Introduction to Machine Learning

Chap I: Basic concepts

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Outline of these lectures

Lectures

Chap I: Basic concepts on ML

Chap II: Regression

Chap III: Classification

Practice sessions

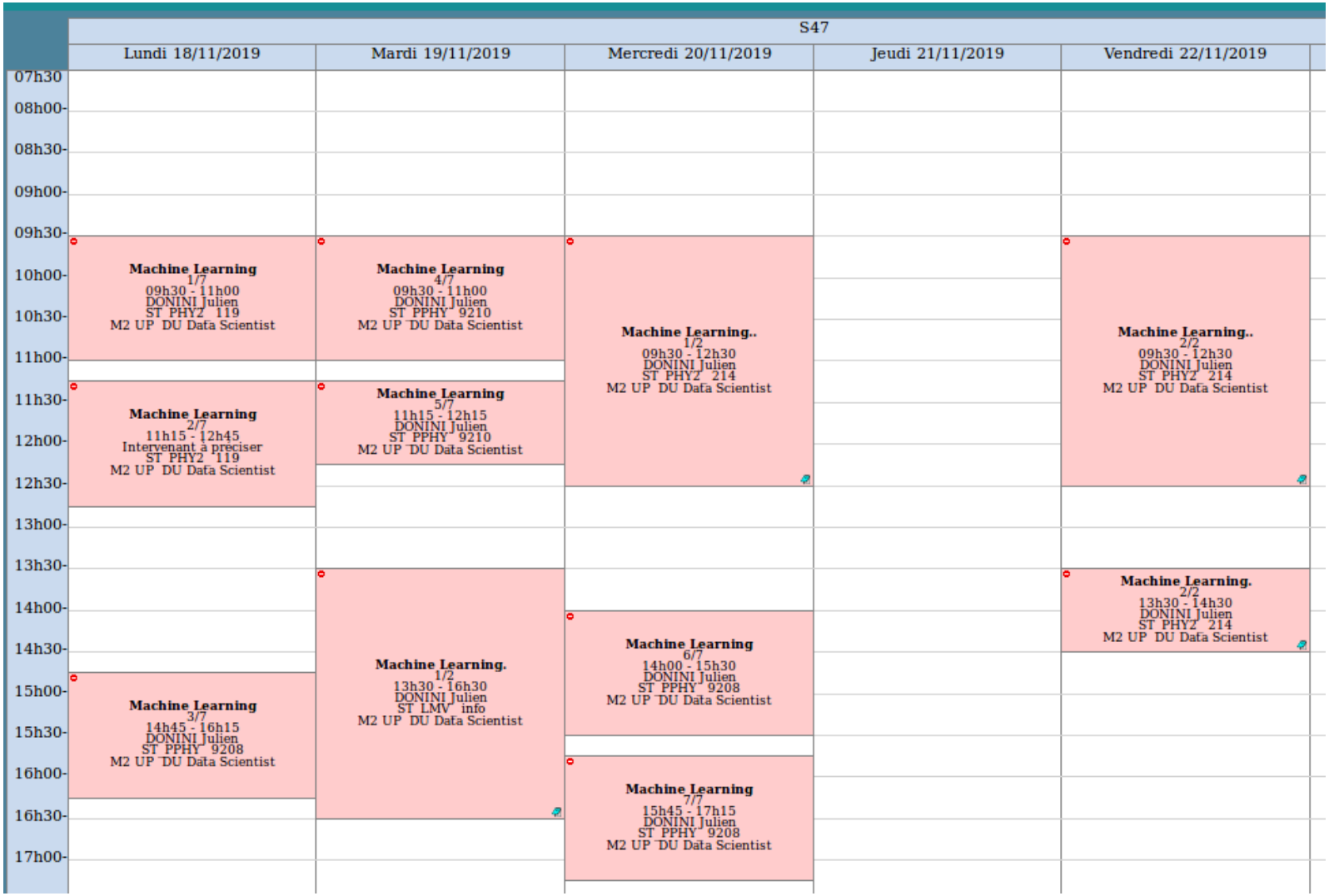
Introduction to Machine Learning

Code on Git: 

https://github.com/judonini/MLcourses2019

Sections marked with (*) are more advanced → non examinable for DU students

This week



Lecture: 4h30 Lecture: 2h30 Practice: 3h Practice: 4h

Practice: 3h Lecture: 3h

References (non exhaustive !) & credits

Classical Machine Learning textbooks

- **Elements of statistical learning** (ESL), Hastie et al., Springer
- **An Introduction to Statistical Learning** (ISLR), Hastie et al. Springer
  - Both books available online: http://web.stanford.edu/~hastie/pub.htm
- **Pattern Recognition and Machine Learning**, Bishop, Springer
- **Deep learning book,** I. Goodfellow et al, http://www.deeplearningbook.org/

A *lot* of courses, lectures and tutorial on the web

- **Online courses**: DataCamp, Coursera, Andrew Ng (http://cs229.stanford.edu/)
- **CERN** lectures (ex: Kagan https://indico.cern.ch/event/619370)
- **2 recommended lectures:**
  - **François Fleuret** (EPFL) **https://fleuret.org/ee559/**
  - **Gilles Louppe** (University Liège)https://github.com/glouppe/info8010-deep-learning
- ML **cheatsheet**: https://ml-cheatsheet.readthedocs.io/en/latest/index.html

Python resources

- A **Crash Course** in Python for Scientists : http://nbviewer.jupyter.org/gist/rpmuller/5920182
- Introduction to **scientific computing** with Python: http://github.com/jrjohansson/scientific-python-lectures
- Python **Tutorial**: https://www.codecademy.com/tracks/python

Notebooks basics

- **Installation** (recommended): https://www.anaconda.com/download
- **Jupyter** Notebook documentation: https://jupyter-notebook.readthedocs.io/en/stable/
- **Interactive** notebooks: https://mybinder.org/
- Introduction with **video** tutorial: https://www.youtube.com/watch?v=Duicsycntdo

Git

- **Git** documentation: https://book.git-scm.com/
- **Github**: https://github.com/
- **GitLab** (CERN) basics: https://gitlab.cern.ch/help/gitlab-basics/start-using-git.md
- **Tutorial** (in FR): https://github.com/clr-info/tuto-git
  https://openclassrooms.com/en/courses/1233741-gerez-vos-codes-source-avec-git

ML software and interfaces

Internal (HEP) tools

ROOT framework for data storage and processing

Multivariate Analysis: TMVA for mostly BDT and (deep) NN

Specific for Neural Networks: NeuroBayes

External tools

Data format: text, csv, images, HDF5, ...

ML libraries: Keras+TensorFlow, Pytorch, scikit-learn (no DL), ...

All kinds of popular algorithms: CNN, GAN, RNN, LSTM, AE, VAE ...

Interfaces and middleware

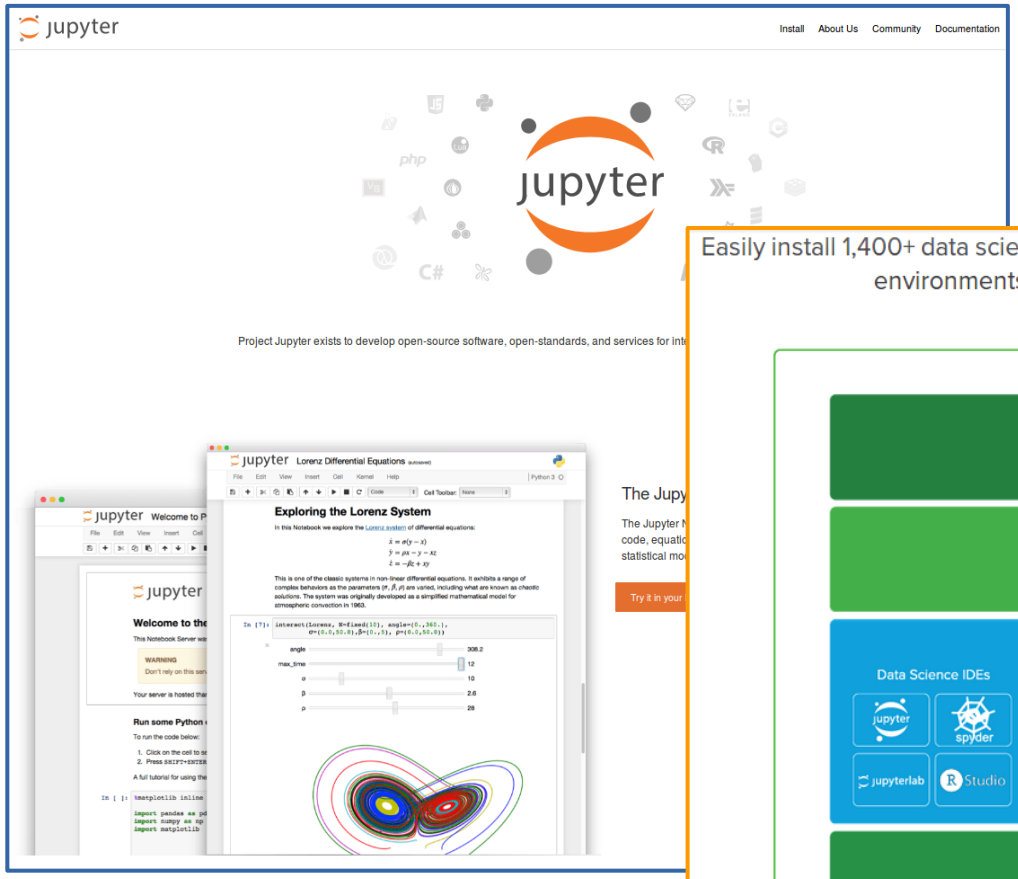
PyMVA: Interface TMVA and Keras

Several middleware file format conversion solutions:

