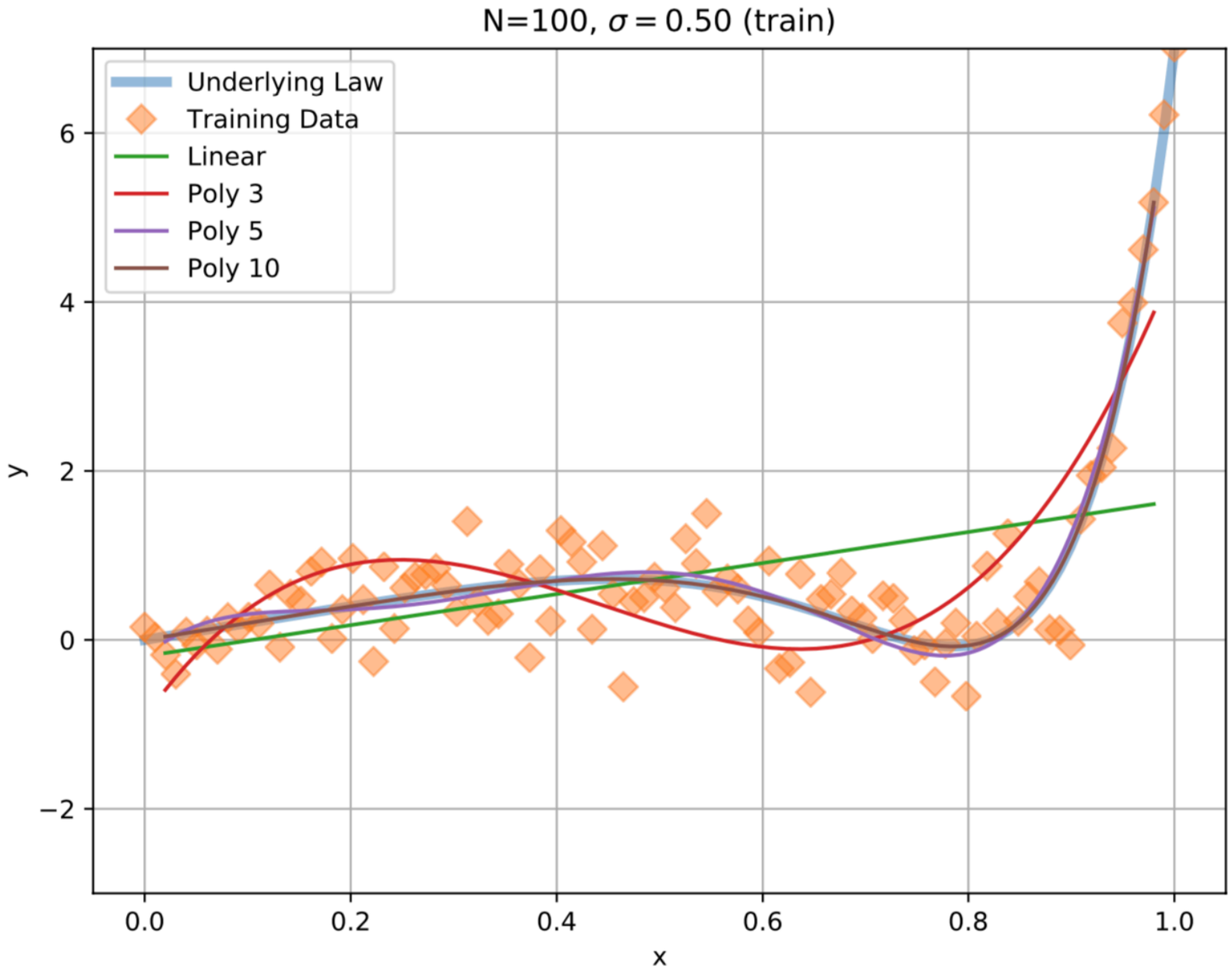
***https://github.com/juanrojochacon/ml-ditp-attp/blob/master/Tutorials/Tutorial1/***

- Generate data with different underlying laws and try to model it using **polynomial regression**

- Study how the cost function to the training data depends on *i)* the complexity of the underlying law, *ii)* the flexibility of the model, *iii)* the number of training points

- Now generate a validation dataset, either within the training data range [0,1] or outside it. Study which model is **more predictive** as a function of the same parameters as before in the two cases

- Can you **identify overfitting**? Can you think of a way of avoiding it?



# Why Machine Learning is difficult

- **Fitting existing data** is conceptually different from **making predictions about new data**

- Increasing the model complexity can improve the description of the training data but **reduce the predictive power** of the model due to overfitting, unless a suitable regularisation strategy is implemented

- For complex and/or small datasets, simple models can be better at prediction than complex models. The ``**right" amount of complexity** cannot in general be determined from first principles

- It is difficult to **generalise** beyond the situations encountered in the training set: the model cannot learn what it has not seen

- Many problems that are **approachable in principle** can become **unfeasible in practice**, e.g. due to computational limitations, lack of convergence, instability

# Supervised Learning: Optimisation Strategies

# Optimisation strategies

problems in **Supervised Machine Learning** are defined by the following ingredients:

