Lecture 1: Introduction

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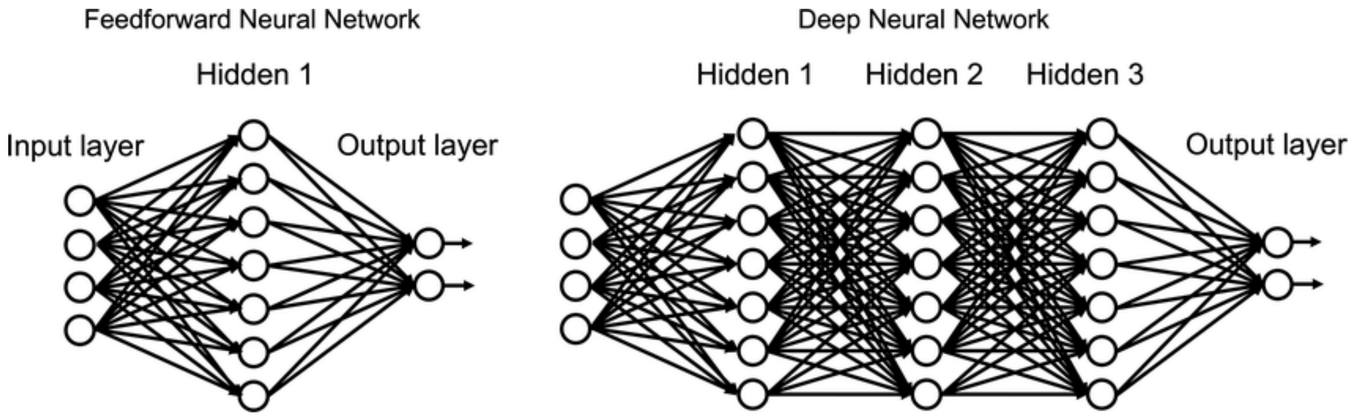
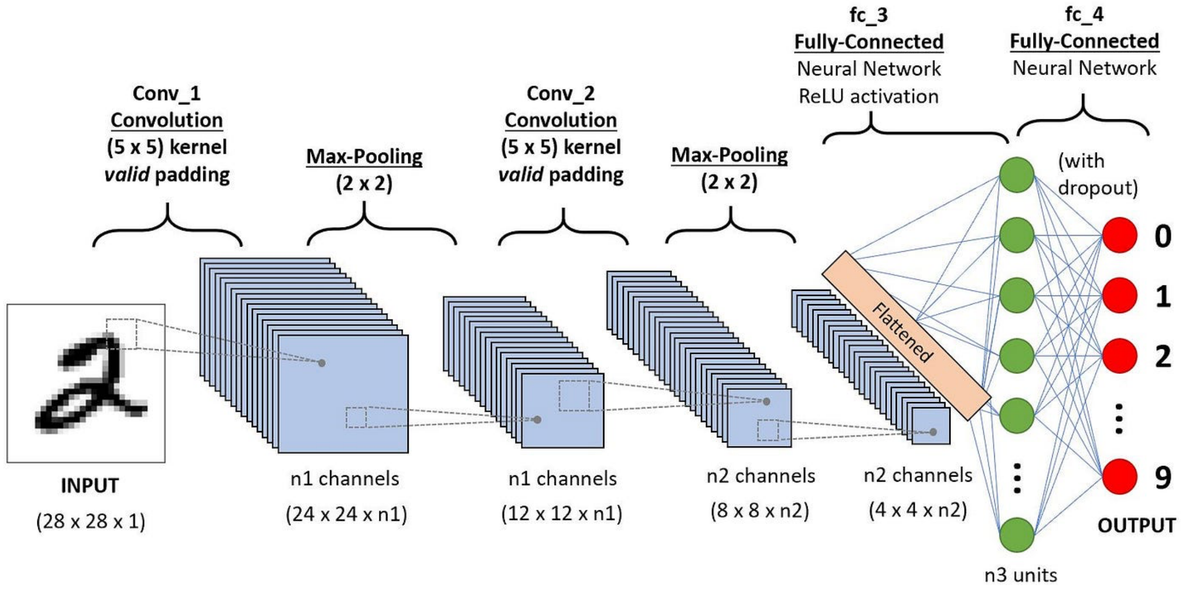
Class Overview

- *This series of lectures will give you an entry point on the quickly evolving domain of Deep Learning, which is driving the recent revolution in AI-related research*
  - *The focus is on applications: we will be light on formalism and will devote some time to discuss Jupyter notebooks with examples*
  - *No scientific background is required: we will use standard datasets like MNIST for most of the activity. Physics concepts, when needed, will be introduced*
  - *Nevertheless, this is a physics course, you will see some (particle) physics related to applications at the Large Hadron Collider*

The topics

- *General introduction to Machine Learning*
- *Deep Learning Architectures*
  - *Fully-connected NNs (aka Dense NNs)*
  - *Convolutional NNs*
  - *Graph NNs*
  - *Tranformers*
  - *Normalizing Flows*
  - *…*
- *Learning processes and applications*
  - *Supervised*
  - *Unsupervised*
  - *Adversarial*
  - *Anomaly Detection*
- *Deep Learning in practice*
  - *Training: How to optimize a model*
  - *Inference: How to deploy and use an algorithm*
  - *Model Compression and edge computing*
  - *…*





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  - *…*

Lectures in blue
Tutorials in red italic

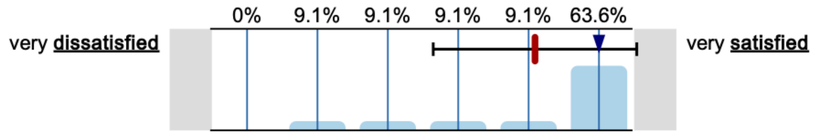
Date	Topic	Tutorial
Sep 16	Intro & class description	Linear Algebra in a nutshell + prob and stat
Sep 23	Basic of machine learning + Dense NN	*Basic jupyter + DNN on mnist (give jet dnn as homework)*
Sep 30	Convolutional NN	*Convolutional NNs with MNIST*
Oct 7	Training in practice: regularization, optimization, etc	*Practical methodology*
Oct 14	*Google tutorial **To Be Confirmed***	
Oct 21	Graph NNs	*Tutorial on Graph NNs*
Oct 28	Unsupervised learning and anomaly detection	*Autoencoders with MNIST*
Nov 4	Generative models: GANs, VAEs, etc	Normalizing flows
Nov 11	Transformers	
Nov 18	Network compression (pruning, quantization, Knoweldge Distillation)	
Nov 25	Tutorial on hls4ml **To Be Confirmed**	
Dec 2	To Be Decided	
Dec 9	Quantum Machine Learning	
Dec 16	**Exams To Be Confirmed**	

Teaching Style: lectures

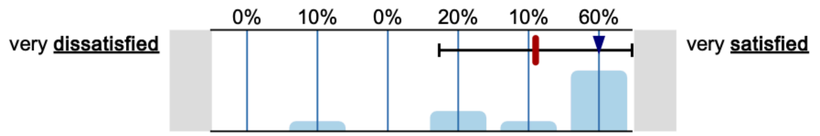
Students' feedback survey. You will be asked to fill one

Overall Satisfaction

How **satisfied** are you with the course overall?



Overall, how **satisfied** are you with the **realization of the course** (e. g., course mode, portion of interactive and asynchronous elements, etc.)?

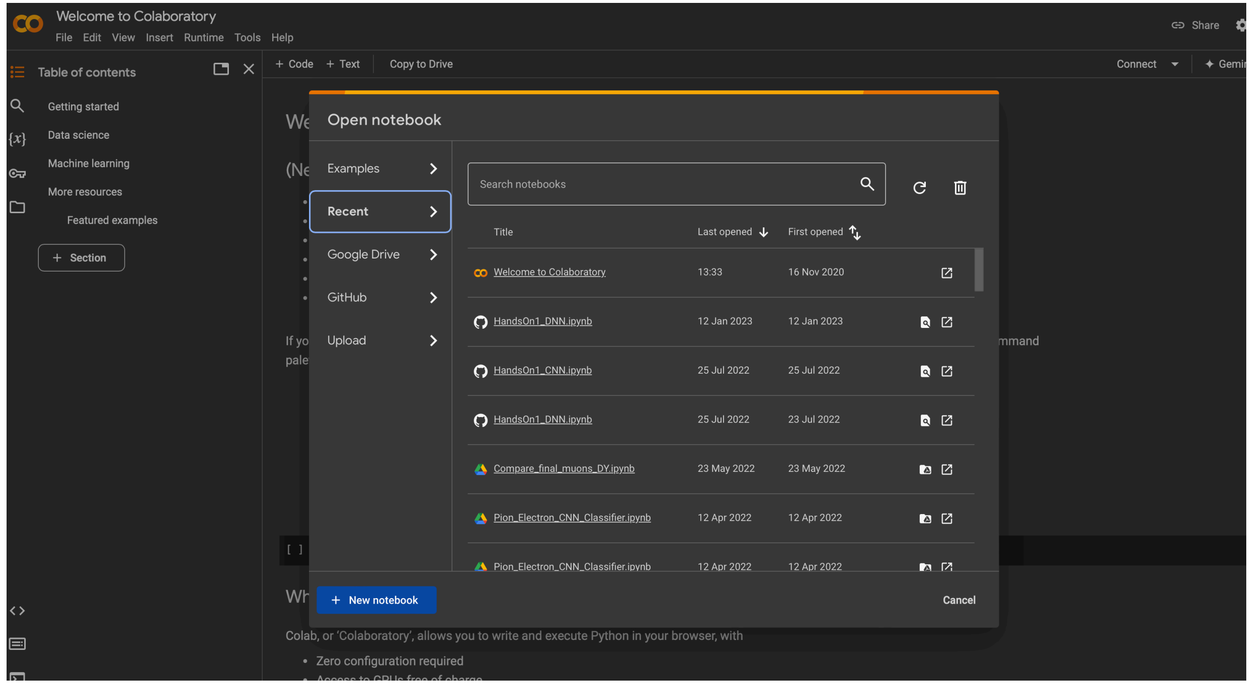


- *The material you will see was already used to teach this course with fair success*
- *The aim is to adapt lectures to students' level and background, which changes year by year*
  - *Parts of these lectures were given to PhD students and high-school teachers/ students with equally fair results*
- *To do so, we need live feedback:* ***interrupt at any time with questions.***
  - *If we hear nothing, we assume that everything is clear and we keep going*
  - *We don't have to get to the end of the lecture series: covering 2/3 of the program with good results is better than rushing to the end*