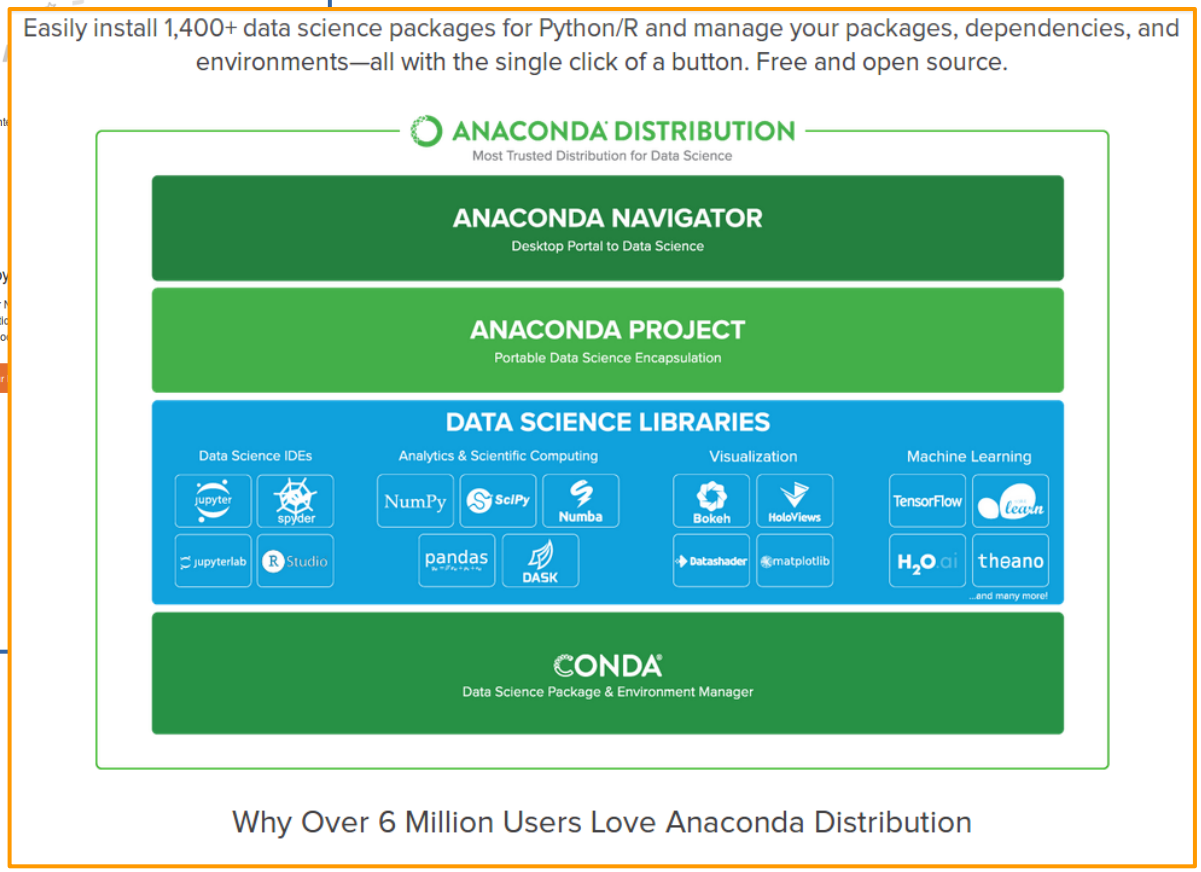
arxiv:1807.02876

PyROOT	Python extension module that allows the user to interact with ROOT data/classes. [69]
root_numpy	The interface between ROOT and NumPy supported by the Scikit-HEP community. [65]
root_pandas	The interface between ROOT and Pandas dataframes supported by the DIANA/HEP project. [70]
uproot	A high throughput I/O interface between ROOT and NumPy. [71]
c2numpy	Pure C-based code to convert ROOT data into Numpy arrays which can be used in C/C++ frameworks. [72]
root4j	The hep.io.root package contains a simple Java interface for reading ROOT files. This tool has been developed based on freehep-rootio. [73]
root2npy	The `go-hep` package contains a reading ROOT files. This tool has been developed based on freehep-rootio. [73]
root2hdf5	Converts ROOT files containing TTrees into HDF5 files containing HDF5 tables. [74]

Jupyter notebooks: jupyter.org



Install using Anaconda: www.anaconda.com



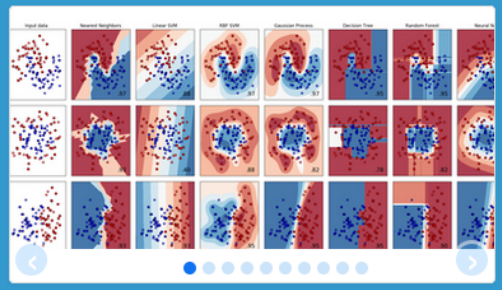
Scikit-learn (scikit-learn.org)

scikit learn

Home Installation Documentation Examples

Google Custom Search Search

Fork me on GitHub



scikit-learn

Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying to which category an object belongs to.

Applications: Spam detection, Image recognition.
Algorithms: SVM, nearest neighbors, random forest, ... — Examples

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.
Algorithms: SVR, ridge regression, Lasso, ... — Examples

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: k-Means, spectral clustering, mean-shift, ... — Examples

Dimensionality reduction

Reducing the number of random variables to consider.

Applications: Visualization, Increased efficiency
Algorithms: PCA, feature selection, non-negative matrix factorization. — Examples

Model selection

Comparing, validating and choosing parameters and models.

Goal: Improved accuracy via parameter tuning
Modules: grid search, cross validation, metrics. — Examples

Preprocessing

Feature extraction and normalization.

Application: Transforming input data such as text for use with machine learning algorithms.
Modules: preprocessing, feature extraction. — Examples

News

On-going development: What's new (Changelog)

Community

About us See authors and contributing

More Machine Learning Find related projects

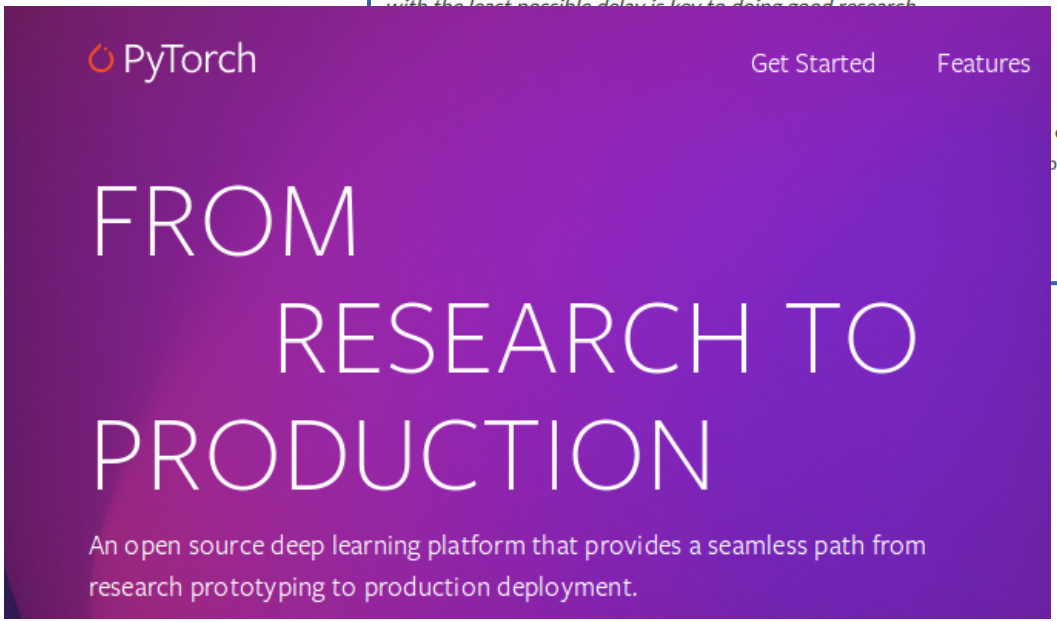
Who uses scikit-learn?

Deep Learning libraries

www.tensorflow.org

Keras.io

Pytorch.org



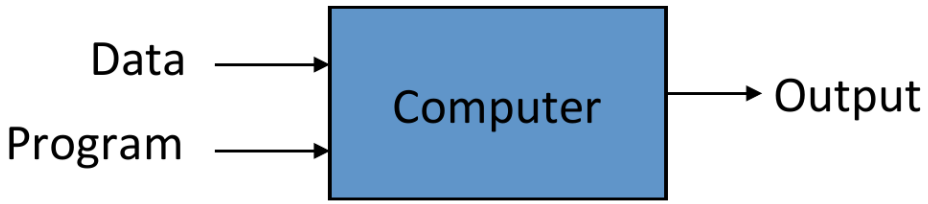
What ML pioneers say

"Giving computer the ability to **learn without training** them" (Arthur Samuel '59)

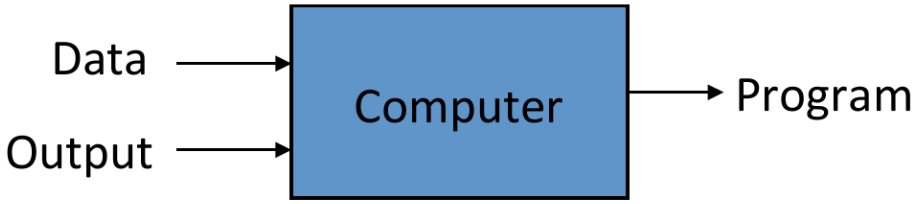
"**Learning** is any process by which a **system improves performance** from **experience**."(Herbert Simon)

"ML is the study of **algorithms** that improve their **performances P** at some **task T** by **Experience E**. A well defined learning task is given by **<P,T,E>**" (T. Mitchell '98)

Traditional Programming



Machine Learning



[P. Domingo]

What is Machine Learning

Based on mathematics, statistics and algorithmics + computer power

- Determine complex **models** from data
- **Prediction** and **inference**

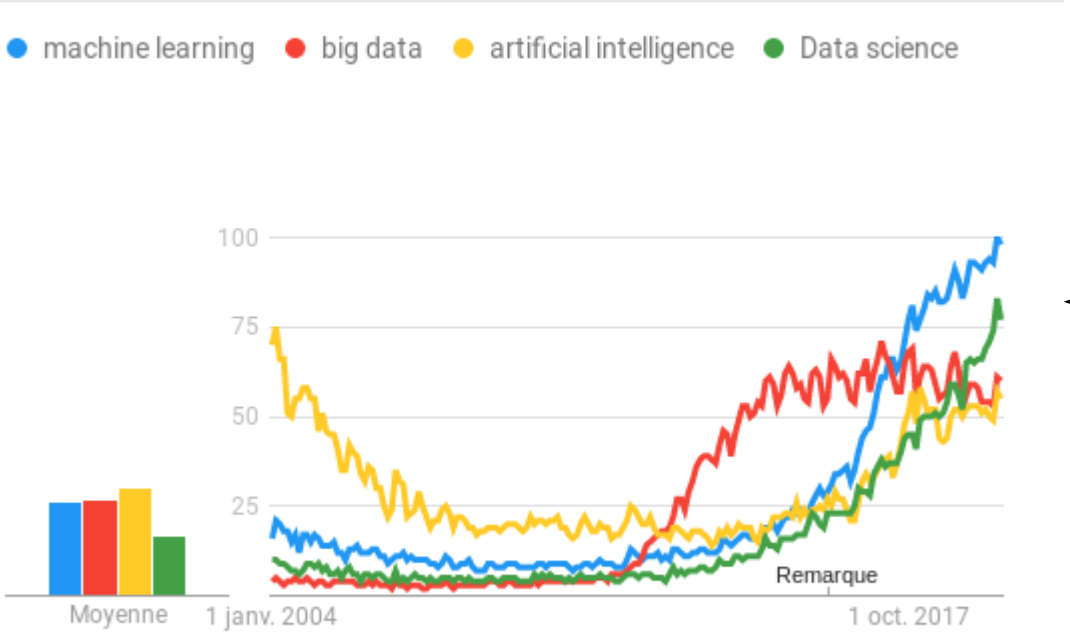
Machine Learning is not recent

- Artificial **Neural Network** (theory 40's, first functional networks 60's)
- Decision **Trees** (~80's)
- Used in **HEP** since many years – but sometime with scepticism.

Renaissance of the field since ~10 years

- **Deep Learning** (first DNN in HEP arxiv:2014.4735)
- **G**raphics **P**rocessing **U**nits for fast and scalable calculations
- New **recent** algorithms: GAN (2014), Adam minimization (2014), ...