***(1) Input dataset:*** $\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$

***(2) Model:*** $f\left(\boldsymbol{X}, \boldsymbol{\theta}\right)$

***(3) Cost function:*** $C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right)$

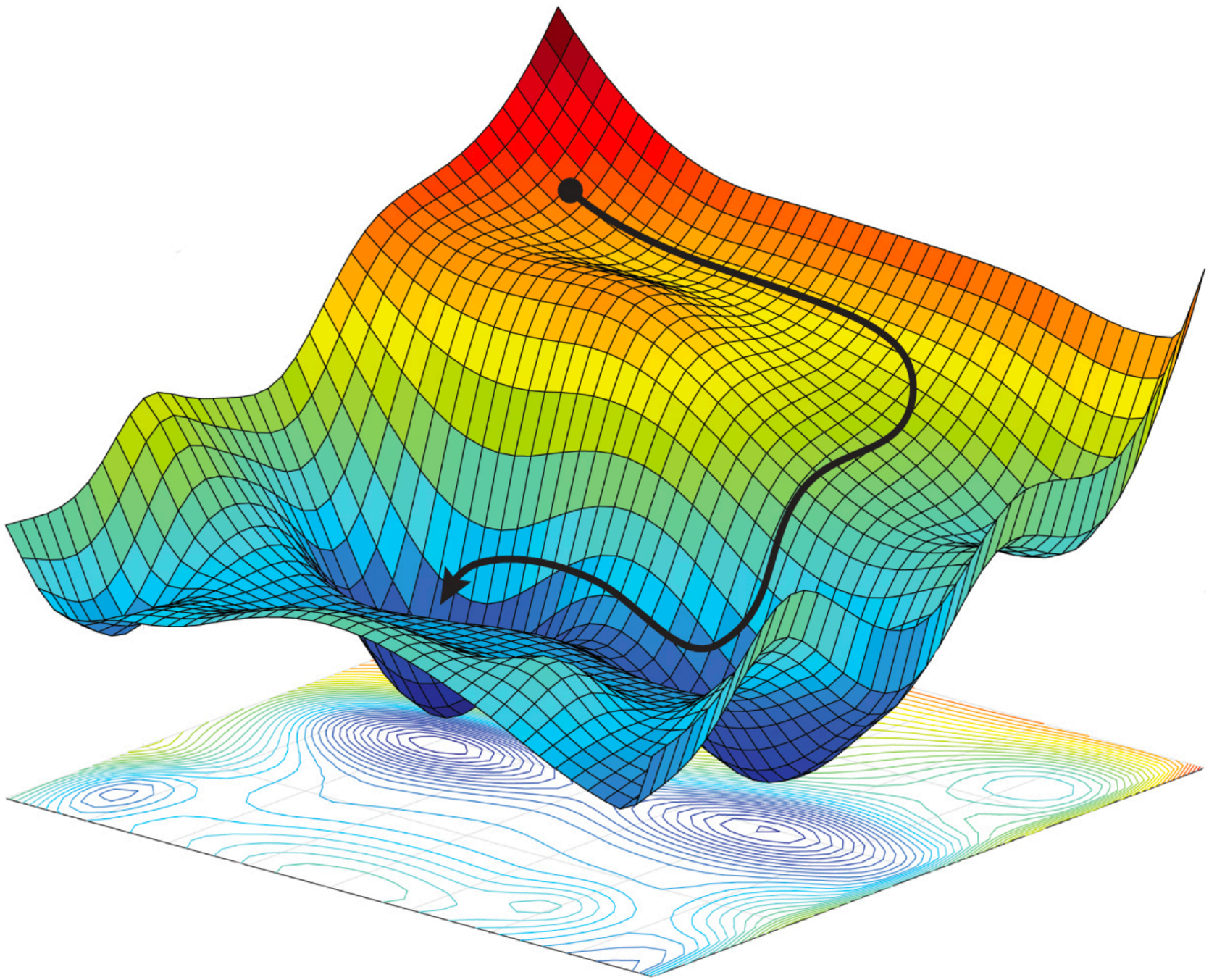
the model parameters are then found by **minimising the cost function**

for simple models (*e.g.* polynomial regression), the solution of this minimisation problem can be found analytically. This is not possible with complex models in realistic applications. In the context of ML studies, there exist two main classes of **minimisers (optimisers)** that are frequently deployed:

- **Gradient Descent** and its generalisations
- **Genetic Algorithms** and its generalisations

# Gradient Descent

basic idea: iteratively adjust the model parameters in the direction where the **gradient of the cost function** is large and negative (**steepest descent direction**)



# Gradient descent

basic idea: iteratively adjust the model parameters in the direction where the **gradient of the cost function** is large and negative (**steepest descent direction**)

Our goal is thus to **minimise an error (cost) function** that can usually be expressed as

$$E\left(\boldsymbol{\theta}\right) = \sum_{i=1}^{n} e_i(x_i;\boldsymbol{\theta})$$

*e.g.* in polynomial regression we had that

$$E(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(y_i - f_\alpha(x_i;\boldsymbol{\theta}_\alpha)\right)^2 \quad \text{so} \quad e_i = \left(y_i - f_\alpha(x_i;\boldsymbol{\theta}_\alpha)\right)^2$$

and we will see that in **logistic regression** (classification problems)

$$E(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(-y_i \ln \sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}) - (1-y_i)\ln[1-\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}]\right)$$

***aka the cross-entropy, relevant for categorisation***

# Gradient descent

starting from a suitable initial condition, GD **iteratively updates** the model parameters:

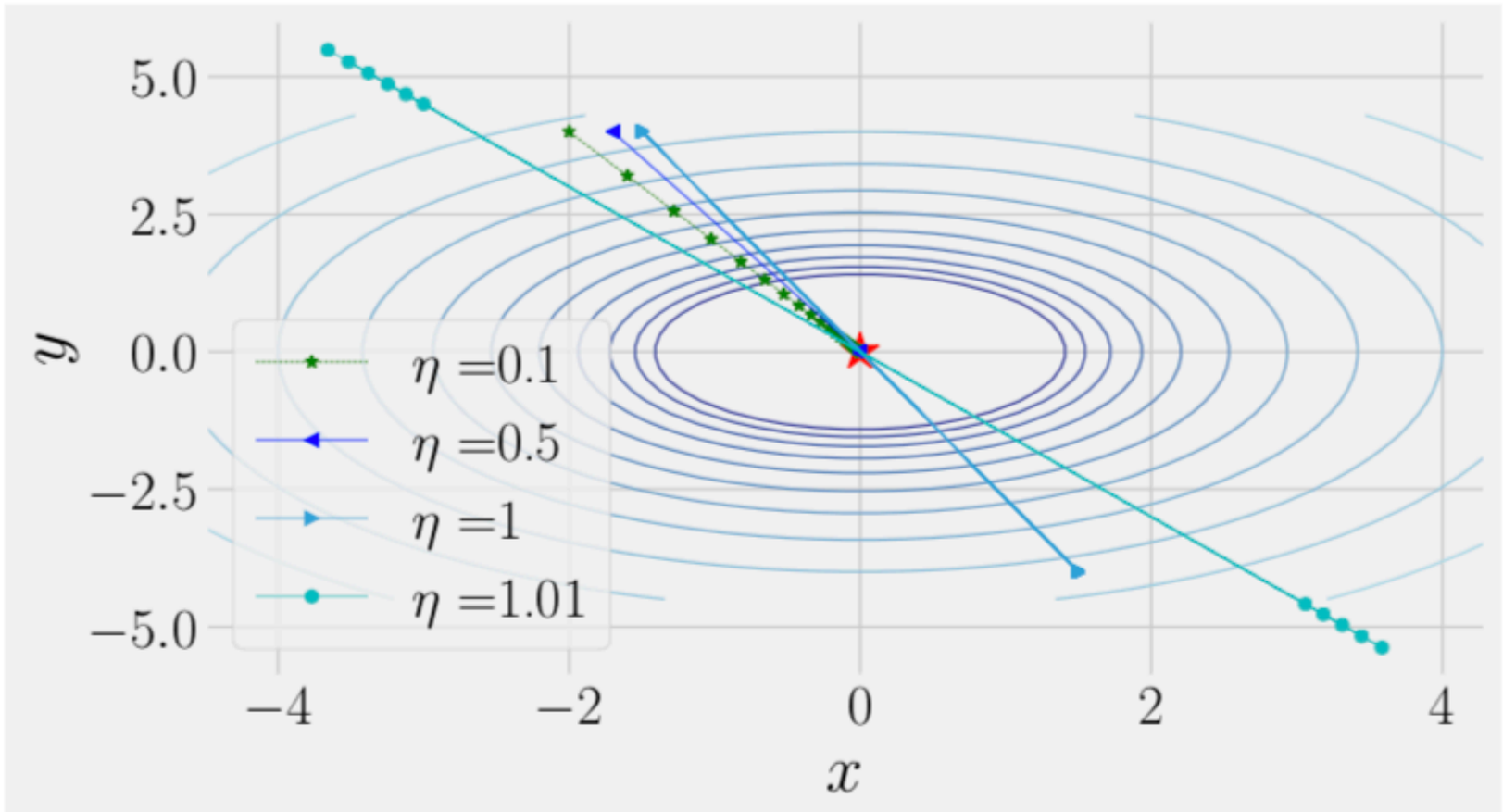
$$\mathbf{v}_t = \eta_t \nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

*learning rate*

*gradient of cost function*

*update of model parameters between iterations **t** and **t+1***

the learning rate determines the size of the step in the direction of the gradient




***small η: guaranteed to find local minimum, at price of large number of iterations***

***large η: can overshoot minimum, problems of convergence***

***nb evaluating gradient can be very cpu-intensive!***

# Gradient descent

starting from a suitable initial condition, GD **iteratively updates** the model parameters:

$$\mathbf{v}_t = \eta_t \nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

*learning rate*

*gradient of cost function*

*update of model parameters between iterations **t** and **t+1***

compare GD with **Newton's method**: first Taylor-expand of cost function for a small change of the model parameters

$$E\left(\boldsymbol{\theta}+\mathbf{v}\right) \simeq E\left(\boldsymbol{\theta}\right) + \nabla_\theta E\left(\boldsymbol{\theta}\right)\cdot\mathbf{v} + \frac{1}{2}\mathbf{v}^T H(\boldsymbol{\theta})\mathbf{v}$$

$$H_{ij}(\boldsymbol{\theta}) = \left\{ \frac{\partial^2 E(\boldsymbol{\theta})}{\partial\theta_i \partial\theta_j} \right\}$$