Teaching Style: tutorials

- *We will spend some time on jupyter notebook sessions*
  - *We are trying to schedule (on Oct 14th?) a long tutorial by the Google ZH AI team*
  - *(Tentatively on Nov 25th) we will have a long tutorial on hls4ml [special lecturers from my team at CERN]*
  - *At the end (Dec 16th?) we will have a class+tutorial on Quantum Machine Learning*
  - *We will use PYTHON jupyter notebooks in COLAB*
    - *You need to have a working google account on COLAB for next week*
    - *The notebooks run on the cloud, so you can use any device with a network (from your smartphone to your laptop)*
  - *To familiarise with the tutorials, you will have to practice at home*
    - *Repeat the tutorial, change things, and try to get a better result*

https://colab.research.google.com/



Python & Jupyter

- *We are assuming some previous knowledge of python*
- *But we will use very minimal python knowledge*
- *Most of what you need to know will be available on keras.io and looking for examples on googles*
- *It might help to refresh your jupiter/ matplotlib skills with some online tutorial*
  - *You could try this (or similar) on colab directly (instructions here)*
  - *Similarly here for matplotlib*

DNN model building

In [ ]:
```
# keras imports
from tensorflow.keras.models import Model
from tensorflow.keras.layers import Dense, Input, Dropout, Flatten, Activation
from tensorflow.keras.utils import plot_model
from tensorflow.keras import backend as K
from tensorflow.keras import metrics
from tensorflow.keras.callbacks import EarlyStopping, ReduceLROnPlateau, TerminateOnNaN
```

In [ ]:
```
input_shape = X_train.shape[1]
dropoutRate = 0.25
```

In [ ]:
```
####
inputArray = Input(shape=(input_shape,))
#
x = Dense(40, activation='relu')(inputArray)
x = Dropout(dropoutRate)(x)
#
x = Dense(20)(x)
x = Activation('relu')(x)
x = Dropout(dropoutRate)(x)
#
x = Dense(10, activation='relu')(x)
x = Dropout(dropoutRate)(x)
#
x = Dense(5, activation='relu')(x)
#
output = Dense(5, activation='softmax')(x)
####
model = Model(inputs=inputArray, outputs=output)
```

In [ ]:
```
model.compile(loss='categorical_crossentropy', optimizer='adam')
model.summary()
```

We now train the model

In [ ]:
```
batch_size = 128
n_epochs = 50
```

In [ ]:
```
# train
history = model.fit(X_train, y_train, epochs=n_epochs, batch_size=batch_size, verbose = 2,
                    validation_data=(X_val, y_val),
                    callbacks = [
                    EarlyStopping(monitor='val_loss', patience=10, verbose=1),
                    ReduceLROnPlateau(monitor='val_loss', factor=0.1, patience=2, verbose=1),
                    TerminateOnNaN()])
```

In [ ]:
```
# plot training history
plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.yscale('log')
plt.title('Training History')
plt.ylabel('loss')
plt.xlabel('epoch')
plt.legend(['training', 'validation'], loc='upper right')
plt.show()
```

Final Exam

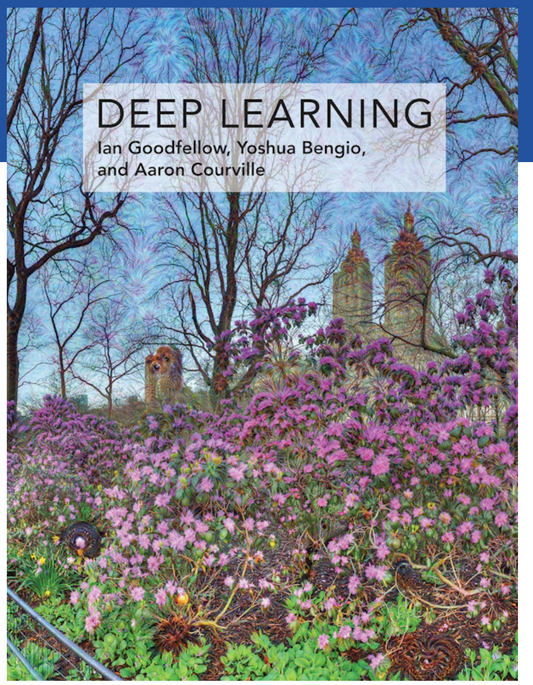
- The final exam will consist of two parts
  - PRACTICAL: you will be asked to demonstrate your capability to design and train a Deep Learning algorithm to solve a task
    - We will assign you a problem on a new dataset
    - You will have to submit a notebook with a solution by the exam
    - The first part of the oral exam will consist in a discussion of your work
  - THEORETICAL: you will have to demonstrate familiarity with the topics discussed in class
    - After the exercise discussion, some Q&A on various topics discussed in classes, not necessarily related to the exercise
- Last year, we scheduled the exam before Xmas, with a second session on early January. Each exams lasts ~ 20 min. A whole session spans up to two days.
- The exam is Pass/Fail. PhD students can give the exam or just receive one credit for acceptance

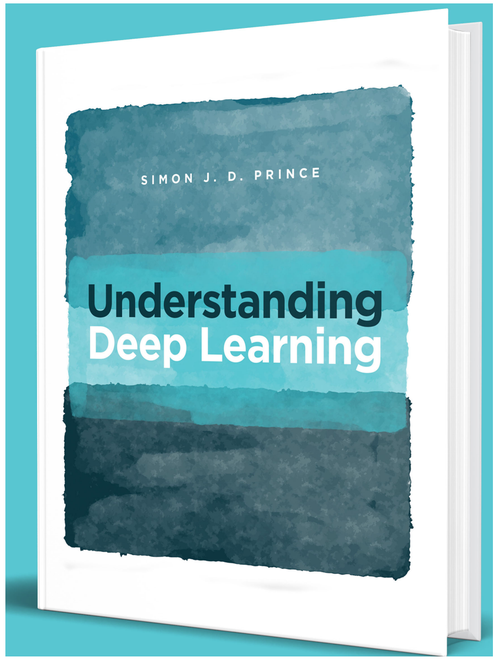
Textbook

- *The main reference for you will be the electronic materials*
  - *Slides*
  - *Tutorial notebooks*

The material will be posted on MP's github progressively

- *In addition, we will loosely follow "Deep Learning" by Goodfellow et al. (MIT Press)*
  - *You can find an html version by the authors here*
  - *You can find it in the library*
- ***For more recent topics (graph, transormers, etc**) we will follow a more recent text: Understanding Deep Learning by Simon J. D. Prince (MIT Press)*





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✔: Parts that we will cover

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Additional Material

- Depending on your interest for various topics, we can provide you with further readings:
  - e.g., reviews on specific topics, e.g. "Graph Neural Networks in Particle Physics"
- For generic topics, you can find very good introductory material on
  - wikipedia.org
  - townrdsdatascience.org
- For code issues
  - You are not the first having the problem you have: check on stackoverflow.co or just google your problem

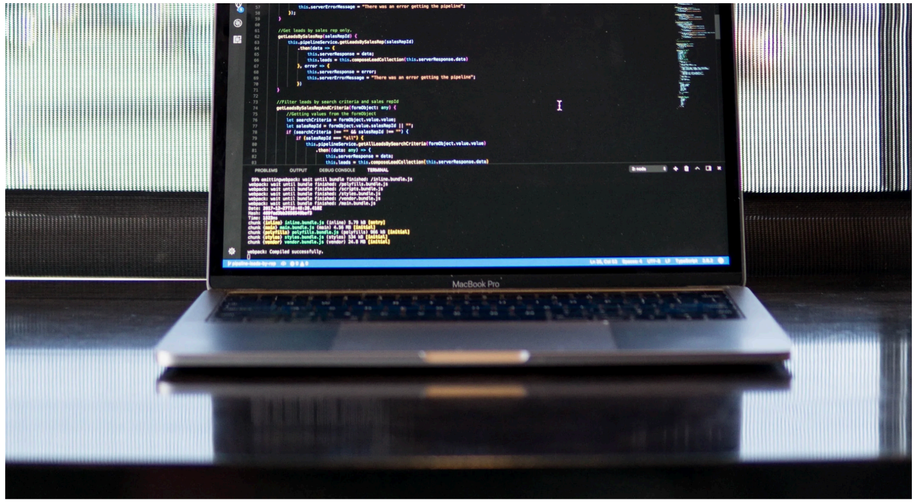
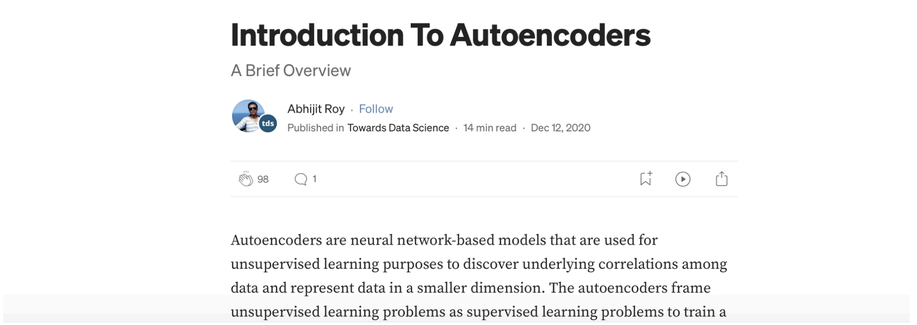