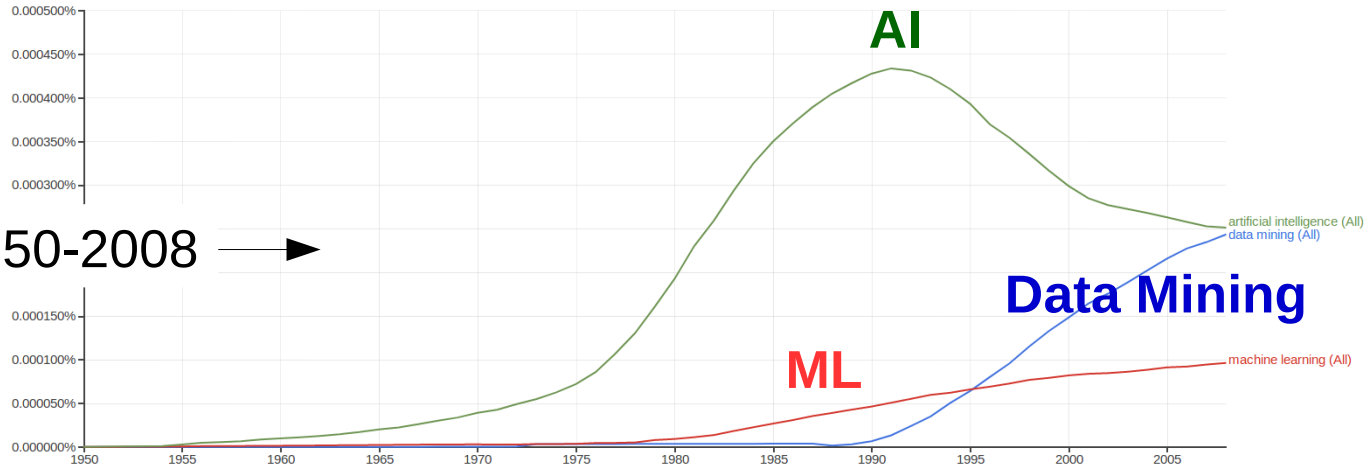
Buzzwords



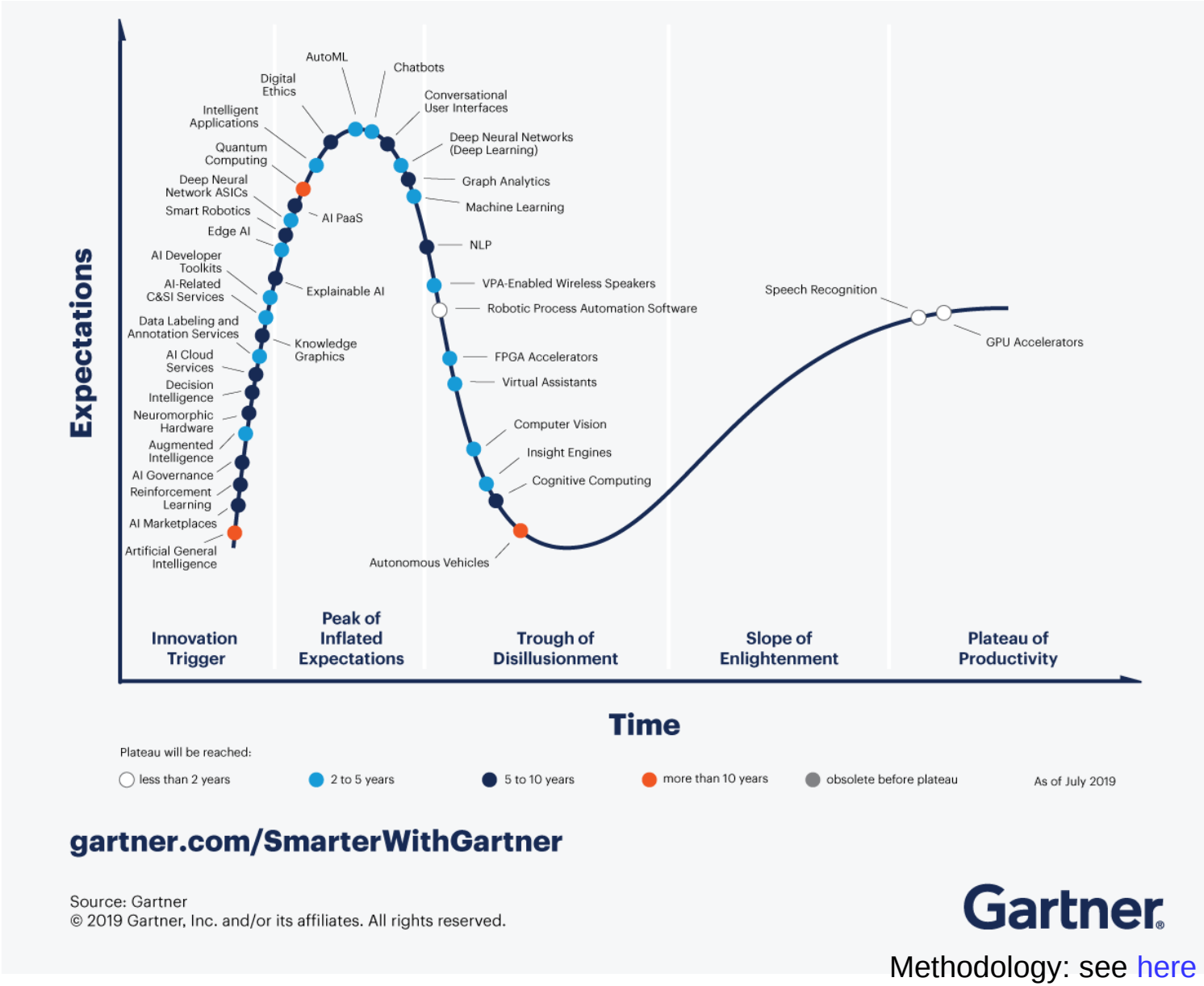
Google trends: 2004-2019

Dans tous les pays. 01/01/2004 – 24/10/2019. Recherche sur le Web.

Google books: 1950-2008



Hype Cycle



Methodology: see here

Applications

- **Speech** and **handwriting** recognition
- **Language** processing
- **Image** recognition
- **Fraud** detection
- **Financial** market analysis
- **Search engines**
- **Spam** and **virus** detection
- **Medical** diagnosis
- **Robotic** control
- **Automation** (self-driving cars)
- **Advertising**
- **Physical** science
- …

MNIST database
60,000 training images
10,000 testing images.

Human error rate ~ 2%

Best ML error rate: 0.2%

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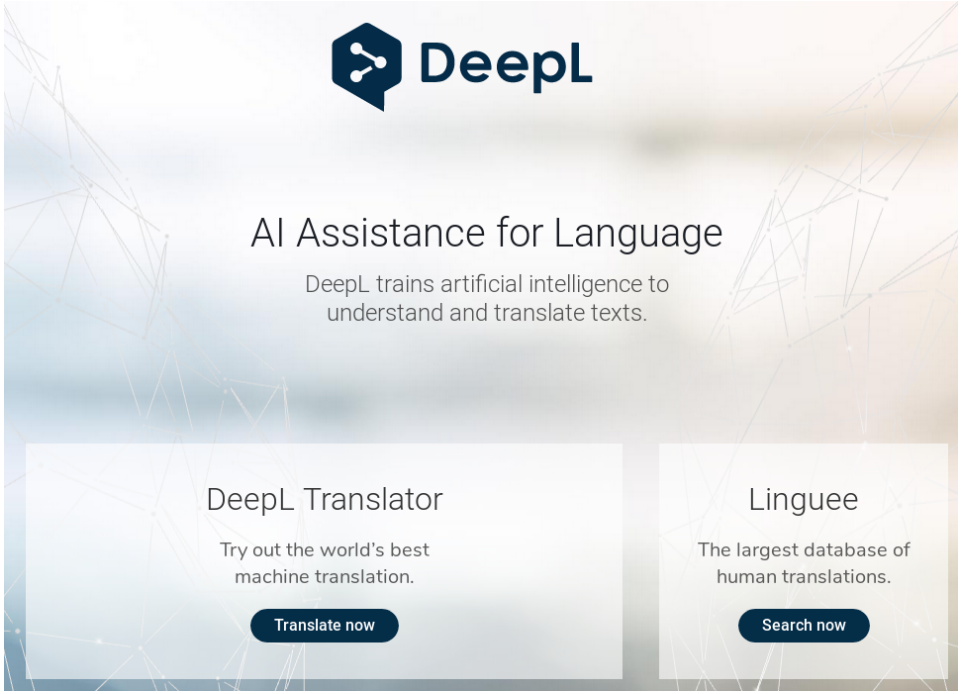

Deep learning translator

https://www.deepl.com

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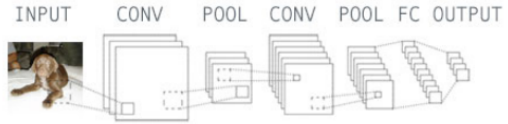

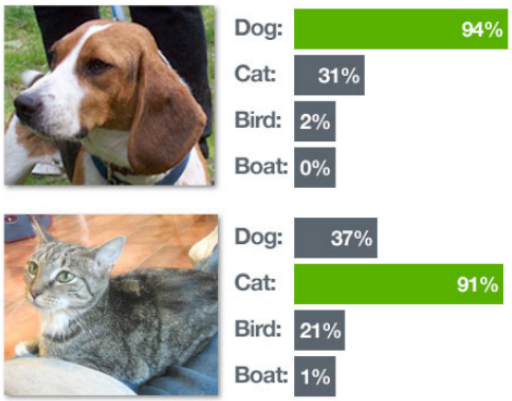

Applications

- **Speech** and **handwriting** recognition
- **Language** processing
- **Image** ~~recognition~~ **generation !**
- **Fraud** detection
- **Financial** market analysis
- **Search engines**
- **Spam** and **virus** detection
- **Medical** diagnosis
- **Robotic** control
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- **Advertising**
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- …

(Arjovsky et al, 2017)

ML and HEP

Data analysis

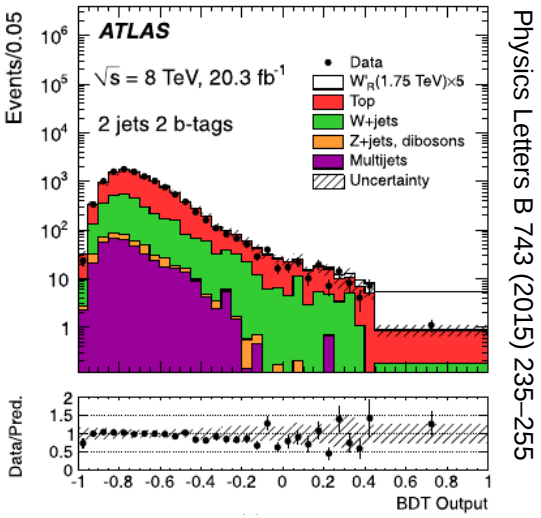
- Precision measurements
- Searches for new physics
- Background rejection
- ...

Performances

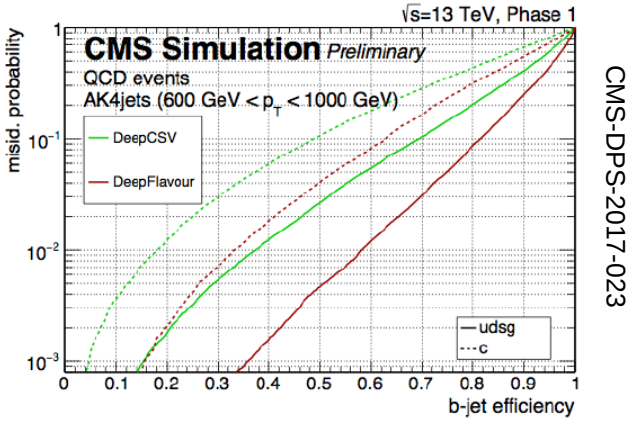
- Trigger and particle identification
- Object reconstruction
- Energy/mass resolution
- Anomaly detection
- ...

Computing

- Best access to popular datasets
- ...