***Hessian matrix (2nd derivatives)***

# Gradient descent

starting from a suitable initial condition, GD **iteratively updates** the model parameters:

$$\mathbf{v}_t = \eta_t \nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

*learning rate*

*gradient of cost function*

*update of model parameters between iterations **t** and **t+1***

compare GD with **Newton's method**: first Taylor-expand of cost function for a small change of the model parameters

$$E\left(\boldsymbol{\theta}+\mathbf{v}\right) \simeq E\left(\boldsymbol{\theta}\right) + \nabla_\theta E\left(\boldsymbol{\theta}\right)\cdot\mathbf{v} + \frac{1}{2}\mathbf{v}^T H(\boldsymbol{\theta})\mathbf{v}$$

and then differentiate with respect to the step requiring that the **linear term vanishes**

$$\left.\frac{\partial E\left(\boldsymbol{\theta}+v\right)}{\partial \mathbf{v}}\right|_{\mathbf{v}_{\text{opt}}} = 0 \longrightarrow \nabla_\theta E\left(\boldsymbol{\theta}\right) + H(\boldsymbol{\theta})\mathbf{v}_{\text{opt}} = \mathbf{0}$$

$$\mathbf{v}_t = H^{-1}(\boldsymbol{\theta}_t)\cdot\nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

# Gradient descent

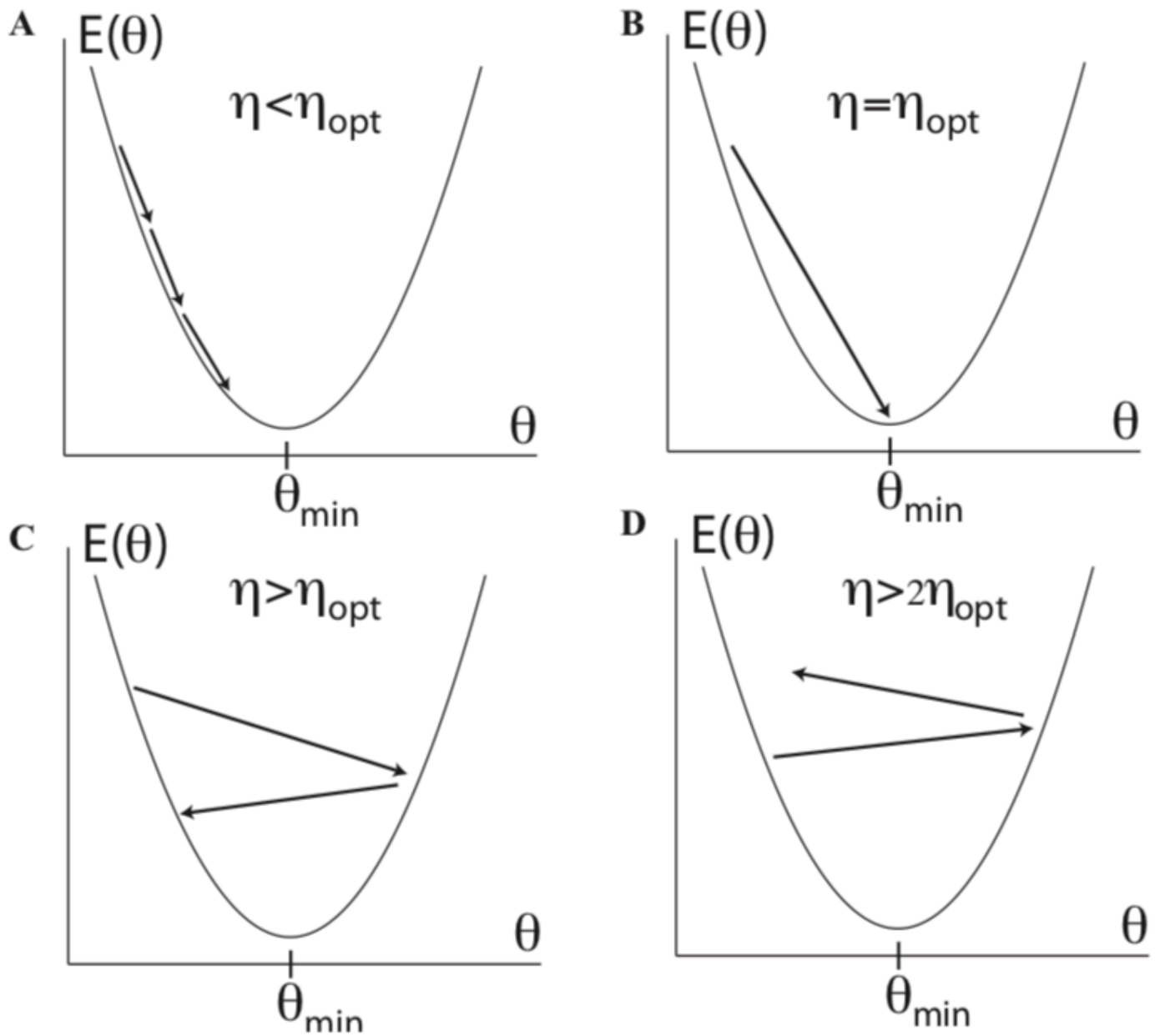
*Gradient Descent* $\longrightarrow$ $\mathbf{v}_t = \eta_t \nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$

*Newton's method* $\longrightarrow$ $\mathbf{v}_t = H^{-1}(\theta_t) \cdot \nabla_\theta E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$

- Newton's method not practical for ML applications: it involves **evaluation and inversion of Hessian matrices with $M^2$ entries**, with $M$ = number of model parameters

- But it provides useful ideas about how to improve GD, for example by **adapting the learning rate to the local curvature** of region of the parameter space