Photo by Maxwell Nelson on Unsplash



Introduction To Autoencoders

A Brief Overview

Abhijit Roy · Follow

Published in Towards Data Science · 14 min read · Dec 12, 2020

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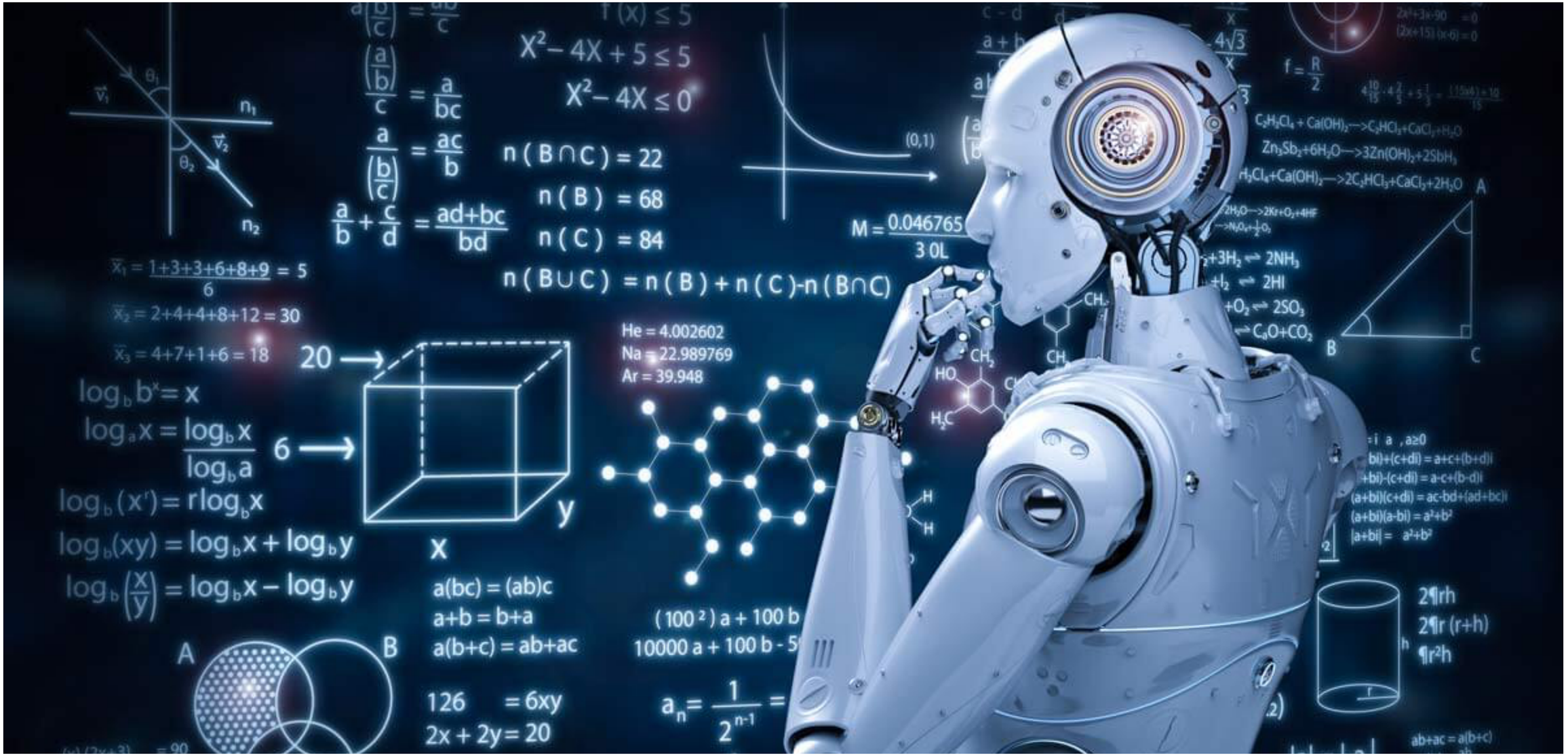
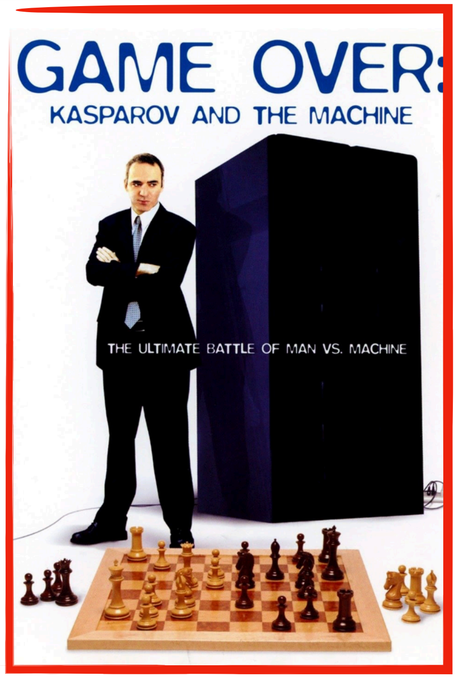
Autoencoders are neural network-based models that are used for unsupervised learning purposes to discover underlying correlations among data and represent data in a smaller dimension. The autoencoders frame unsupervised learning problems as supervised learning problems to train a

What is Machine Learning ?



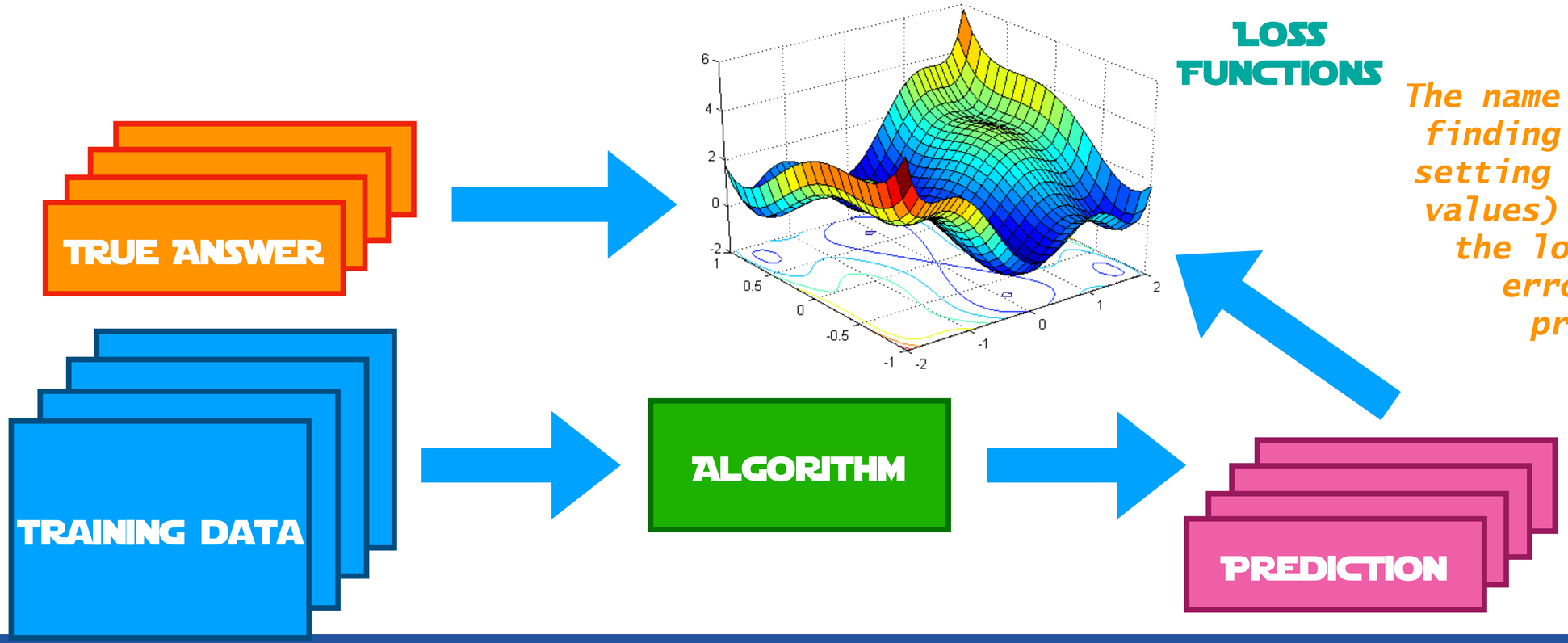
A historical perspective

- *Since (at least) ancient Greece, humankind has been dreaming about the concept of a thinking machine*
- *This idea was revamped in ‘800, when programmable computers appear*
- *This fuelled research in AI during/after WWII*
  - *Very quickly, it was possible to solve human hard problems that are trivial for computers (e.g., when formulated as simple mathematical rules). Most of these solutions are so-called **“rule-based” algorithms***
  - *The challenge of AI is in solving human hard problems which are difficult to formalise as a list of mathematical rules*
  - *Machine Learning is the field of research between AI, Computer Science and Statistics that addresses this issue with a **learn-by-example methodology***



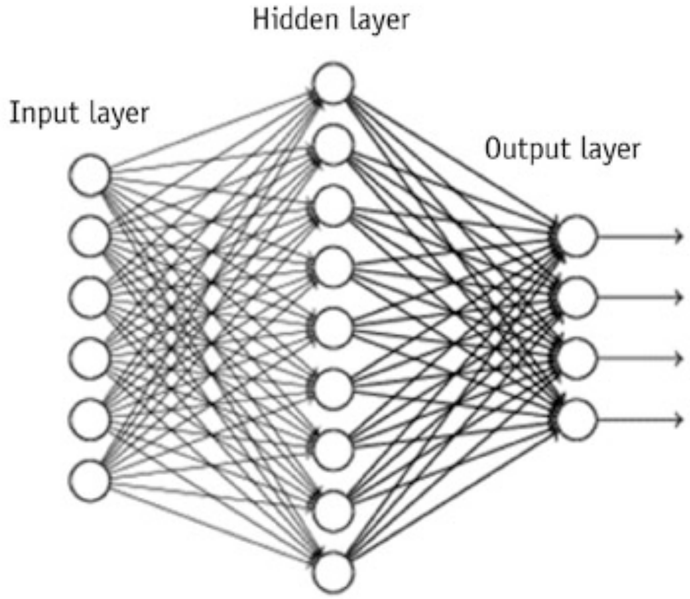
A definition

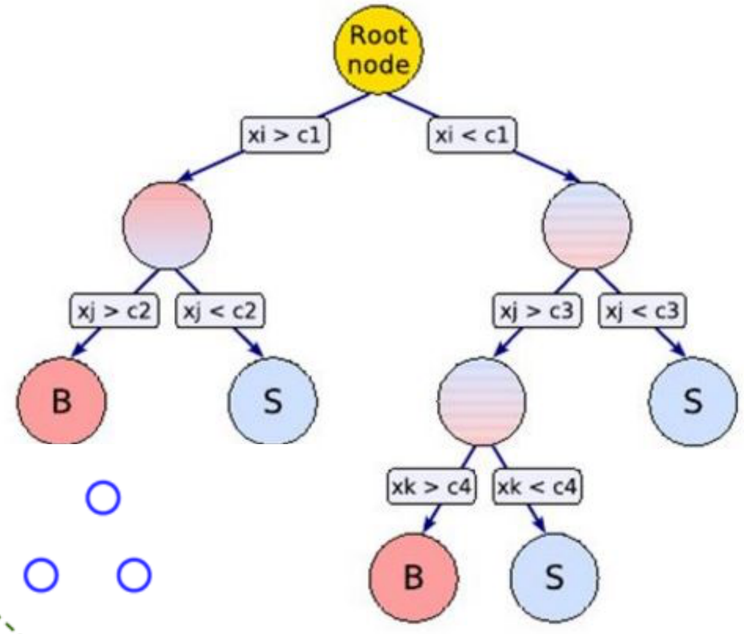
Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to progressively improve their performance on a specific task. Machine learning algorithms build a mathematical model of sample data, known as "training data", in order to make predictions or decisions without being explicitly programmed to perform the task.