Physics Letters B 743 (2015) 235–255



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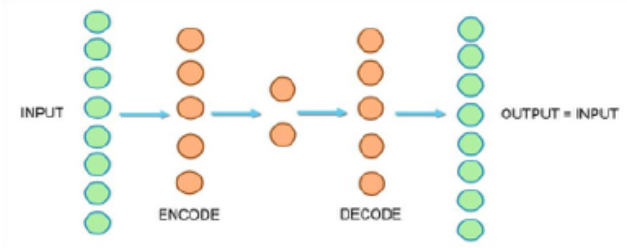


Machine Learning Challenge

www.kaggle.com

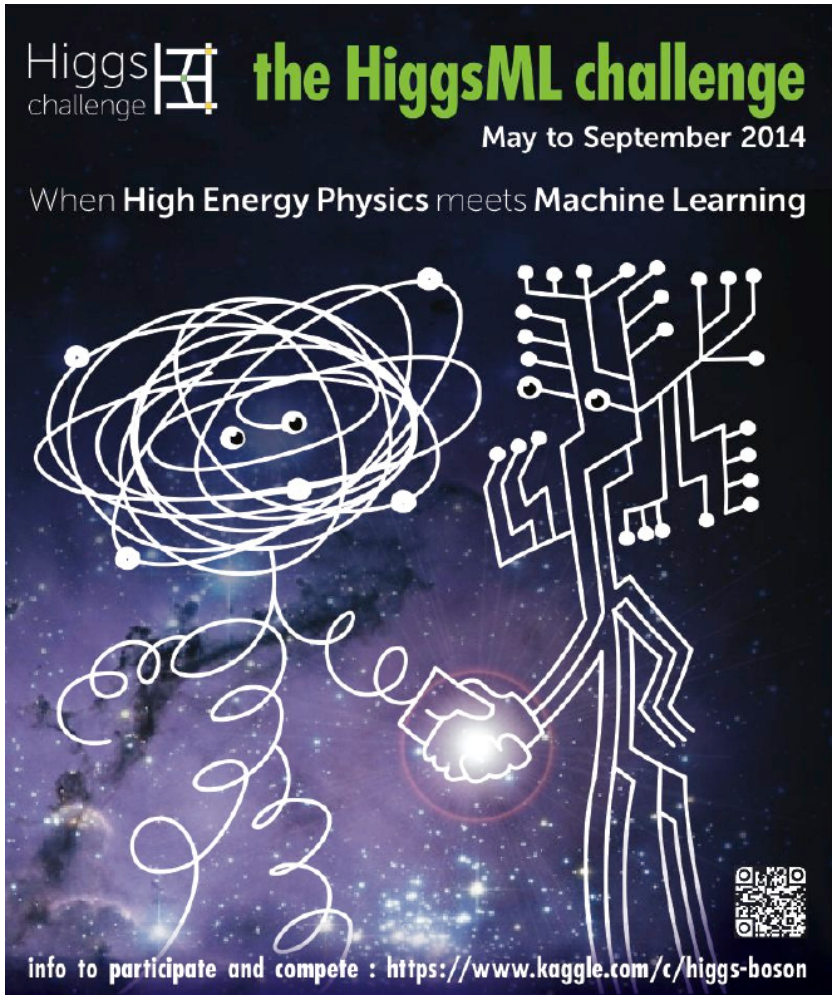
Higgs Boson Machine Learning Challenge
Use the ATLAS experiment to identify the Higgs boson
Featured · 3 years ago

Homesite Quote Conversion
Which customers will purchase a quoted insurance plan?
Featured · a year ago

Forest Cover Type Prediction
Use cartographic variables to classify forest categories
Playground · 2 years ago

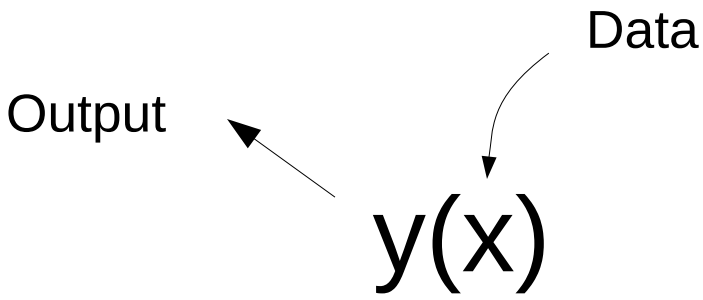
TalkingData Mobile User Demographics
Get to know millions of mobile device users
Featured · 8 months ago

Amazon.com - Employee Access Challenge
Predict an employee's access needs, given his/her job role
Featured · 4 years ago



1800 teams - 2000 participants – 36000 proposed solutions

What is Machine Learning

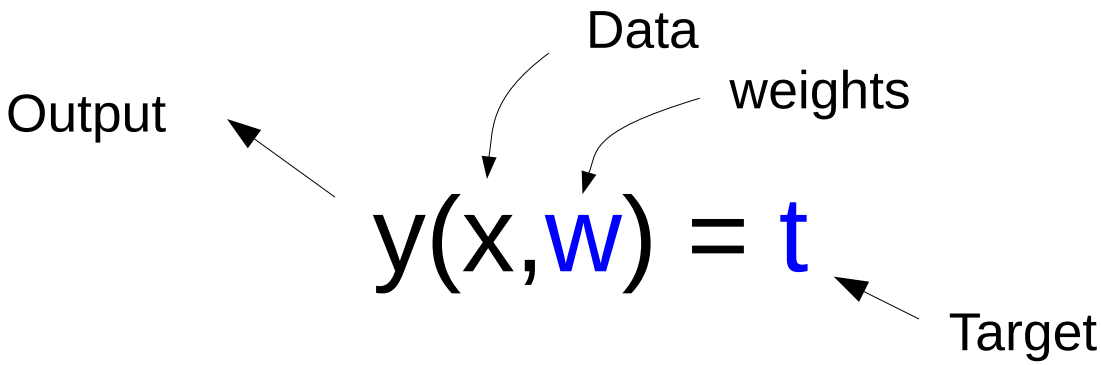


x: input **data** of (multidimensional) variables

y(x): **output** (multidimensional) values

where y is determined by “machine”

What is Machine Learning



Training phase

Input data generally consist of a set of:

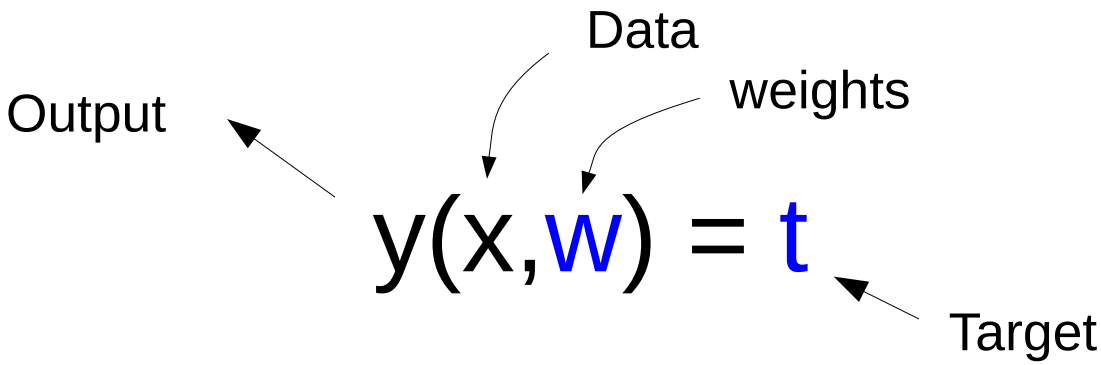
- x_i: known input **features (or variables)**
- t_i: known **target** values **(or label)**

→ **Learn y(x) to reproduce t: determine weights w**

Testing

determine **y** (therefore **t**) for a any new set of **x** values

What is Machine Learning



Examples

- **X** = {age, year, education, …} → **t**: income
- **X** = {image pixel values} → **t**: face recognition
- **X** = {list of words} → **t**: spam detection
- **X** = {E, p, …} → **t**: particle detection

...

Type of learning

Supervised learning

- Given: **training data** and **labels** (i.e type of data)
- **Training** and **testing** phases, generalization

→ Regression, classification ...

Unsupervised learning

- Given: **training data** and **no label**

→ Clustering, dimensionality reduction, ...

Semi-supervised learning

- A **mix** of the above, ex: training data + few labels

Variants

- Reinforcement learning (learn by trial and errors)
- Representation learning / Deep learning
- ...

Regression

Given **training data** $\{x_i,t_i\}$, **learn** a function y(x) to predict t given x.

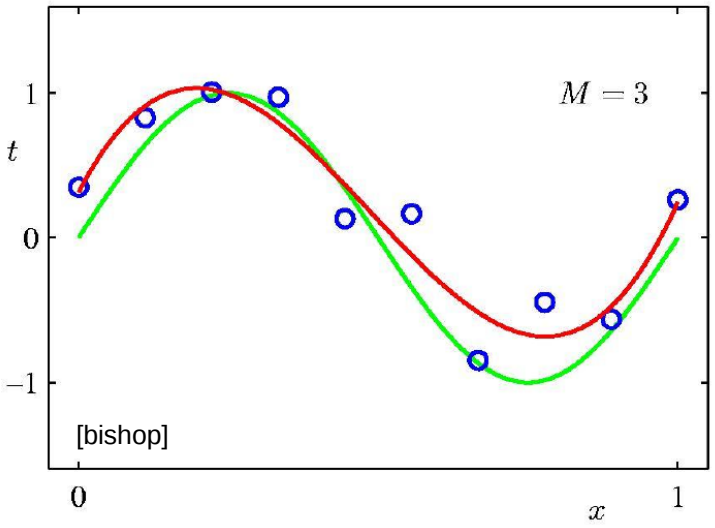
Output **y** consists of one (or more) **continuous** variables → **Regression**

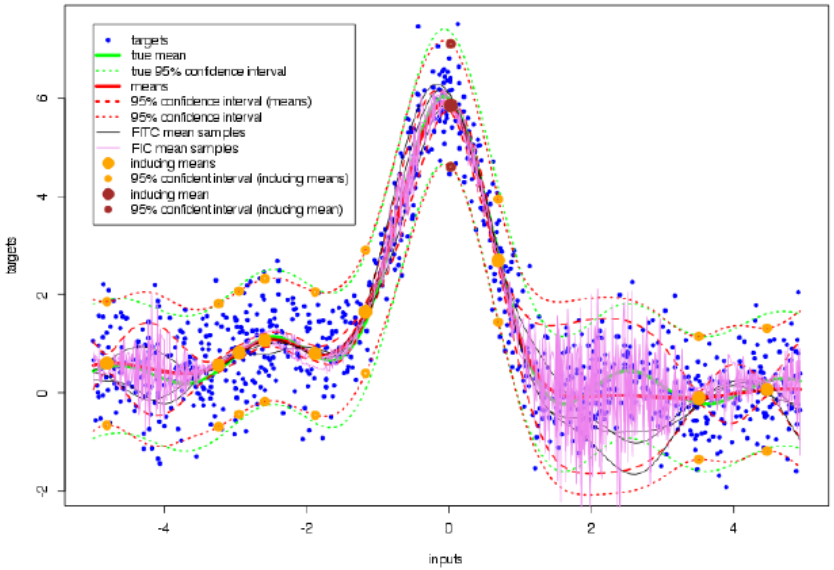
- Ex: linear regression: data is fit with a **linear** function of **weights**

$$y(x; w_1, .., w_M) = \sum_{i=1}^{M} w_i h_i(x)$$

w_i: **weights** (coefficients)