***suggest improvements of GD!***



# Advanced gradient descent

the simplest implementation of GD, unsurprisingly, has several limitations

- It converges to **local, rather than global**, minima of the cost function

***poor performance for realistic applications***

# Advanced gradient descent

the simplest implementation of GD, unsurprisingly, has several limitations

- It converges to **local, rather than global**, minima of the cost function

***poor performance for realistic applications***

- Evaluating gradients is **computationally expensive** for large datasets

$$E(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(y_i - f_\alpha(x_i; \boldsymbol{\theta}_\alpha)\right)^2$$

***involves sum over all n data points***

# Advanced gradient descent

the simplest implementation of GD, unsurprisingly, has several limitations

- It converges to **local, rather than global**, minima of the cost function

***poor performance for realistic applications***

- Evaluating gradients is **computationally expensive** for large datasets

$$E(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left( y_i - f_\alpha(x_i; \boldsymbol{\theta}_\alpha) \right)^2$$

***involves sum over all n data points***

- Very sensitive to choice of **learning rates**

***Ideally one would like an adaptive learning rate***

# Advanced gradient descent

the simplest implementation of GD, unsurprisingly, has several limitations

- It converges to **local, rather than global**, minima of the cost function

***poor performance for realistic applications***

- Evaluating gradients is **computationally expensive** for large datasets

$$E(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left(y_i - f_\alpha(x_i; \boldsymbol{\theta}_\alpha)\right)^2$$

***involves sum over all n data points***

- Very sensitive to choice of **learning rates**

***Ideally one would like an adaptive learning rate***

- Treats **uniformly all directions** in the parameter space

***we would like to use info also on curvature (as in Newton's method)***

**Generalised Gradient Descent methods** have been developed to address these shortcomings and are at the basis of **modern deep learning methods**

# Stochastic gradient descent

**Stochasticity** can be added to GD by approximating the gradient on a subset of the training data, called a **mini-batch**

$$\nabla_\theta E(\boldsymbol{\theta}) = \sum_{i=1}^{n} \nabla_\theta e_i(\boldsymbol{x}_i;\boldsymbol{\theta}) \simeq \nabla_\theta E^{\mathrm{MB}}(\boldsymbol{\theta}) \equiv \sum_{i\in B_k} \nabla_\theta e_i(\boldsymbol{x}_i;\boldsymbol{\theta})$$

$k = 1,\ldots,n/K$ ← *# points per batches*

*# batches*

We then **cycle over all mini-batches**, updating the model parameters at each step *k*

$$\mathbf{v}_t = \eta_t \nabla_\theta^{\mathrm{MB}} E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

A full iteration over all *n* data points (over the *n/K* batches) is called an **epoch**

benefits of SGD: stochasticity prevents getting stuck in local minima, the calculation of the gradient is speed up & stochasticity acts as natural regulariser

# Adding momentum to SGD

SGD can be used with a **momentum term** that provides some **memory** on the direction in which one is moving in the parameter space

$$\mathbf{v}_t = \gamma \mathbf{v}_{t-1} + \eta_t \nabla_\theta^{\mathrm{MB}} E(\boldsymbol{\theta}_t)\,, \qquad \boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \mathbf{v}_t$$

*momentum parameter ( 0 < ɣ < 1)*

$$\Delta\boldsymbol{\theta}_{t+1} = \gamma \Delta\boldsymbol{\theta}_t - \eta_t \nabla_\theta E(\boldsymbol{\theta}_t), \qquad \Delta\boldsymbol{\theta}_t = \boldsymbol{\theta}_t - \boldsymbol{\theta}_{t-1}$$

*proposed parameter change in iteration t+1*

*proposed parameter change in iteration t*

momentum in SGD helps to **gain speed in directions with persistent but small gradients**, while suppressing oscillations in high-curvature directions.

# Adaptative Gradient Descent

**Adaptative GD** varies the learning rate to reflect the **local curvature** of the parameter space without the need to evaluate the Hessian matrix

**RMSprop**: keep track also of the **second moment of gradient**, similar as how the momentum term is a running average of previous gradients

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta_t \frac{\boldsymbol{g}_t}{\sqrt{\boldsymbol{s}_t + \epsilon}}$$

*regulator to avoid numerical divergences*

$$\boldsymbol{g}_t = \nabla_\theta E(\boldsymbol{\theta})$$

*gradient at iteration t*

$$\boldsymbol{s}_t = \beta \boldsymbol{s}_{t-1} + (1-\beta)\boldsymbol{g}_t^2$$

*controls averaging time of 2nd moment of gradient*

$$\boldsymbol{s}_t = \mathbb{E}[\boldsymbol{g}_t^2]$$

*2nd moment of gradient (averaged over iterations)*

$$\beta = 1 \rightarrow \boldsymbol{s}_t = \boldsymbol{s}_{t-1}$$
$$\beta = 0 \rightarrow \boldsymbol{s}_t = \boldsymbol{g}_t^2$$

*effective learning rate reduced in directions where gradient is consistently large*

# Adaptative Gradient Descent

**Adaptative GD** varies the learning rate to reflect the **local curvature** of the parameter space without the need to evaluate the Hessian matrix

**ADAM:** adaptively change the parameters from information on **running averages** of first and second moments of the gradient

$$\boldsymbol{g}_t = \nabla_\theta E(\boldsymbol{\theta})$$

$$\boldsymbol{m}_t = \beta_1 \boldsymbol{m}_{t-1} - (1-\beta_1)\boldsymbol{g}_t \qquad \boldsymbol{s}_t = \beta_2 \boldsymbol{s}_{t-1} + (1-\beta_2)\boldsymbol{g}_t^2$$

$$\widehat{\boldsymbol{m}}_t = \frac{\boldsymbol{m}_t}{1-(\beta_1)^t} \qquad \widehat{\boldsymbol{s}}_t = \frac{\boldsymbol{s}_t}{1-(\beta_2)^t}$$