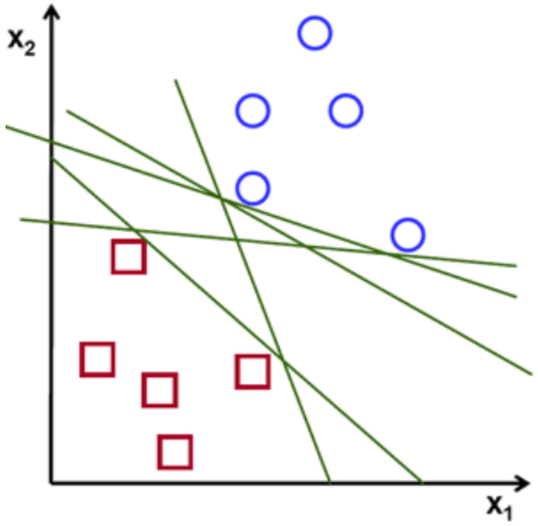


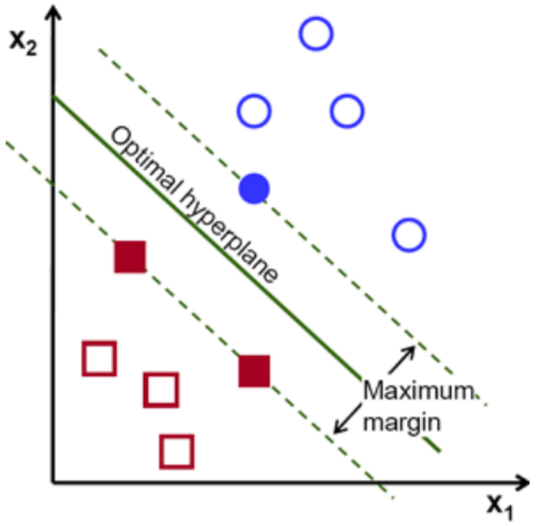
Many ML algorithms

- *In different moments, different algorithms were at the edge of ML research*
  - *(Shallow) neural networks dominated the scene up to the 80's*
  - *Alternatives emerged in the 90's*
    - *Support vector machine*
    - *Boosting of decision trees*
- *These classes of ML algorithms can be used for various tasks*



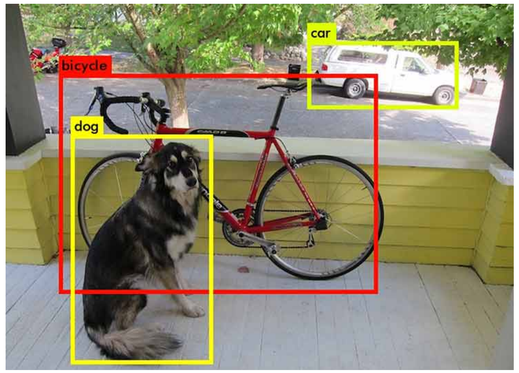


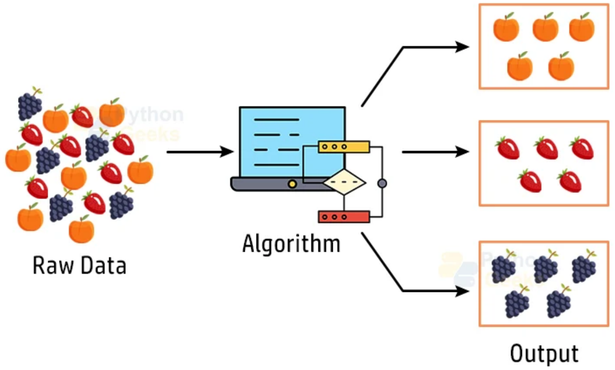


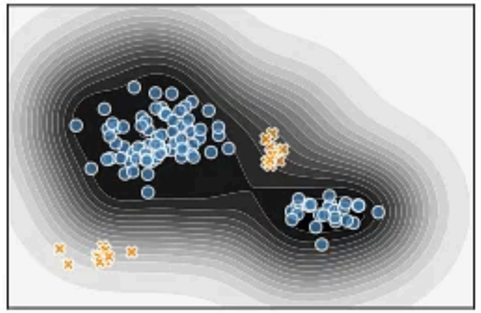


Many Problems to Solve

- ***Classification***: *given an image, identify the object represented*
- ***Regression***: *given an image with an object, estimate its coordinates*
- ***Clustering***: *given a dataset, group dataset entries which are alike*
- ***Anomaly/outlier detection***: *given a reference dataset and a list of test entries, identify the entries not belonging to the dataset*
- ***Generation***: *given a dataset, generate new entries that belong to the dataset*



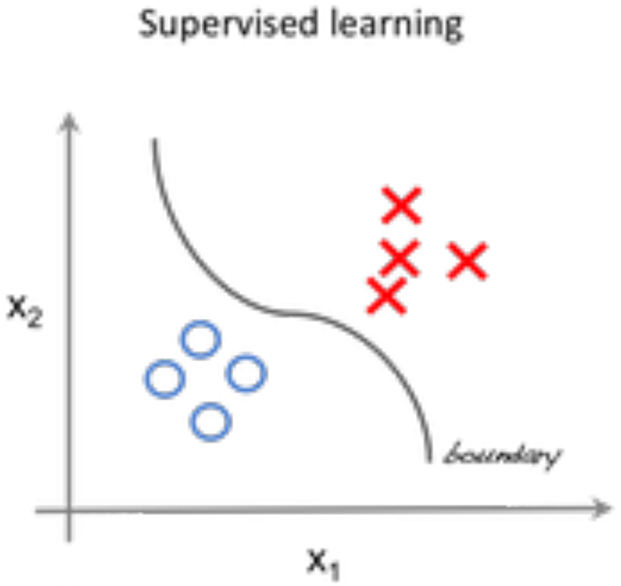


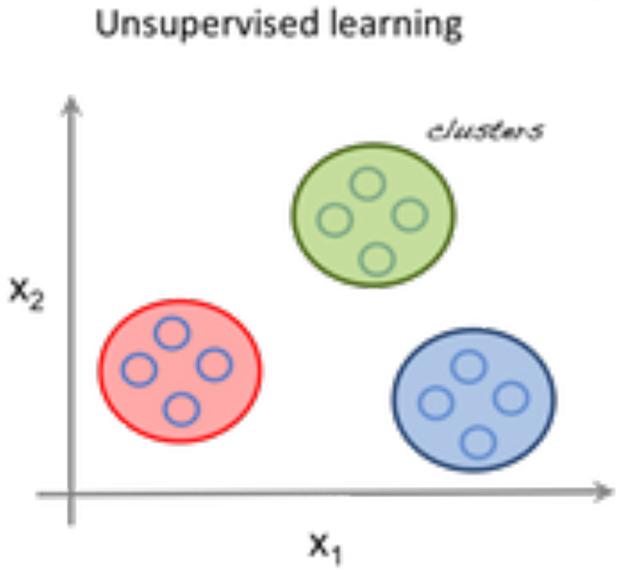


https://thispersondoesnotexist.com/

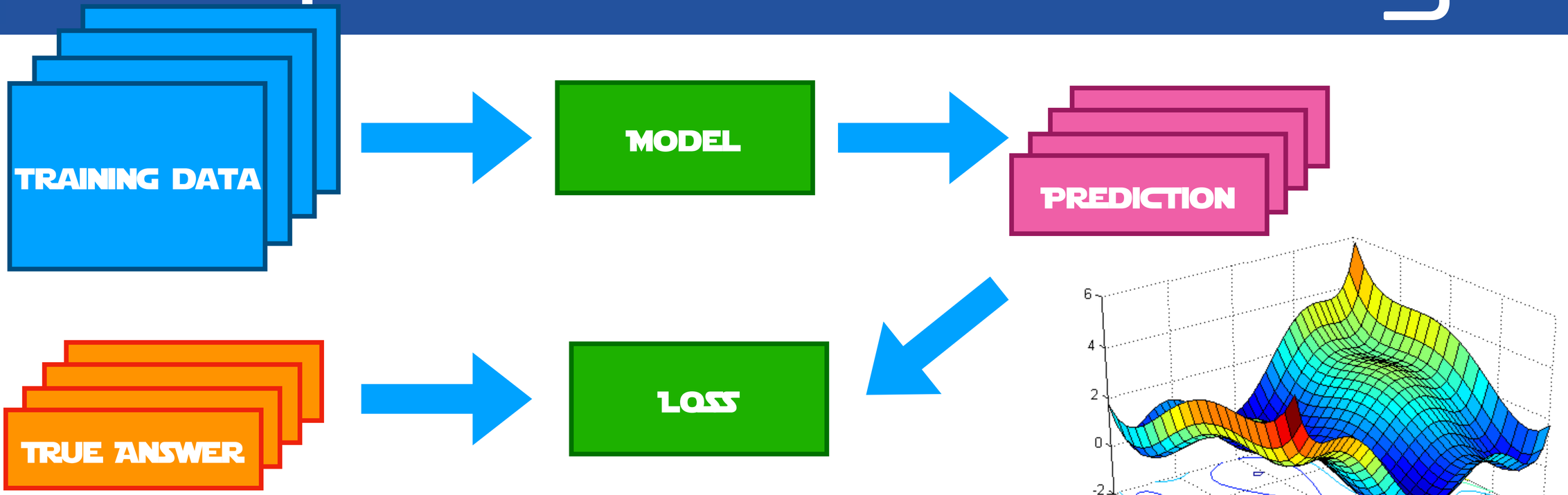
Many kinds of learning

- ***Supervised:*** *the dataset X comes with the right answer y (right class in a classification problem). The algorithm learns the function*
- ***Unsupervised****: the dataset X comes with no label. The algorithm learns structures in the data (e.g., alike events in a clustering algorithm)*
- ***Various intermediate flavors*** *(weekly supervised, semisupervised, etc.)*
- ***Adversarial*** *train a network against another network design for a competing task*
- ***Reinforcement Learning:*** *learn a series of actions and develop a decision-taking algorithm, based on some action/reward model (we will not cover this)*