$h_i(x)$: **any** function of x

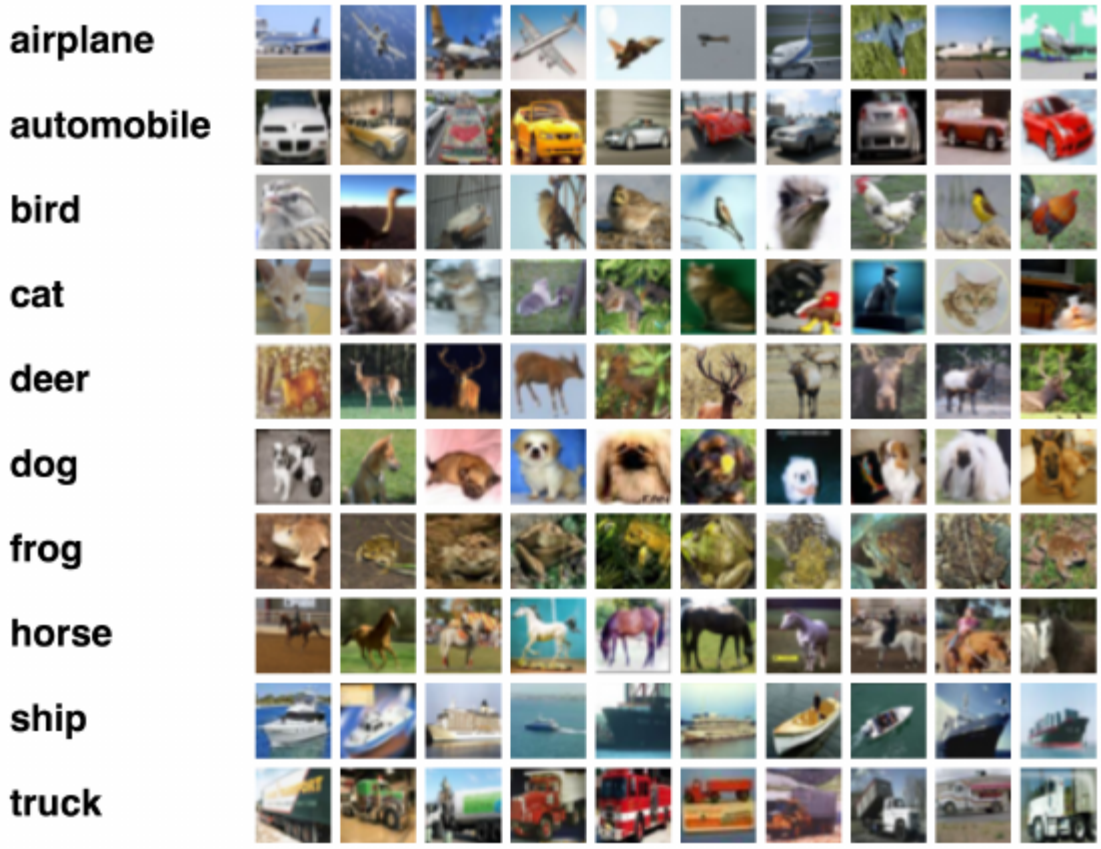




Classification

Given **training data** $\{x_i, t_i\}$, **learn** a function y(x) to predict t given x.

Output **y** consists of one (or more) **categories** → **Classification**



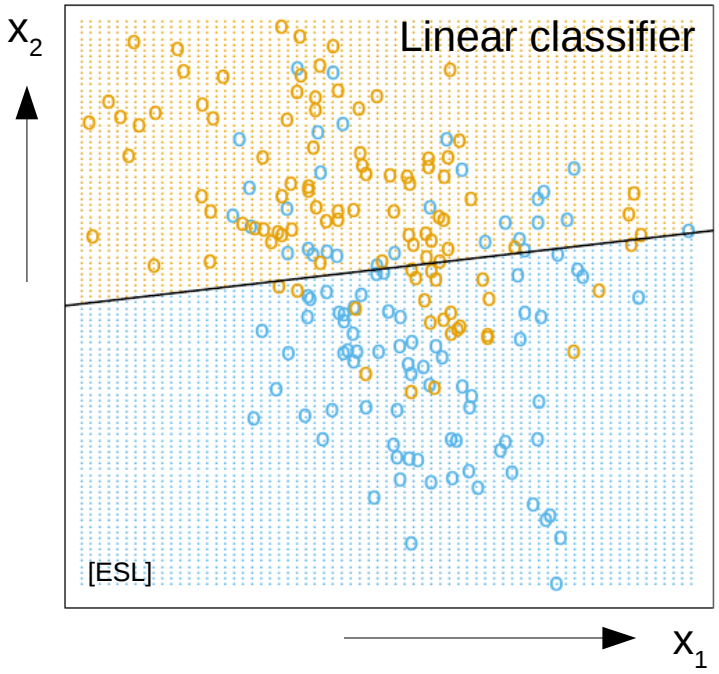
Classification

Given **training data** $\{x_i,t_i\}$, **learn** a function y(x) to predict t given x.

Output **y** consists of one (or more) **categories** → **Classification**

Example (2D):

Data coded as a binary variable (BLUE = 0, ORANGE = 1), and then fit by a function.



$$\begin{cases} y(x_1,x_2) > 0.5 \rightarrow \text{ORANGE} \\ y(x_1,x_2) < 0.5 \rightarrow \text{BLUE} \end{cases}$$

Boundary: $y(x_1,x_2) = 0.5$

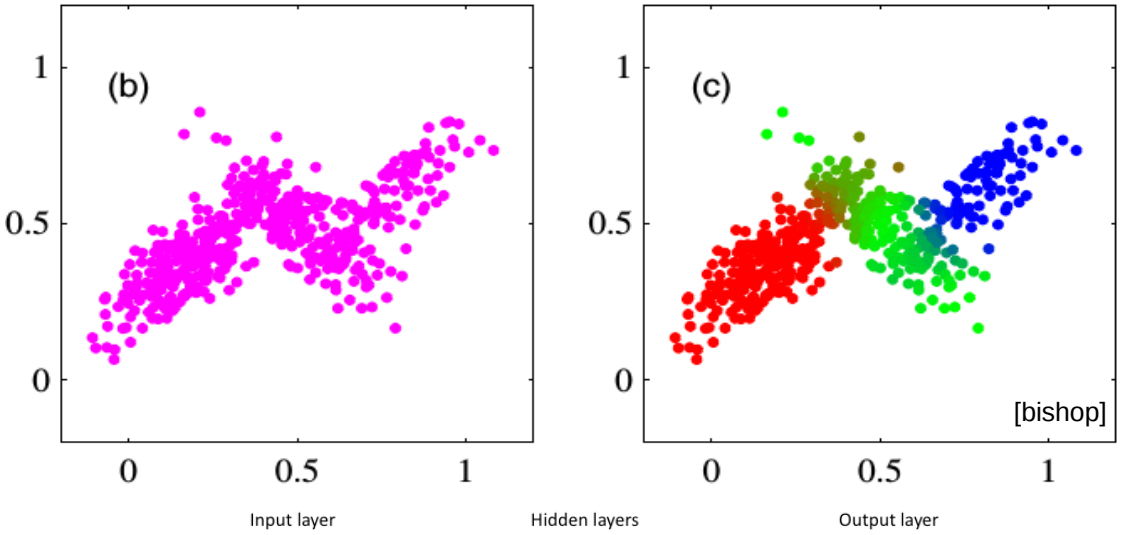
Orange shaded region: space classified as ORANGE

Blue region: space classified as BLUE.

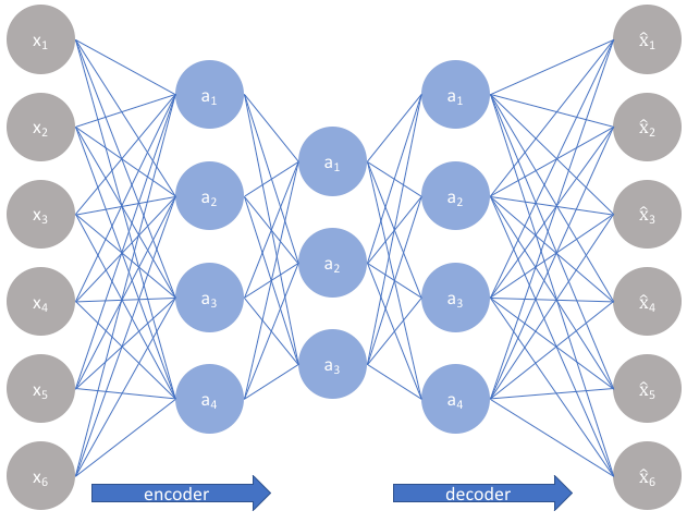
Unsupervised learning

Unsupervised learning = no labels

Clustering

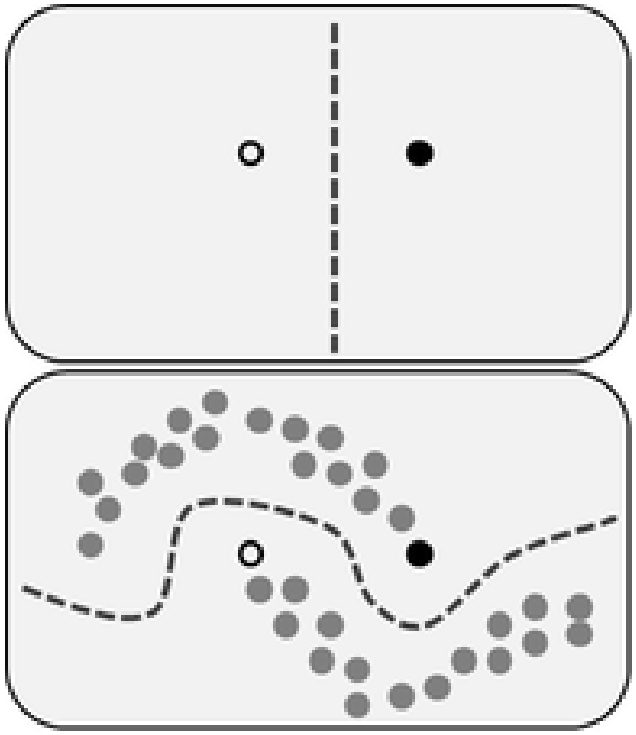


Dimensionality reduction



Semi-supervised learning

Semi-supervised learning = unlabelled data + few labels



[wikipedia]

Example of the influence of unlabelled data in semi-supervised learning.

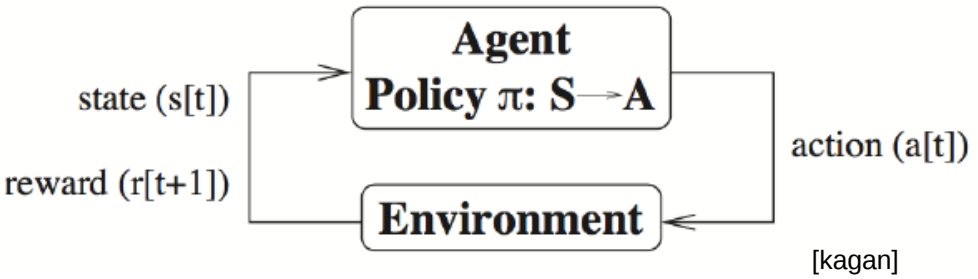
The unlabelled data (grey dots) influence the separation of the two classes (decision surface)