*sets lifetime of first moment*

*sets lifetime of second moment*

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta_t \frac{\widehat{\boldsymbol{m}}_t}{\sqrt{\widehat{\boldsymbol{s}}_t + \epsilon}}$$

# Adaptative Gradient Descent

**Adaptative GD** varies the learning rate to reflect the **local curvature** of the parameter space without the need to evaluate the Hessian matrix

**ADAM** has two main advantages: *(i)* adapting step size to cut off large gradient directions (prevent oscillations) and *(ii)* measuring gradients in a natural length scale

to see this, express the ADAM update rules in terms of the **variance in parameter space**

$$\sigma_t = \hat{s}_t - \left(\hat{m}_t\right)^2$$

and we can see that the update rule for one of the parameters reads now

$$\Delta\theta_{t+1} = -\eta_t \frac{\hat{m}_t}{\sqrt{\sigma_t^2 + \hat{m}_t^2} + \epsilon}$$

***small fluctuations of gradient***

$$\Delta\theta_{t+1} \to -\eta_t$$

***large fluctuations of gradient***

$$\Delta\theta_{t+1} = -\eta_t \hat{m}_t / \sigma_t^2$$

***learning rate promotional to signal-to-noise ratio***

# Tutorial 1 Exercise 1b

starting point is the **Python script** that you will find in

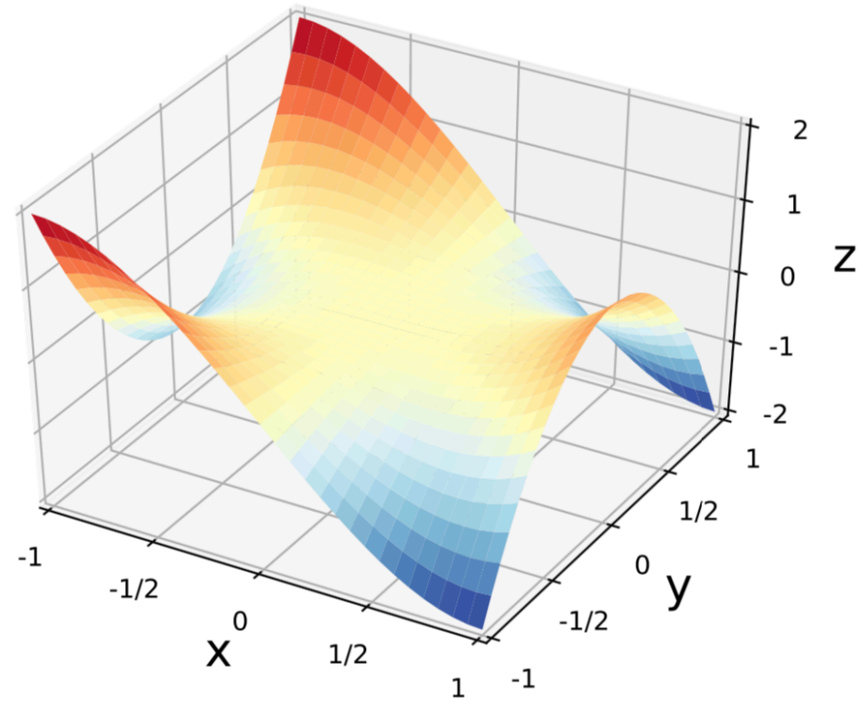
***https://github.com/juanrojochacon/ml-ditp-attp/blob/master/Tutorials/Tutorial1/***

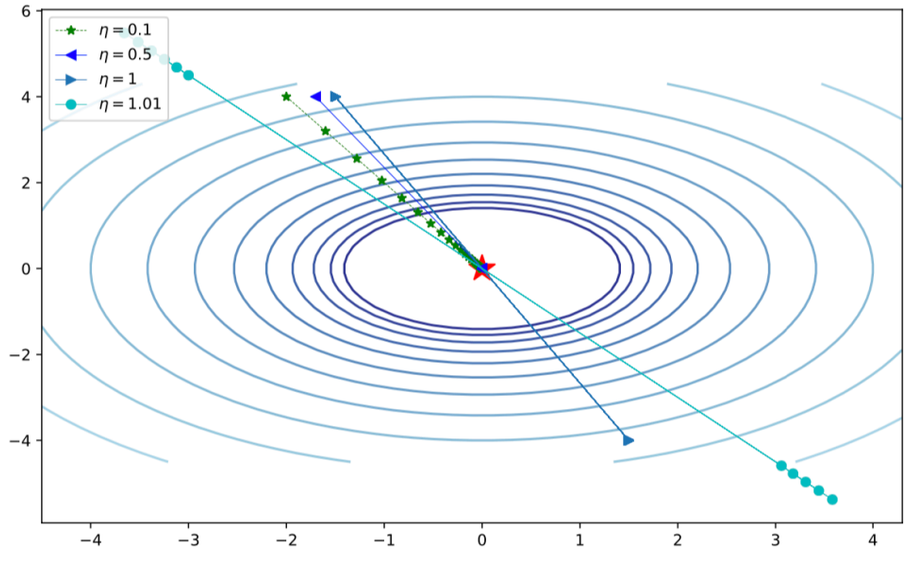
- Study different optimisation algorithms based on GD for simple 2D functions