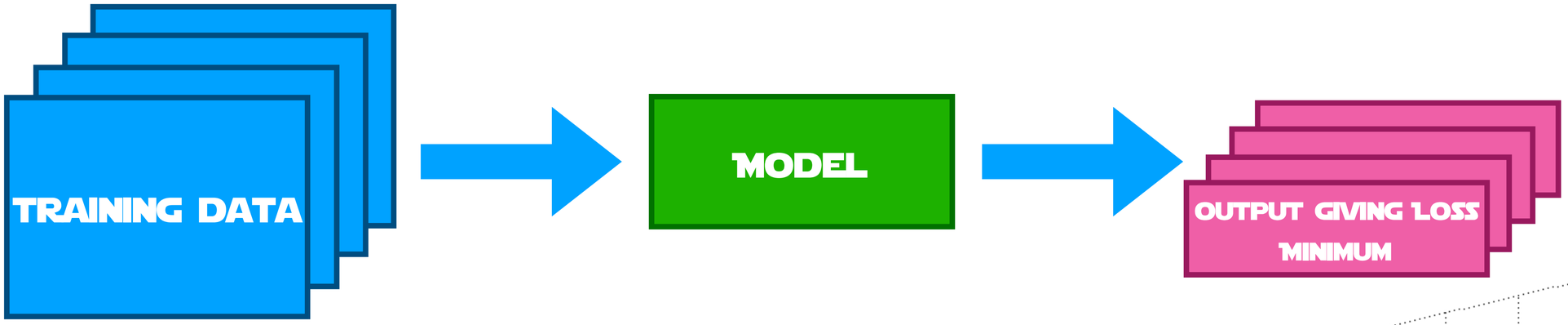


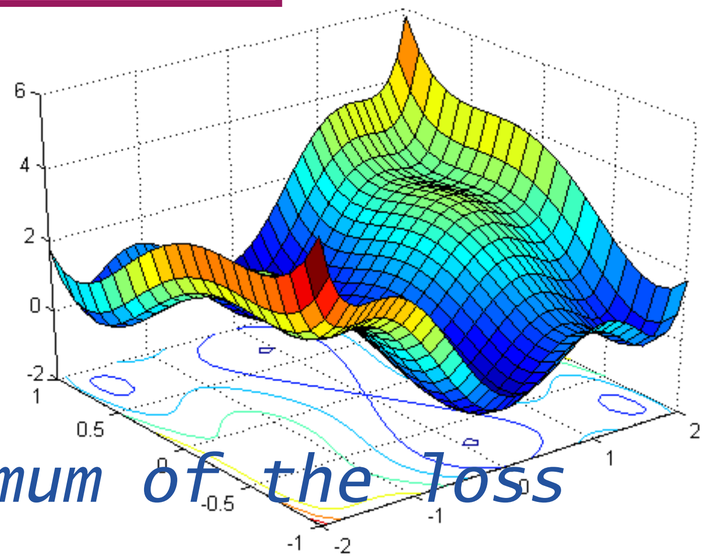
Supervised Learning



- *A training dataset* ***x***
- *A target y*
- *A model to go from* ***x*** *to y*
- *A loss function quantifying how wrong the model is*
- *A minimisation algorithm to find the model h that corresponds to the minimal loss*

Unsupervised Learning

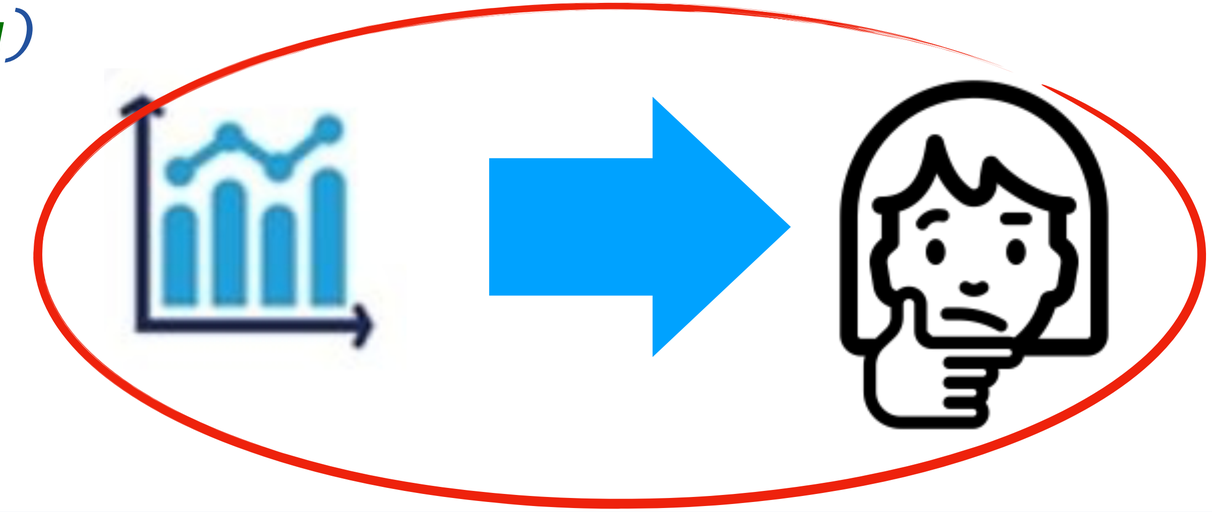


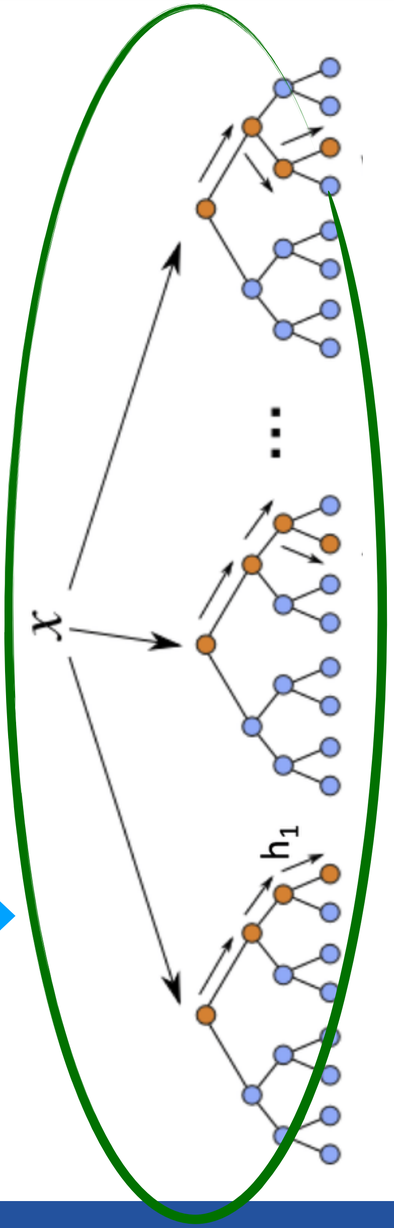


- *A training dataset* ***x***
- *No target y*
- *A model providing an output y at the minimum of the loss*
- *A loss function of x and y specifying the task*
  - *e.g., clustering: group similar objects together*

A pre-DL workflow

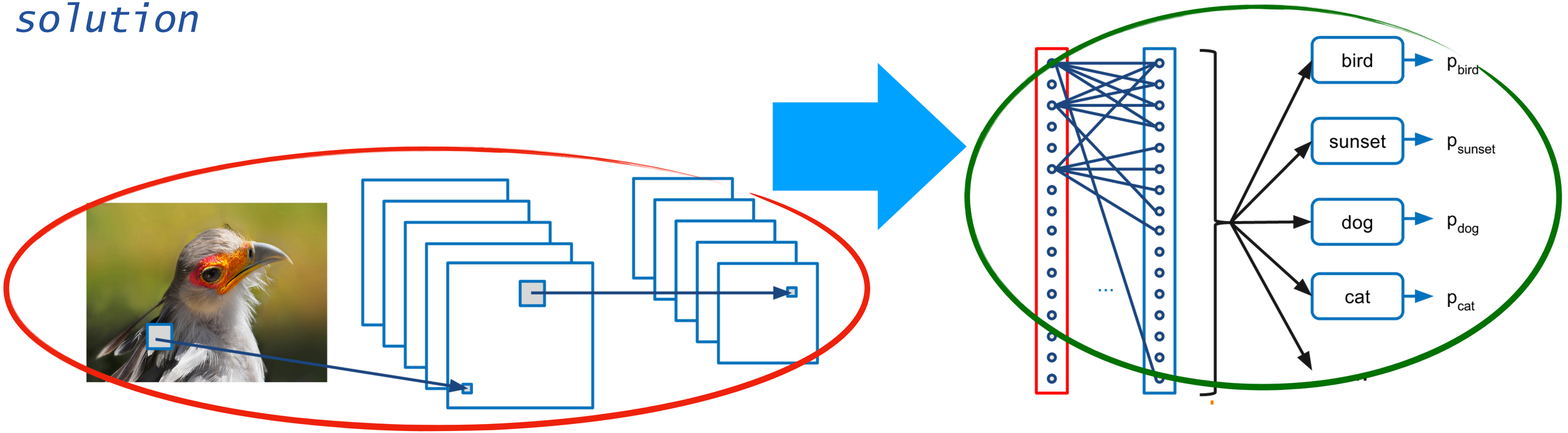
- *A ML practitioner is given task and a dataset*
- *She would*
  - *compute from the data a set of quantities that would be relevant to solve the problem (feature engineering by domain knowledge)*
  - *pass these quantities to a ML algorithm for training (task solving)*





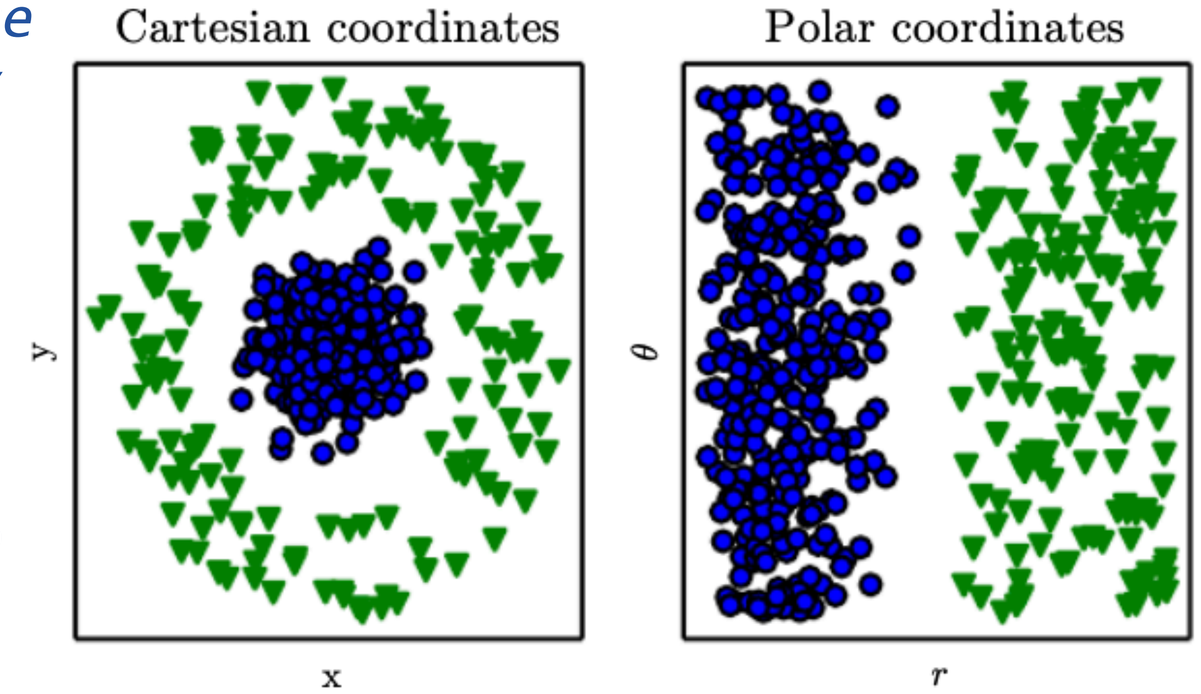
A DL workflow

- *The first part of the network processes the raw data and learns the feature engineering*
- *The second part of the network performs the task solving*
- *The simultaneous training of the two steps guarantees optimal solution*