Reinforcement learning

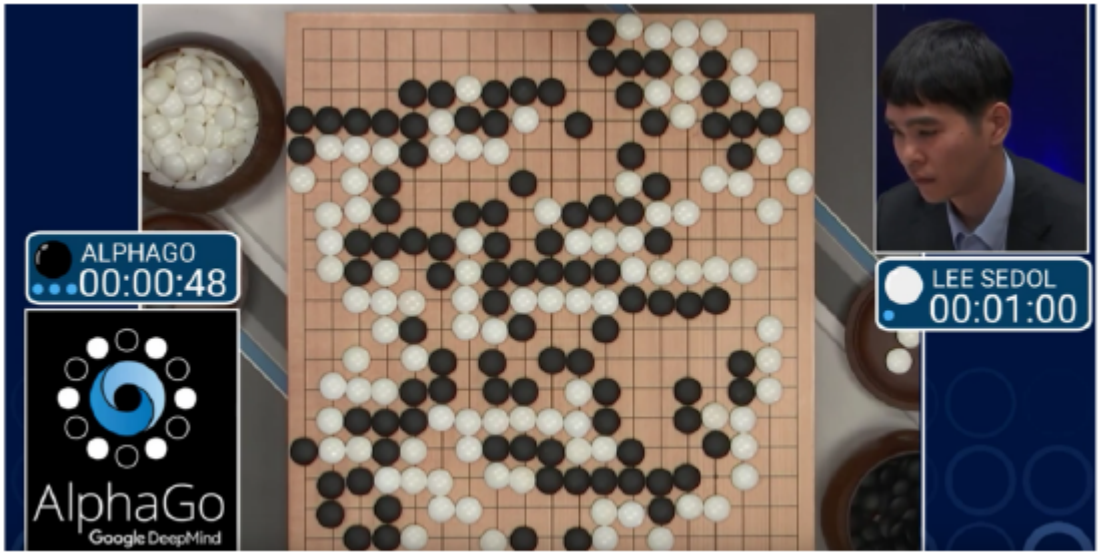
Model for **agents** that take **actions** depending on current **state**

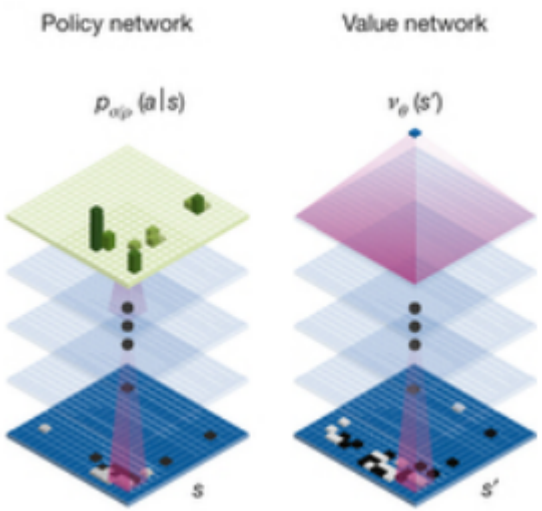
Action imply **reward** and modify state

Learn to make best sequences of **decisions**.



[kagan]





Nature 529, 484–489 (28 January 2016)

Representation learning

Representation is how we present the information (data) to solve a problem

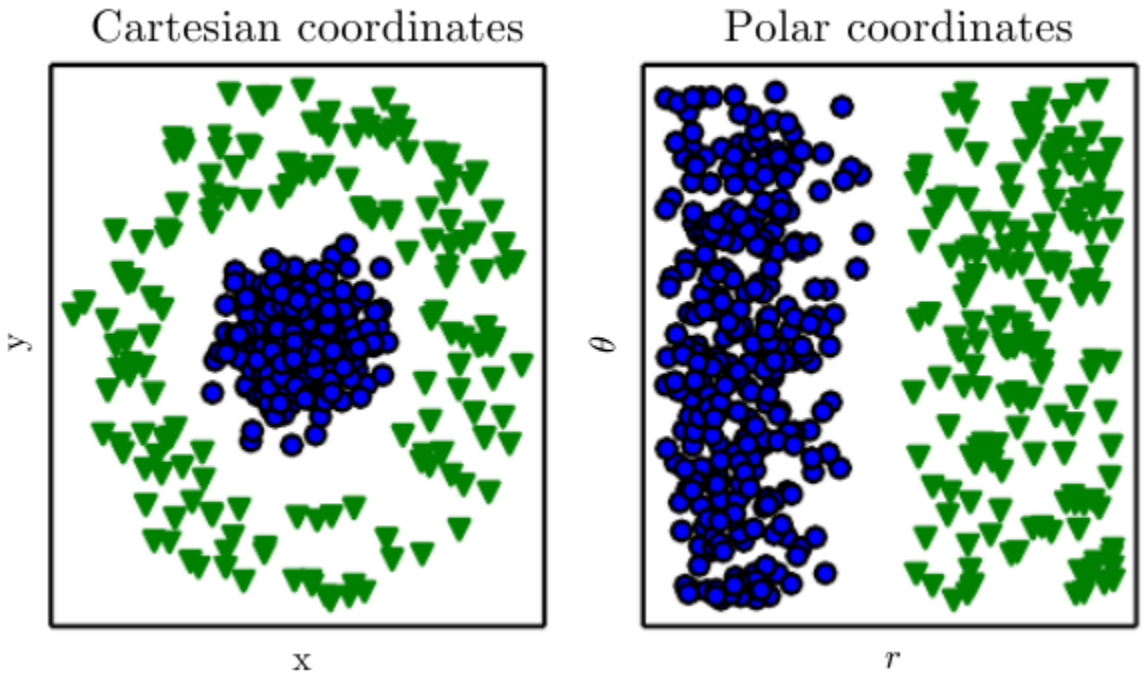
Example: what is the best number representation to perform this division ?

Decimal	121 : 11
Roman	CXXI / XI
Binary	1111001 : 1011
Hex	79 : B
ASCII	y : VT

Representation learning

Representation is how we present the information (data) to solve a problem

Example: what are the best coordinates to separate this data ?



[deeplearningbook]

Representation learning

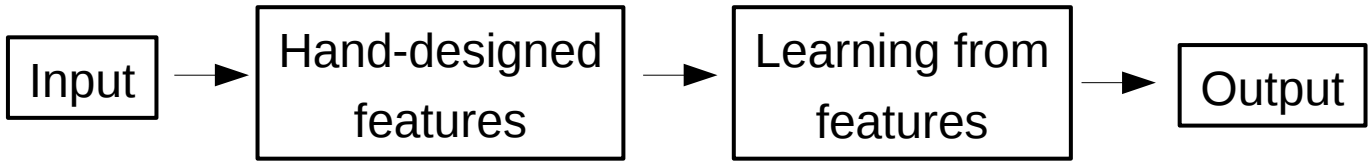
Representation is how we present the information (data) to solve a problem

For ML a good representation is one that makes the **learning task easier**

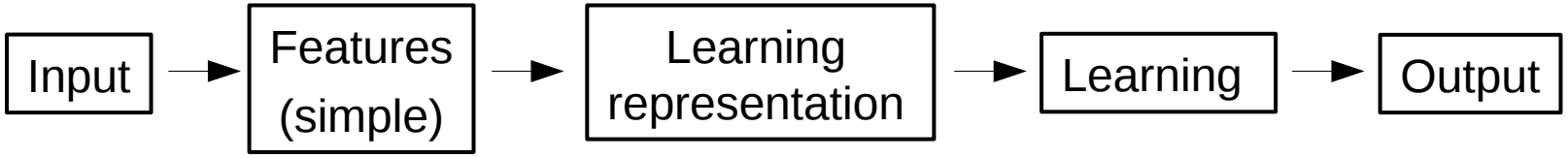
ML algorithms can also learn best representation: **representation learning**