- Visualise the **path of GD algorithms in parameter space**

- Determine which choices of the parameters allow reaching the minima quicker

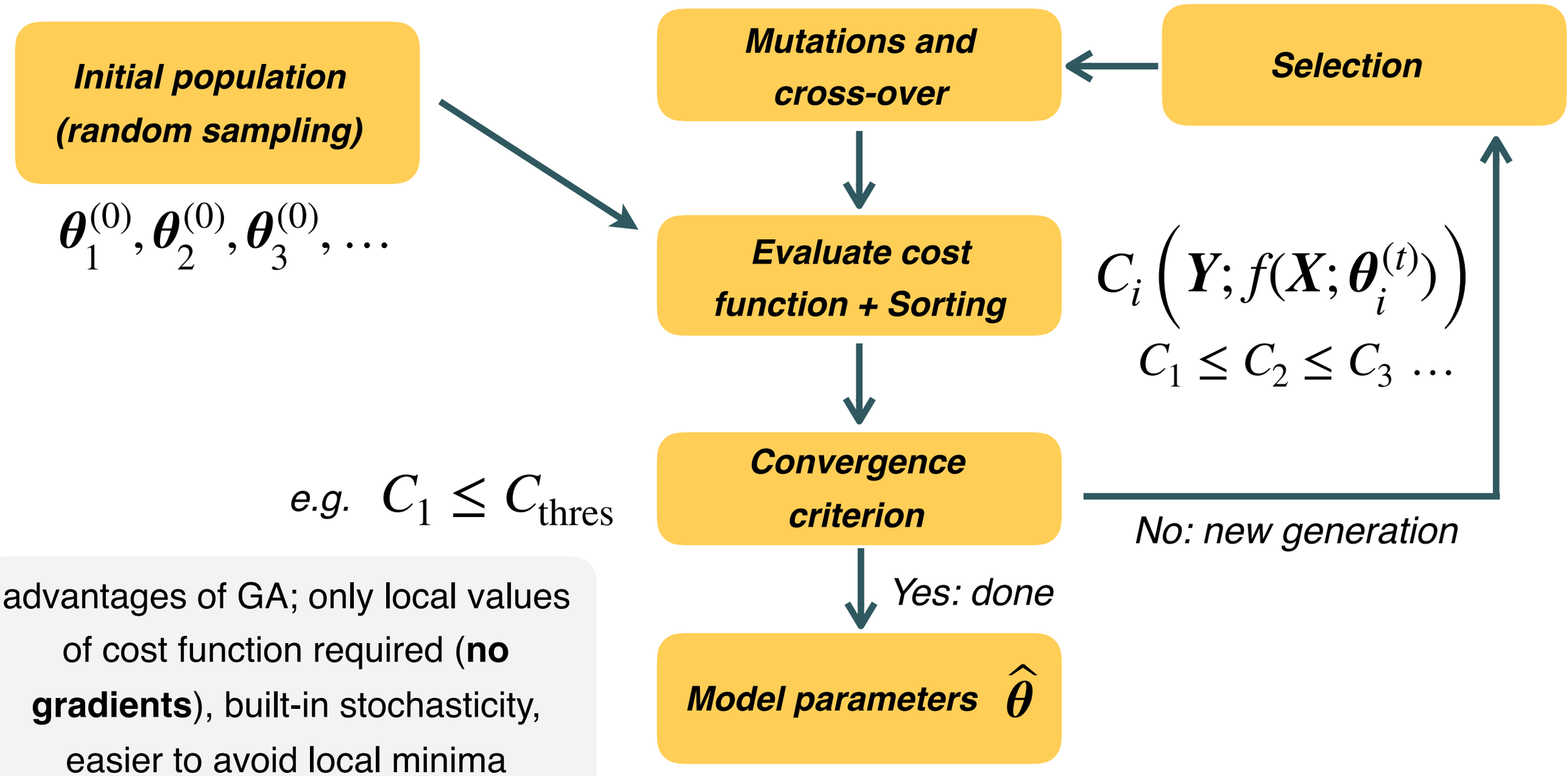
- Given new 2D functions, show that you can **tune GD to find all the minima**, and compare with the analytical results



# Genetic Algorithms

GAs combine **stochastic and deterministic ingredients** to explore the model parameter space and minimise the cost function




*e.g.* $C_1 \leq C_{\text{thres}}$

advantages of GA; only local values of cost function required (**no gradients**), built-in stochasticity, easier to avoid local minima

# Genetic Algorithms

GAs combine **stochastic and deterministic ingredients** to explore the model parameter space and minimise the cost function

***mutations***

$$\theta_{i,j}^{(t+1)} = \theta_{i,j}^{(t)} \left(1 + \eta_j^{(t)}\right) , \quad j = 1 \ \ldots, m, i = 1, \ldots, M$$