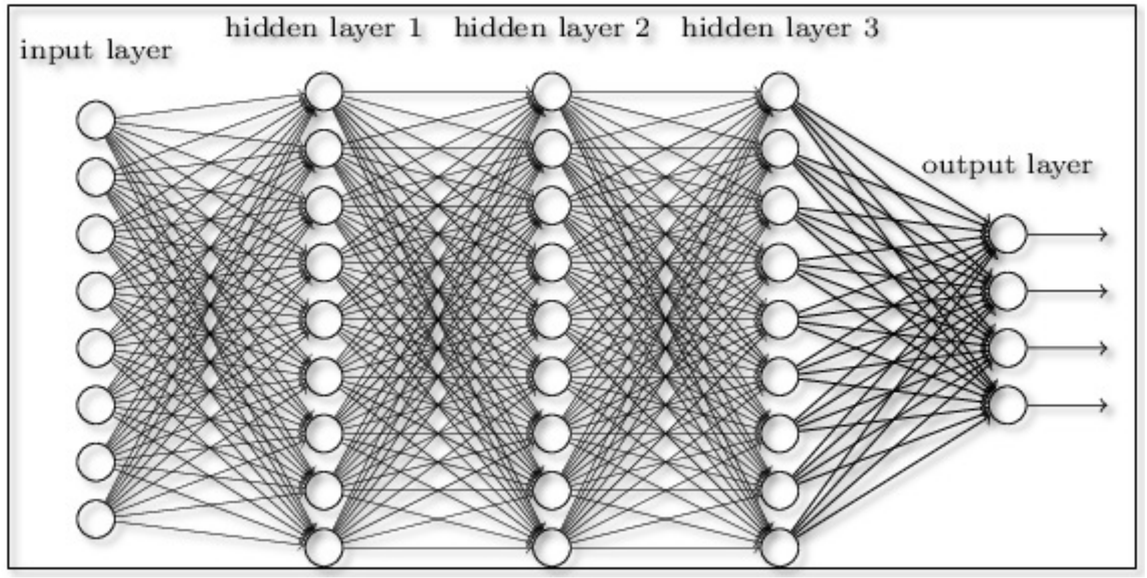
Representation Learning

- *Performance may change depending on how inputs are presented*
- *Imagine the following problem: separate two populations with a linear boundary*
  - *Depending on the coordinate system, this might be possible or not. One might have to look at data from the right angle*
  - *When the right angle is unknown, one can learn it*
    - *Use NNs to define functions f of the input x such that the problem is easier when starting from f(x)*



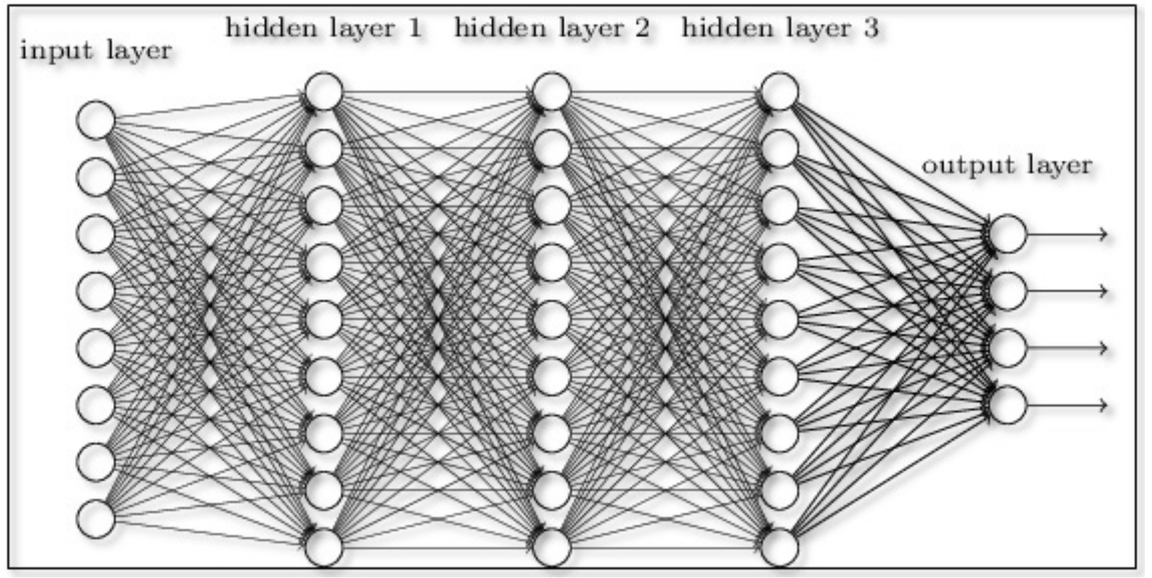
Feed-Forward NNs

- *Feed-forward neural networks have hierarchical structures:*
  - *inputs enter from the left and flow to the right*
  - *no closed loops or circularities*
- *Deep neural networks are feed-fwd NNs with more than one hidden layer*
- *Out of this "classic idea, new architectures emerge, optimised for computing vision, language processing, etc*



Feed-Forward NNs

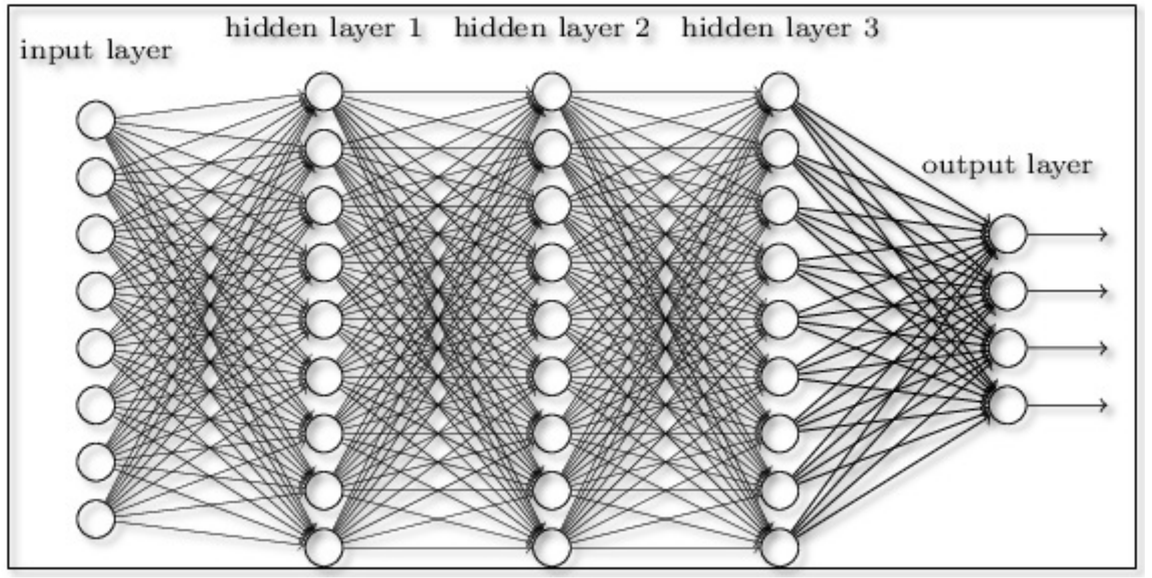
- ***Each input is multiplied by a weight***
- *The weighted values are summed*
- *A bias is added*
- *The result is passed to an activation function*



$$w_{ij}x_j$$

Feed-Forward NNs

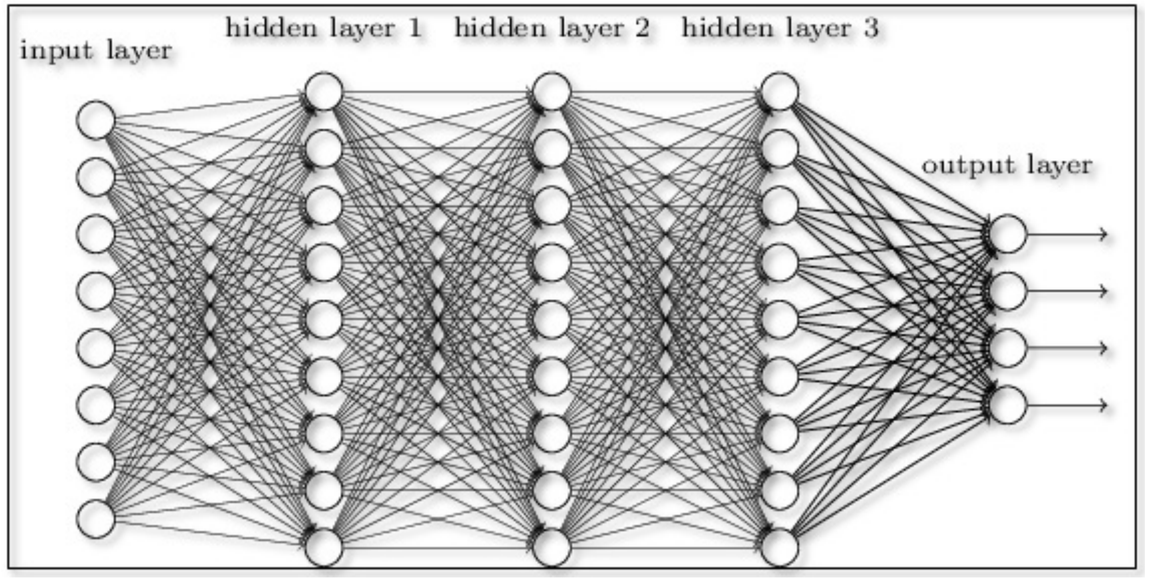
- *Each input is multiplied by a weight*
- ***The weighted values are summed***
- *A bias is added*
- *The result is passed to an activation function*