→ Central to **deep learning** : learn complex representation from simpler ones

Classic ML

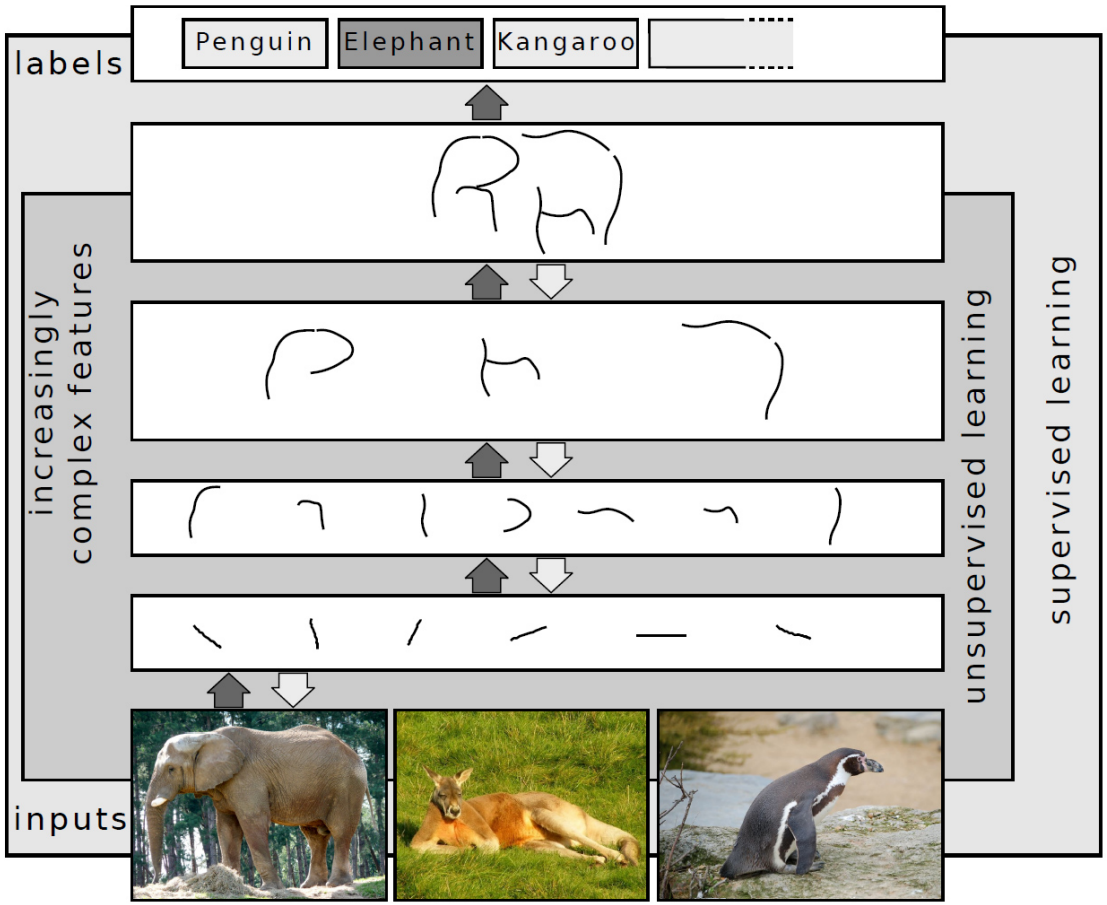


Deep learning



Deep learning

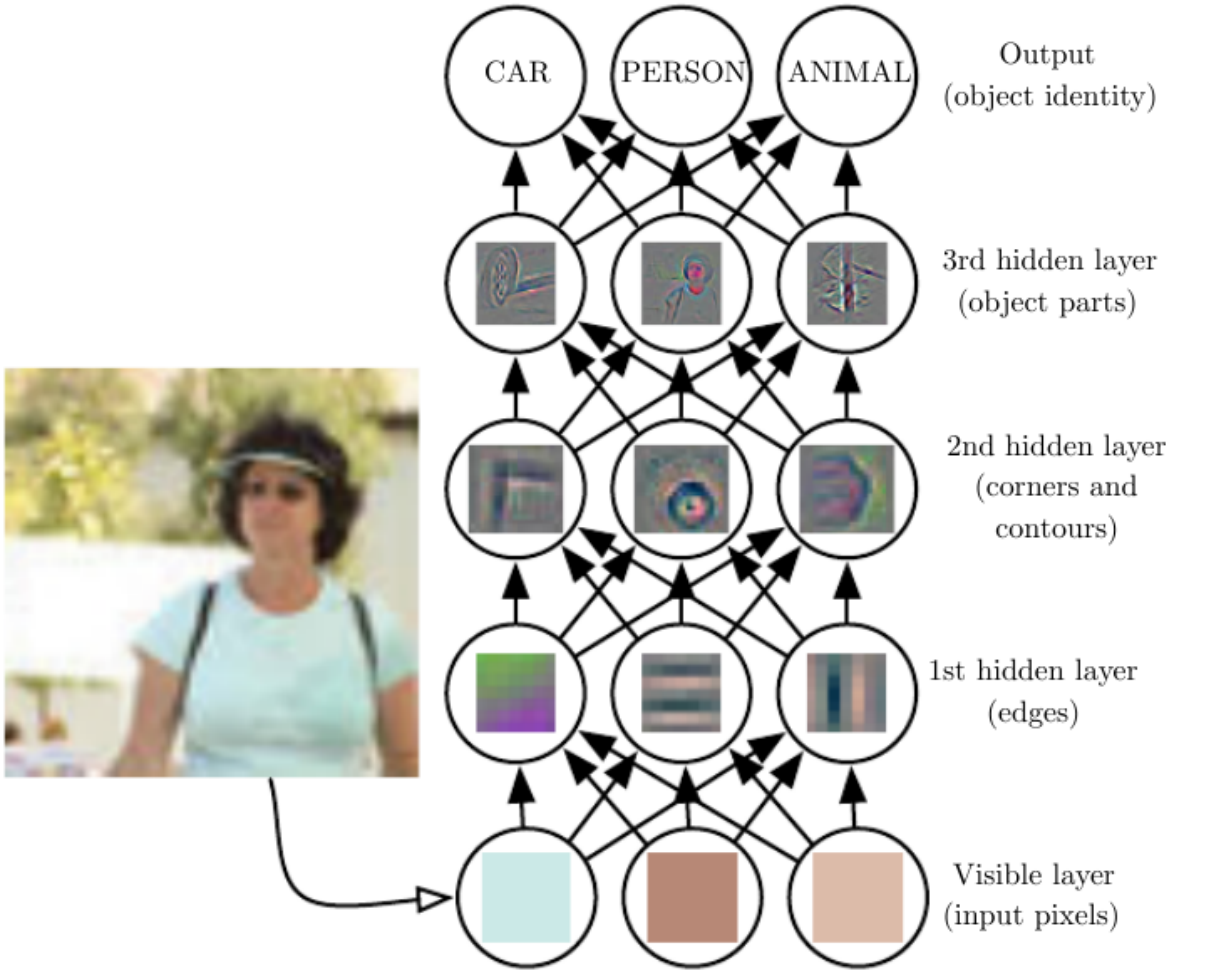
Class of **ML algorithms** (in general artificial neural networks) that use **multiple layer** to **extract higher level features** from raw data



[wikipedia]

Deep learning

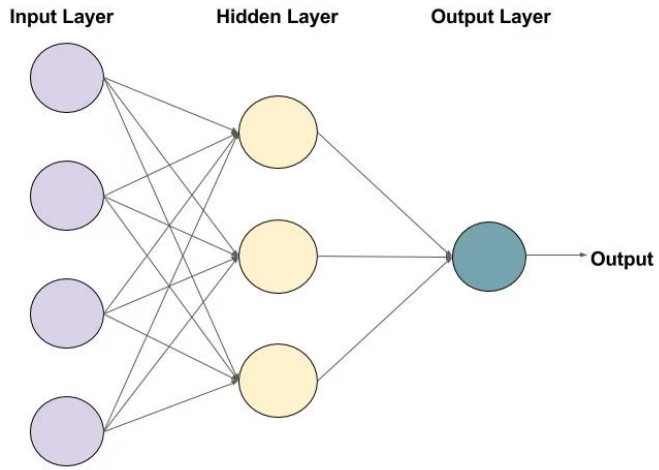
Class of **ML algorithms** (in general artificial neural networks) that use **multiple layer** to **extract higher level features** from raw data

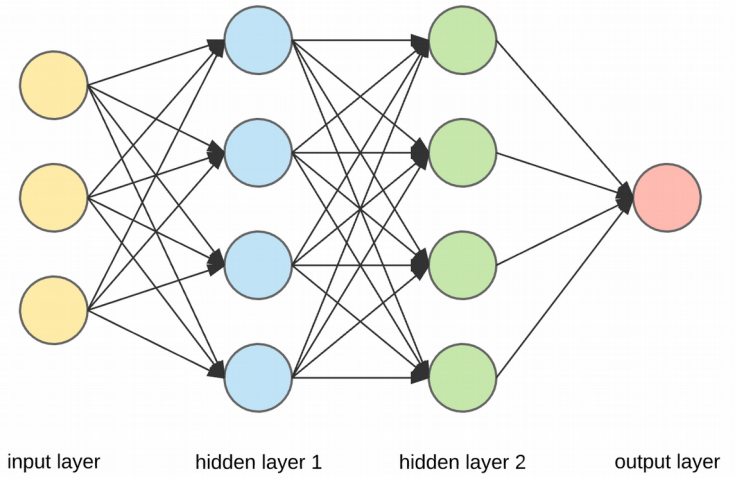


[deeplearningbook]

Shallow Neural Networks

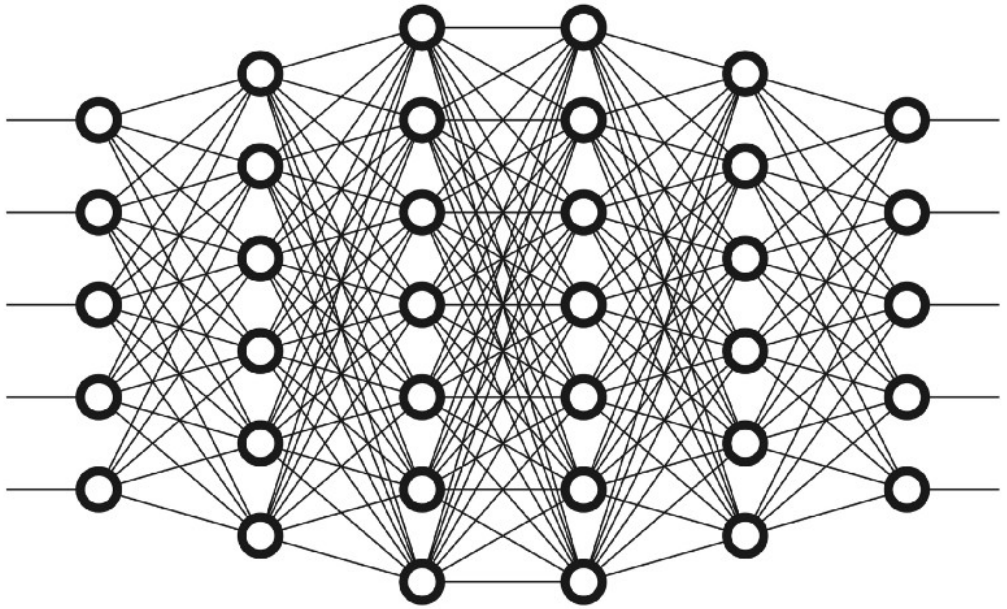
(1 or 2 hidden layers)



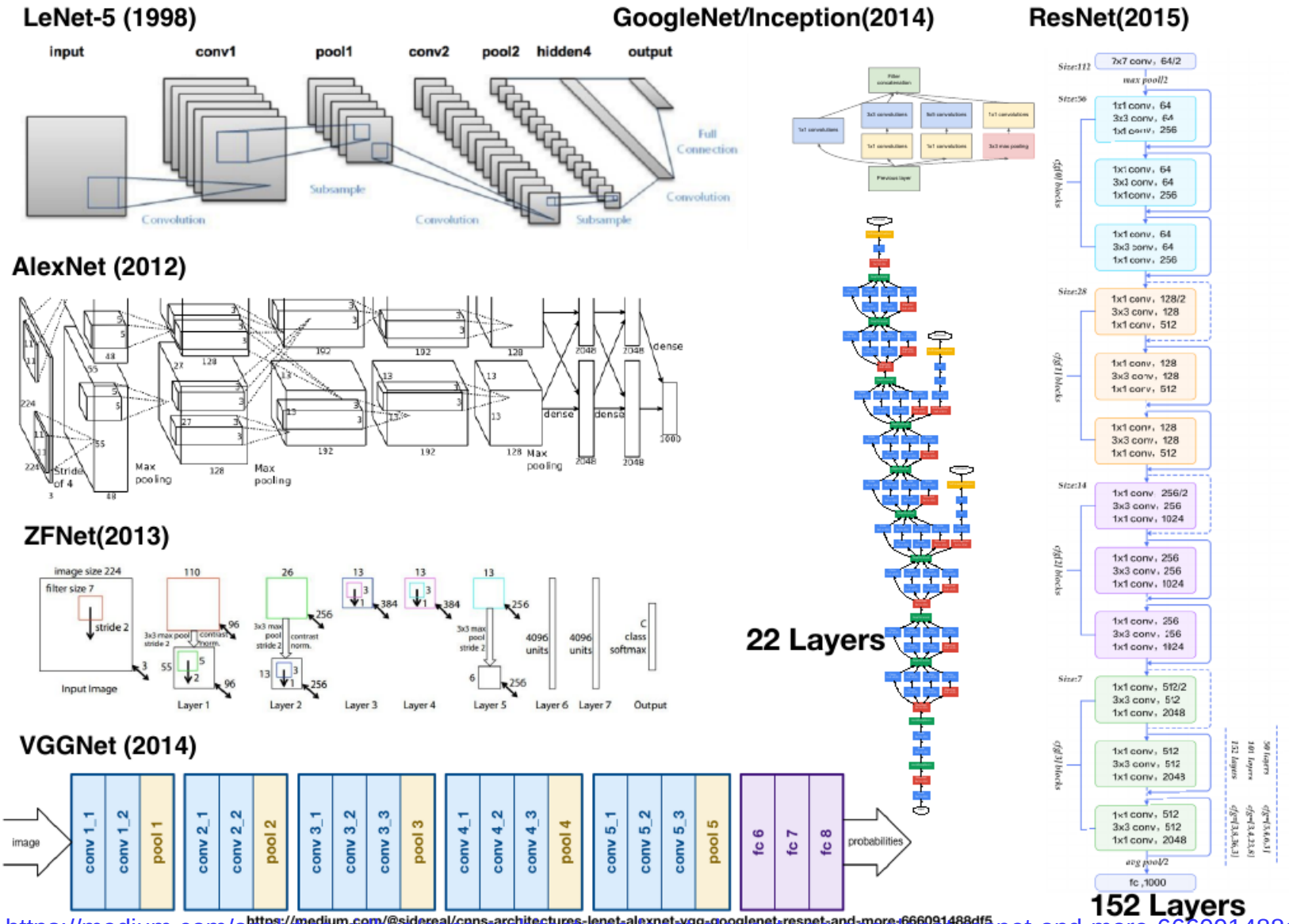


Deep Neural Network

(more layers)