*learning rates (depends in generation and parameter)*

*# model parameters*

*# mutants*

***crossover***

$$\boldsymbol{\theta}_i^{(t)} = \left(\theta_{i,1}^{(t)}, \theta_{i,2}^{(t)}, \ldots, \theta_{i,m}^{(t)}\right) \rightarrow \left(\theta_{i,1}^{(t)}, \theta_{i,2}^{(t)}, \ldots, \theta_{i,p-1}^{(t)}, \theta_{k,p}^{(t)}, \ldots, \theta_{k,m}^{(t)}\right)$$

$$\boldsymbol{\theta}_k^{(t)} = \left(\theta_{k,1}^{(t)}, \theta_{k,2}^{(t)}, \ldots, \theta_{k,m}^{(t)}\right) \rightarrow \left(\theta_{k,1}^{(t)}, \theta_{k,2}^{(t)}, \ldots, \theta_{k,p-1}^{(t)}, \theta_{i,p}^{(t)}, \ldots, \theta_{i,m}^{(t)}\right)$$

*children inherit part of the DNA of each parent*

# Genetic Algorithms

GAs combine **stochastic and deterministic ingredients** to explore the model parameter space and minimise the cost function

***mutations***

$$\theta_{i,j}^{(t+1)} = \theta_{i,j}^{(t)} \left(1 + \eta_j^{(t)}\right) , \quad j = 1 \ \ldots, m, i = 1, \ldots, M$$

***learning rates (depends in generation and parameter)***

***# model parameters***

***# mutants***

***crossover***

| | |
|---|---|
| Chromosome1 | 11011\|00100110110 |
| Chromosome2 | 11011\|11000011110 |
| Offspring1 | 11011\|11000011110 |
| Offspring2 | 11011\|00100110110 |

***children inherit part of the DNA of each parent***

# Genetic Algorithms

# The CMA-ES algorithm

Improve the efficiency of simple GAs by incorporating global (in addition to local) information on the parameter space

One example is the **Covariance matrix Adaptation - Evolutionary Strategy** (CMA-ES)

- Start by randomly initialising the model parameters using a Gaussian distribution

$$\boldsymbol{\theta}^{(0)} \sim \mathcal{N}\left(0, \mathbf{C}^{(0)}\right)$$

- At every generation, we generate ***M* mutants** according to the following distribution

$$\boldsymbol{a}_k^{(t)} \sim \boldsymbol{\theta}^{(t-1)} + \boldsymbol{\sigma}^{(t-1)} \mathcal{N}\left(0, \mathbf{C}^{(t-1)}\right), \quad k = 1, \ldots, M$$

*step size*

*covariance matrix of search distribution*

*tuned during fit*

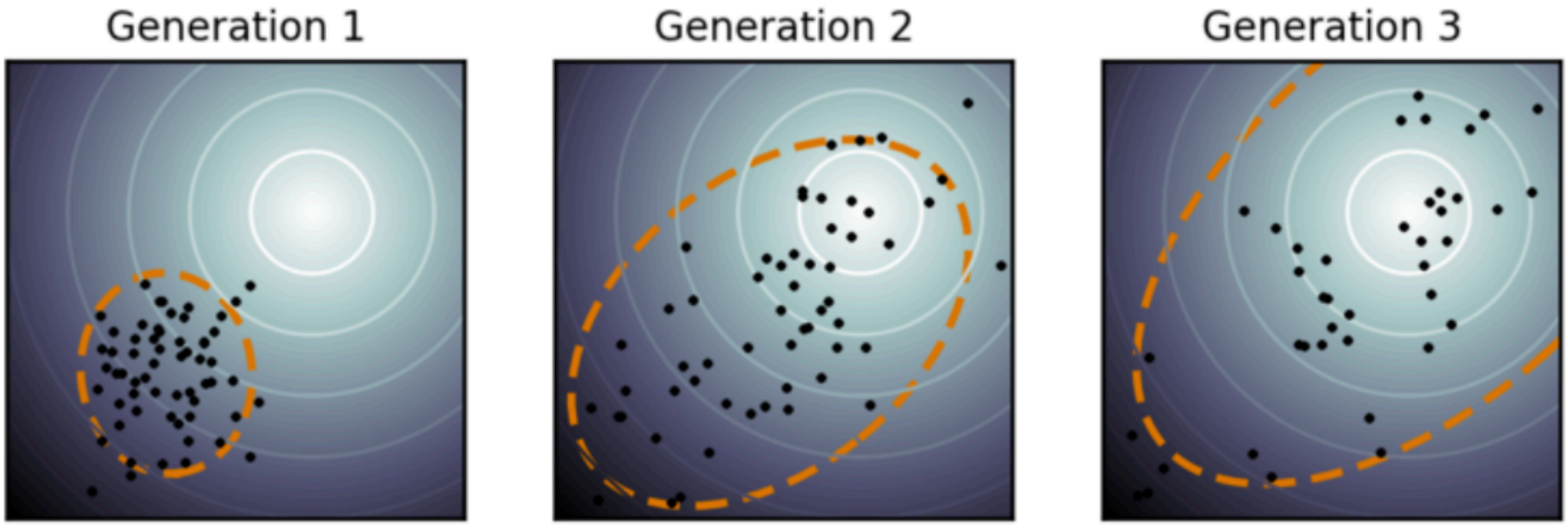
- The **new search centre** is computed as weighted average over fraction of best mutants

$$\boldsymbol{\theta}^{(t)} = \boldsymbol{\theta}^{(t-1)} + \sum_{k=1}^{\mu} W_k (\boldsymbol{a}_k - \boldsymbol{\theta}^{(t-1)})$$

*Parameters of the algorithms*

**adaptation** as the parameter space is explored is key feature of CMA-ES

# The CMA-ES algorithm




***main advantages: (i) information on gradients never required, only local values of cost function, (ii) information on whole set of mutants (not only best ones) used to tune step size and search covariance matrix***