$$\Sigma_j w_{ij} x_j$$

Feed-Forward NNs

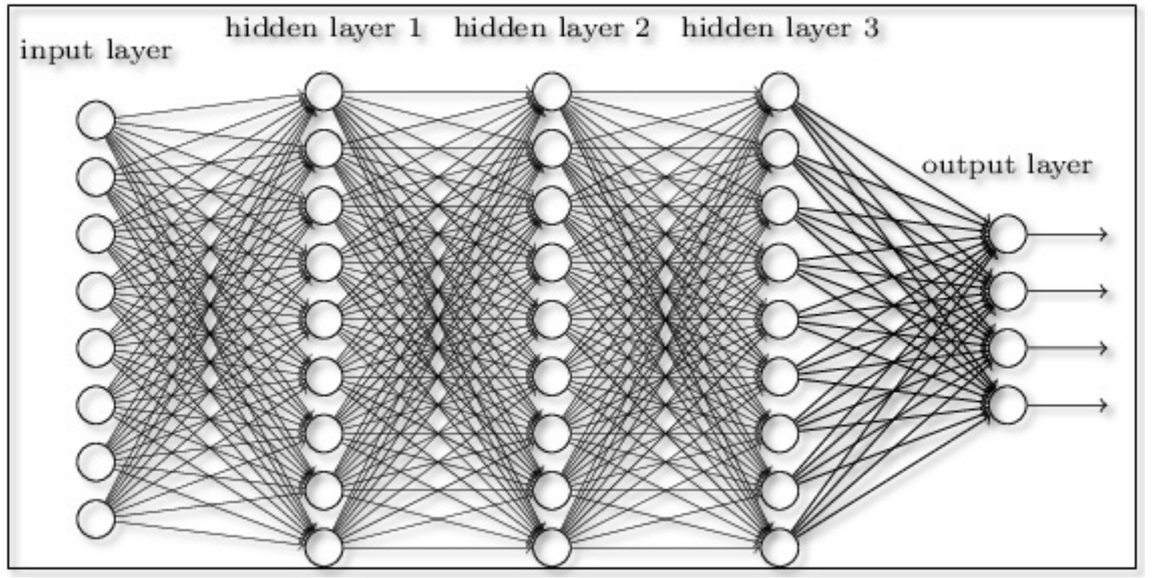
- *Each input is multiplied by a weight*
- *The weighted values are summed*
- ***A bias is added***
- *The result is passed to an activation function*



$$\Sigma_j w_{ij} x_j + b_i$$

Feed-Forward NNs

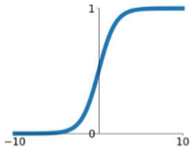
- *Each input is multiplied by a weight*
- *The weighted values are summed*
- *A bias is added*
- ***The result is passed to an activation function***



Activation Functions

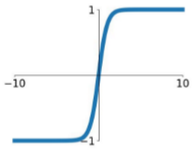
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



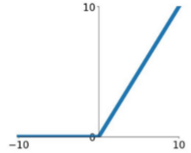
tanh

$\tanh(x)$



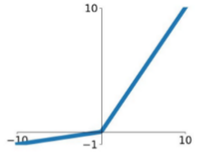
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

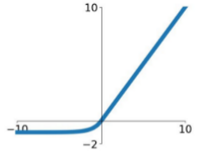


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

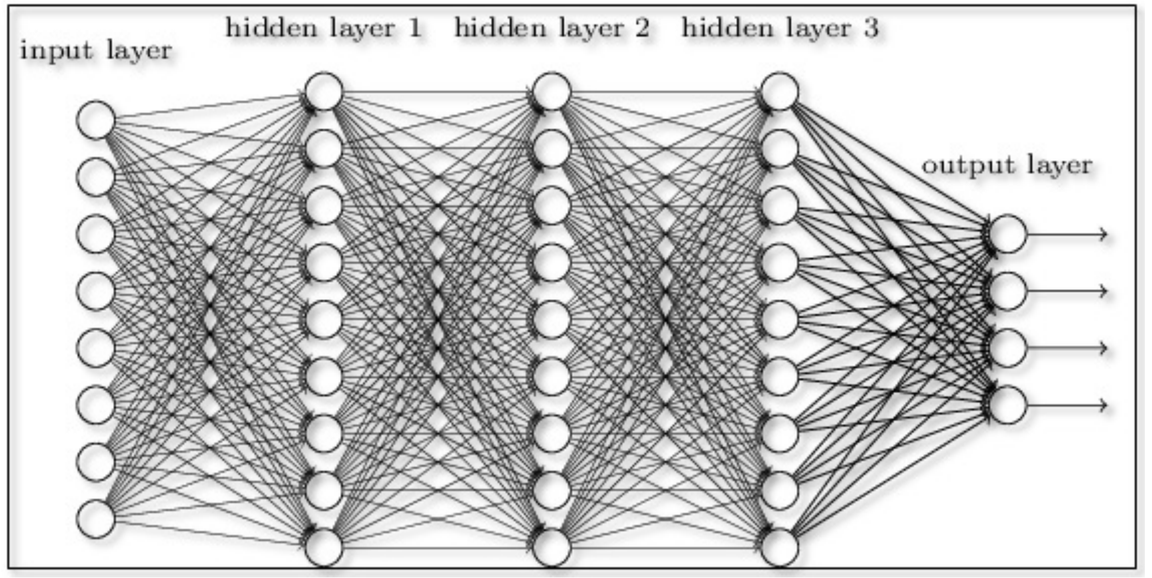
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



$$\hat{y}_i = f(\Sigma_j w_{ij} x_j + b_i)$$

Feed-Forward NNs

- In a feed-forward chain, each node processes what comes from the previous layer
- The final result (depending on the network geometry) is K outputs, given N inputs

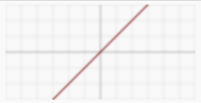
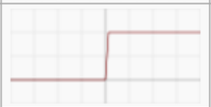
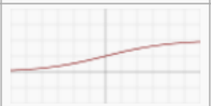
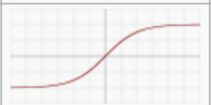
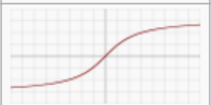
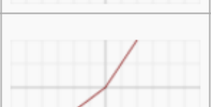


$$\hat{y}_3 = f^{(3)}(\Sigma_l w_{jl}^{(3)} f^{(2)}(\Sigma_k w_{lk}^{(2)} f^{(1)}(\Sigma_i w_{ki}^{(1)} x_i + b_k^{(1)}) + b_l^{(2)}) + b_j^{(3)})$$

- One can show that such a mechanism allows to learn generic $\mathbb{R}^N \to \mathbb{R}^K$ smooth functions

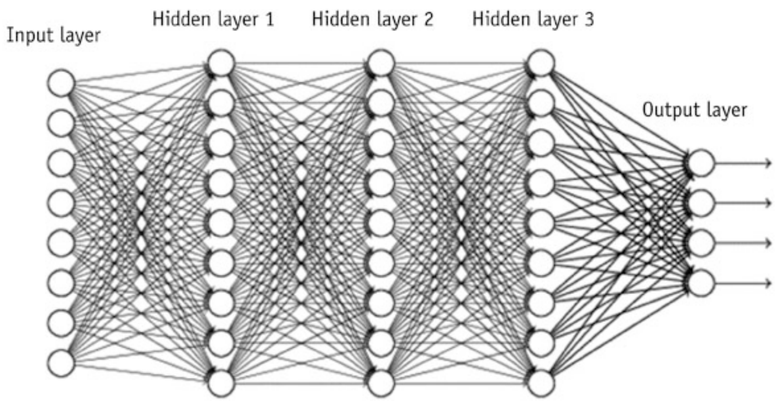
The role of the activation functions

- *Activation functions are the essential ingredient to NNs complexity*
  - *w/o non-linear activation functions, DNNs would just rotate and shift the inputs -> could only solve linear problems*
  - *The choice of the activation function is a hyperparameter*
  - *The last-layer activation function plays a special role. e.g., a classifier would use sigmoid/softmax*
  - *In practice, the fastest is the function, the more efficient is the learning*

Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)(1-f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1+e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$

A technology-driven revolution

- *Deep neural networks have >1 inner layer, hence more complexity thanks to more parameters*
- *Thanks to GPUs, it is now possible to train them efficiently, which boosted the revival of neural networks in the years 2000*
- *In addition, new architectures emerged, which better exploit the new computing power*



Large-scale Deep Unsupervised Learning using Graphics Processors

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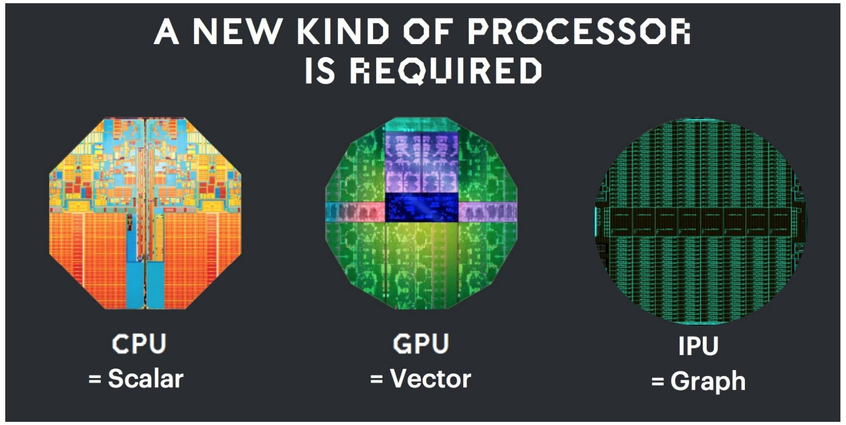


Training in practice

- The network score (i.e., the output) is a function of the network parameters $(\vec{w}, \vec{b})$ and the data

$$\hat{y}_3 = f^{(3)}(\Sigma_l w_{jl}^{(3)} f^{(2)}(\Sigma_k w_{lk}^{(2)} f^{(1)}(\Sigma_i w_{ki}^{(1)} x_i + b_k^{(1)}) + b_l^{(2)}) + b_j^{(3)})$$

- The loss is a function of the score and the data (the input x and, for supervised learning, the truth y)

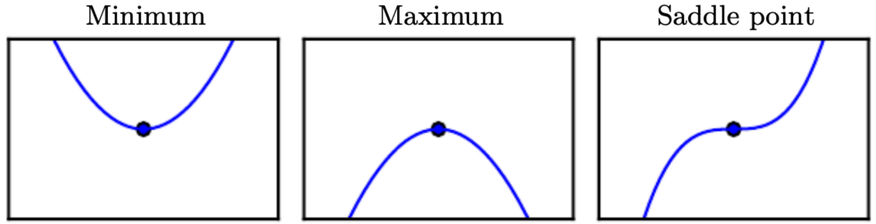
$$\mathscr{L} = \sum_i |y^i - \hat{y}^i(x, w, b)|^2$$

- One can then think that, for a given dataset (and its truth), the loss is a function of the weights

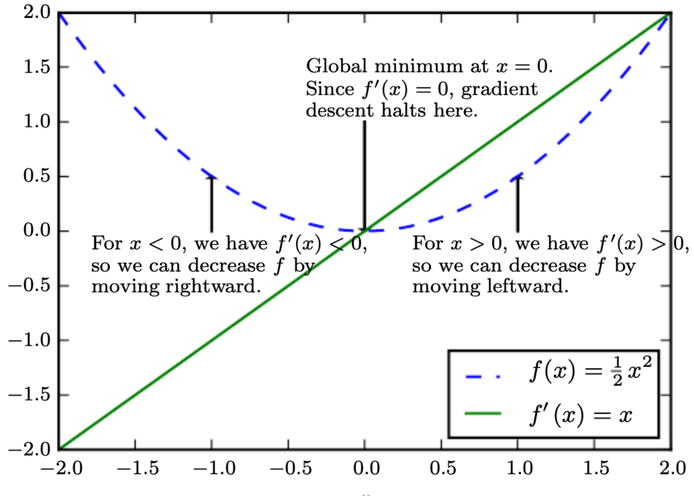
$$\mathscr{L} = f(w, b \,|\, x, y)$$

Minimisation through derivation

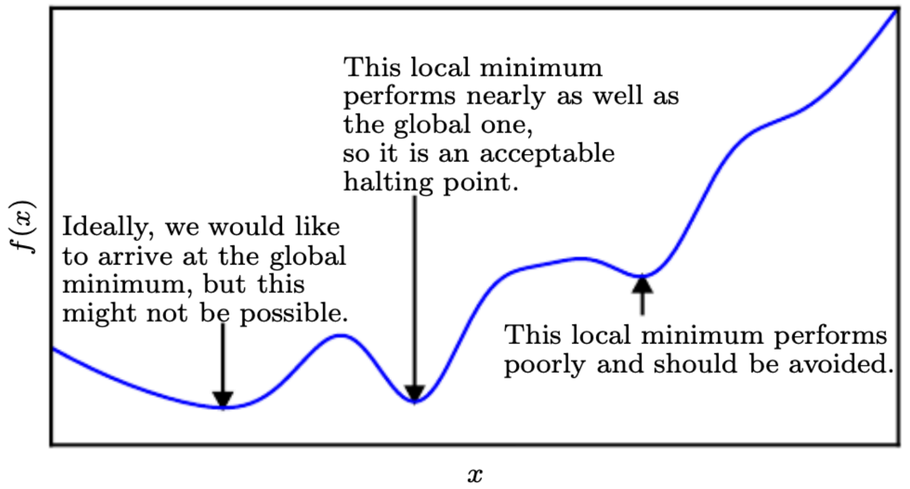
- We can find the minimum of a function looking for zeros of the derivative
  - But keep in mind that not all the zeros are minima



- With multi-dimensional function, we need partial derivatives
  - Compute the derivative wrt every dimension
    - This gives the gradient vector
  - The scalar product of the gradient and a direction vector tells us how fast the function changes in that direction (directional derivative)
  - We want to find the direction of maximal directional derivative and move opposite to it
  - How much should we move? The step size is called **learning rate** and it is a hyperparameter of your training



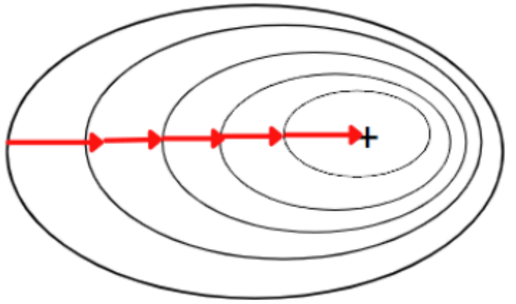
$$\boldsymbol{x}' = \boldsymbol{x} - \epsilon \nabla_{\boldsymbol{x}} f(\boldsymbol{x})$$



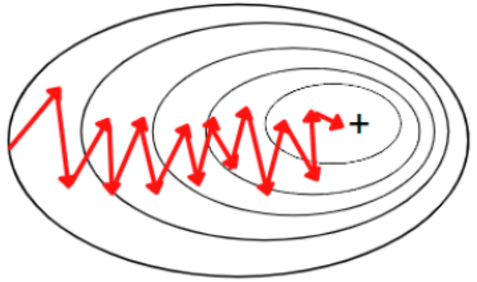
Training in practice

- *The training is then a minimisation problem: one starts from a random point in the (w, b) space and tries to walk down towards the minimum*
  - *Gradient descent: one computes the maximum gradient and takes a step in the opposite direction*
- *Various kinds of gradient descents:*
  - ***batch gradient descent**: compute the gradient in parallel for small chunks of data and take the average. Update the model once all data are processed*
  - ***stochastic gradient descent**: update the model after each example. More noisy, less prone to get stuck to a local minimum, but more computationally expensive*
  - ***mini-batch gradient descent**: like sgd, but update the model only after a batch of examples. Compromise between the previous two*

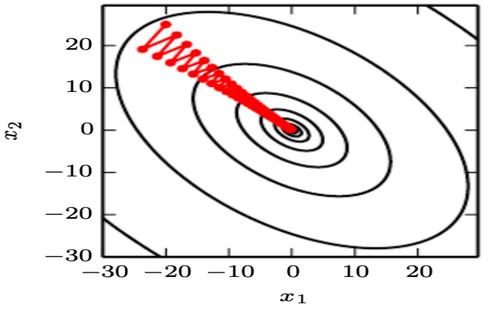
Batch Gradient Descent



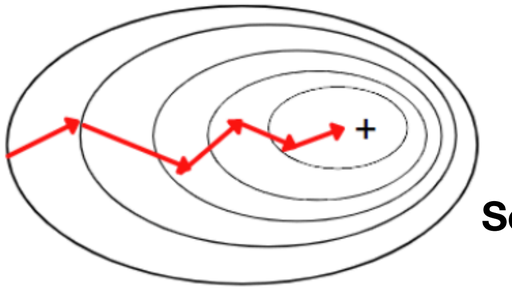
Stochastic Gradient Descent



Stochastic Gradient Descent with too small learning rate



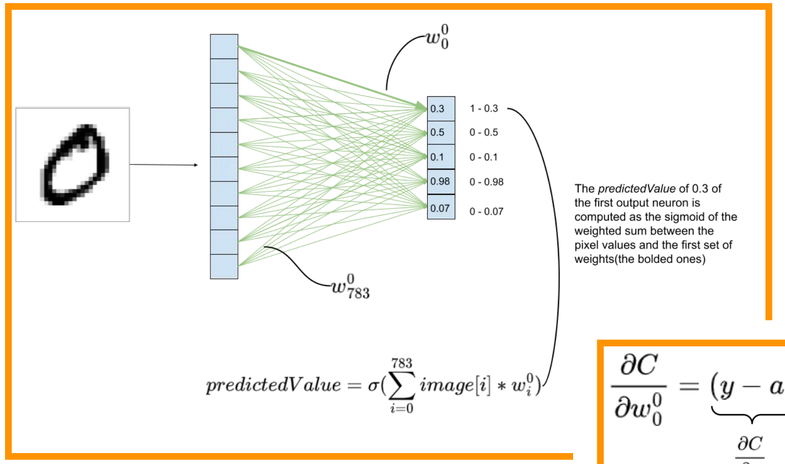
Mini-Batch Gradient Descent



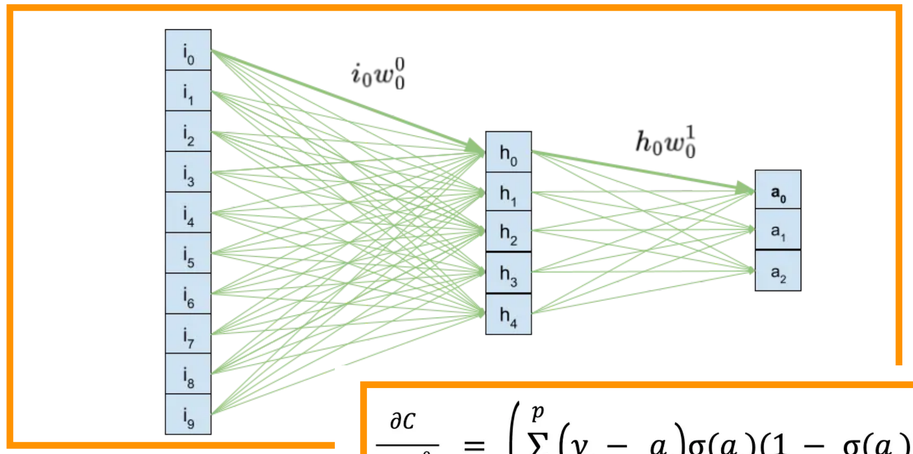
See section 4.3 in the book for considerations on second derivative (Hessian, Netwon's approximation, etc.)

Backpropagation

- Backpropagation allows to speed up sgd exploiting the gradient chain rule
  - one goes back from the activation function to the argument, to the input, using derivative chain rule
  - Adding layers just makes the chain longer, but the concept is the same
- You can find here a useful walkthrough, that will become more clear in a few lectures (when you will be familiar with all the ingredients)
  - with many useful tips, e.g., on the choice of the activation function



$$\frac{\partial C}{\partial w_0^0} = \underbrace{(y-a)}_{\frac{\partial C}{\partial a}}\underbrace{\sigma(z)(1-\sigma(z))}_{\frac{\partial a}{\partial z}}\underbrace{image[0]}_{\frac{\partial z}{\partial w_0^0}}$$



$$\frac{\partial C}{\partial w_0^0} = \left(\sum_{i=0}^{p}\left(y_i - a_i\right)\sigma(a_i)(1-\sigma(a_i))w_i^1\right)\sigma(h_0)(1-\sigma(h_0))i_0$$

Summary

- *Deep Learning is the latest evolution of Machine Learning*
- *Technological progress with gradient computation on distributed computing architectures allowed to use higher complexity architectures*
- *Various kinds of problems, architectures, and learnings*
- *Dense Neural Networks are the simplest architecture*
- *More than brute force: one needs insight for best architecture choice, best choice of hyperparameters, and best data representations to facilitate the feature extraction*