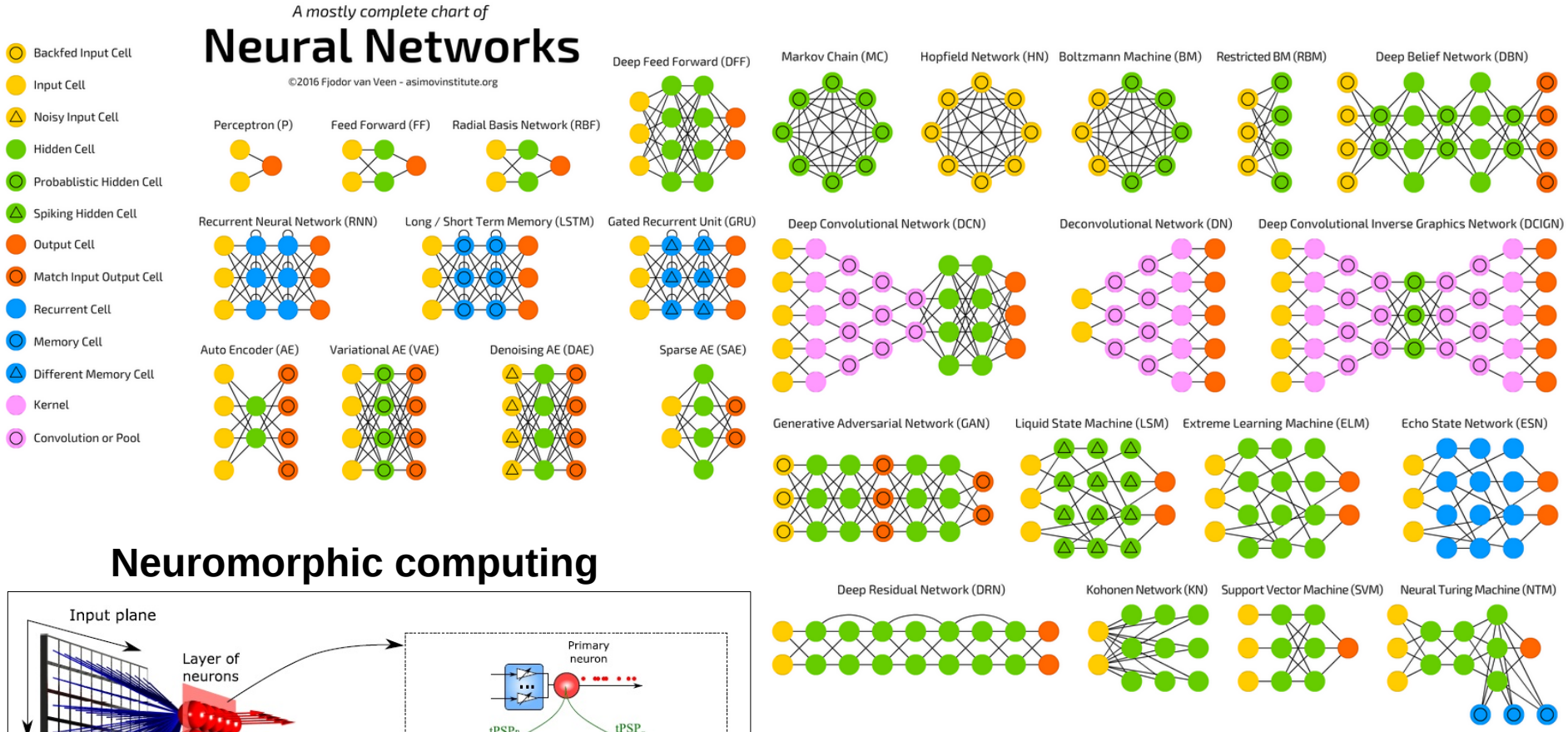
Deep Learning



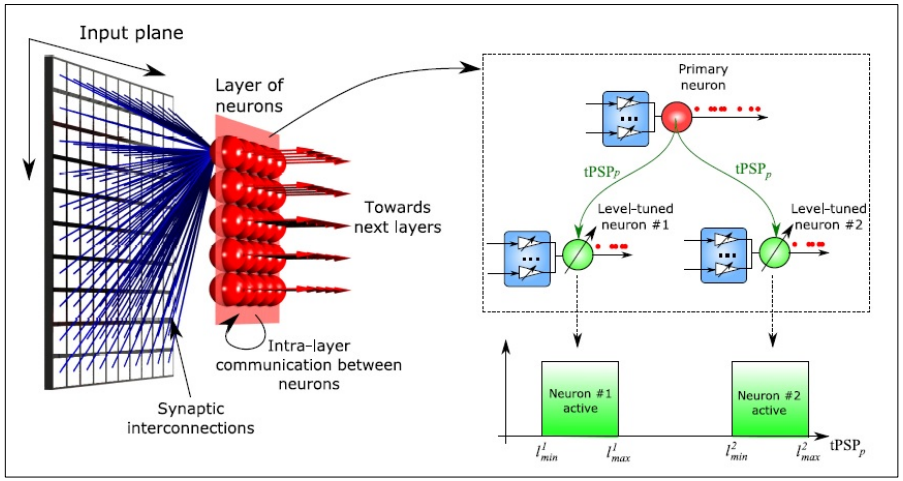
https://medium.com/@sidereal/cnns-architectures-lenet-alexnet-vgg-googlenet-resnet-and-more-666091488df5

https://medium.com/analytics-vidhya/cnns-architectures-lenet-alexnet-vgg-googlenet-resnet-and-more-666091488df5

Neural Networks today

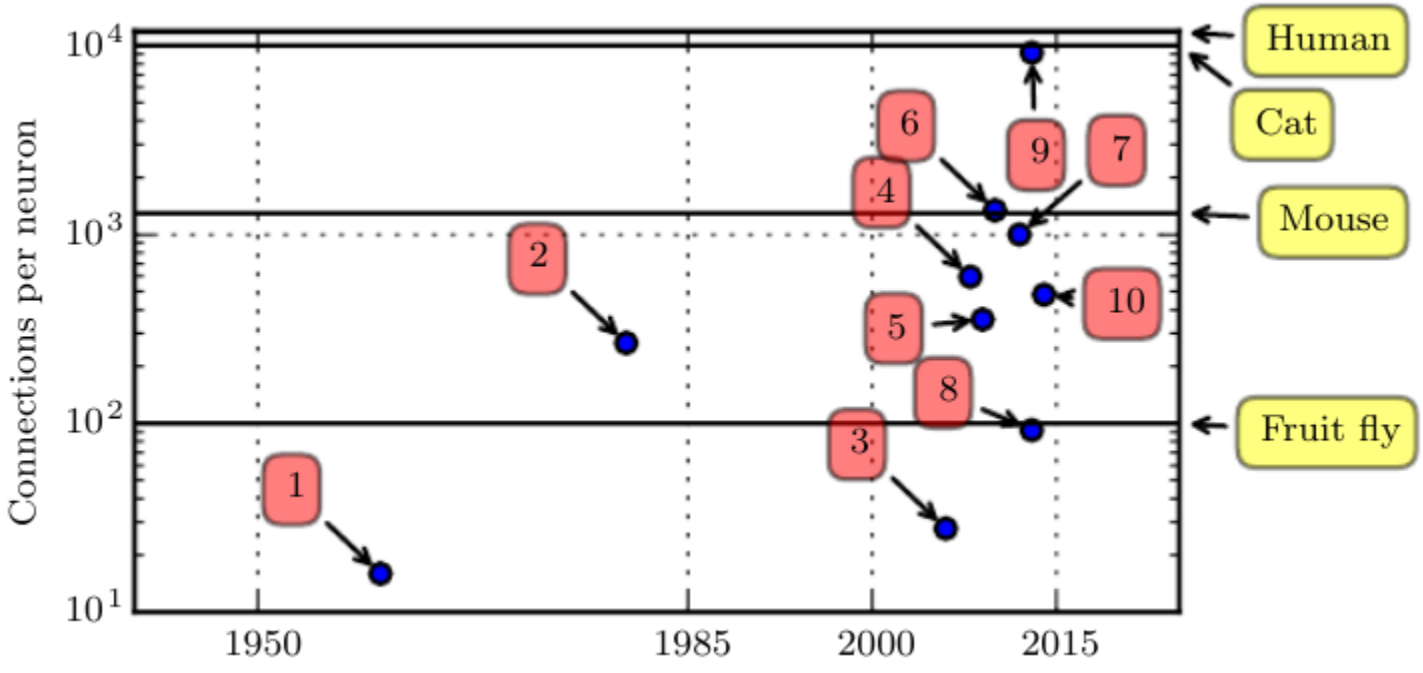


Neuromorphic computing



http://www.asimovinstitute.org/neural-network-zoo/

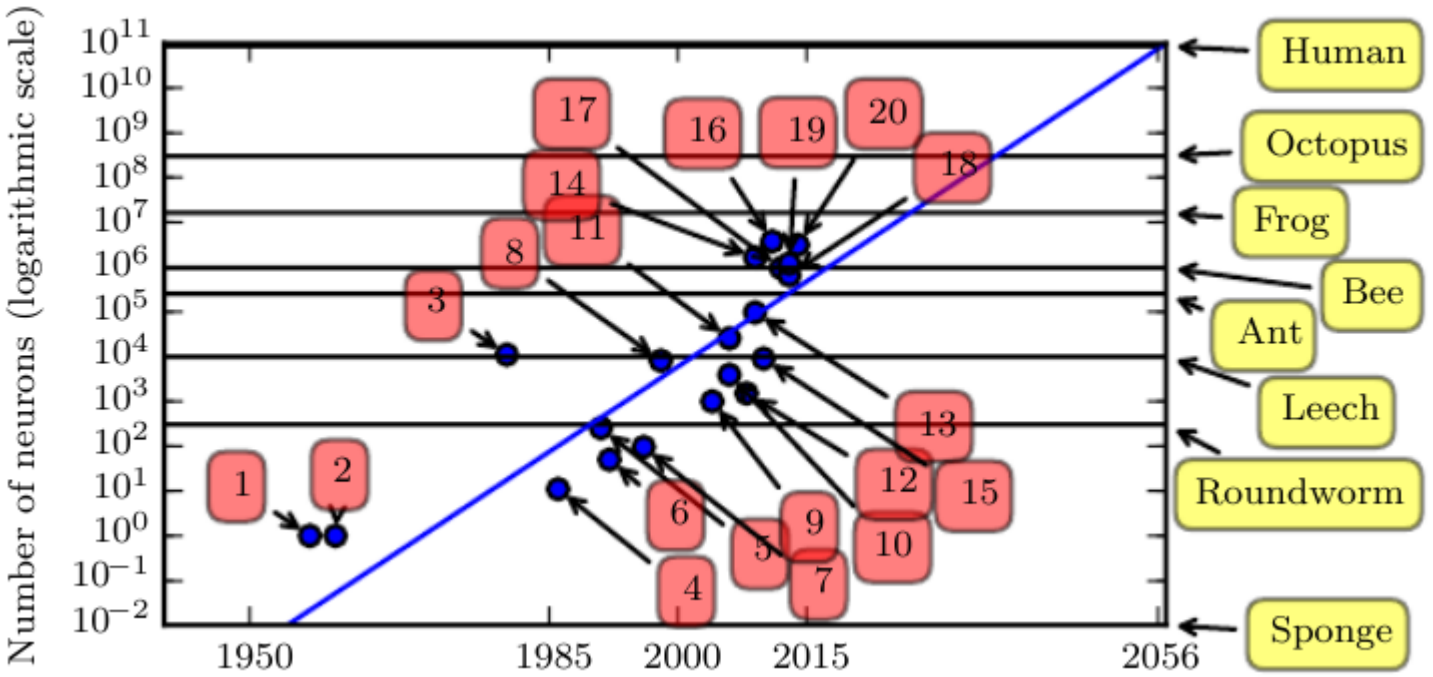
Connections per neuron



[deeplearningbook]

1. Adaptive linear element (Widrow and Hoff, 1960)
2. Neocognitron (Fukushima, 1980)
3. GPU-accelerated convolutional network (Chellapilla et al., 2006)
4. Deep Boltzmann machine (Salakhutdinov and Hinton, 2009a)
5. Unsupervised convolutional network (Jarrett et al., 2009)
6. GPU-accelerated multilayer perceptron (Ciresan et al., 2010)
7. Distributed autoencoder (Le et al., 2012)
8. Multi-GPU convolutional network (Krizhevsky et al., 2012)
9. COTS HPC unsupervised convolutional network (Coates et al., 2013)
10. GoogLeNet (Szegedy et al., 2014a)

Number of neurons



[deeplearningbook]

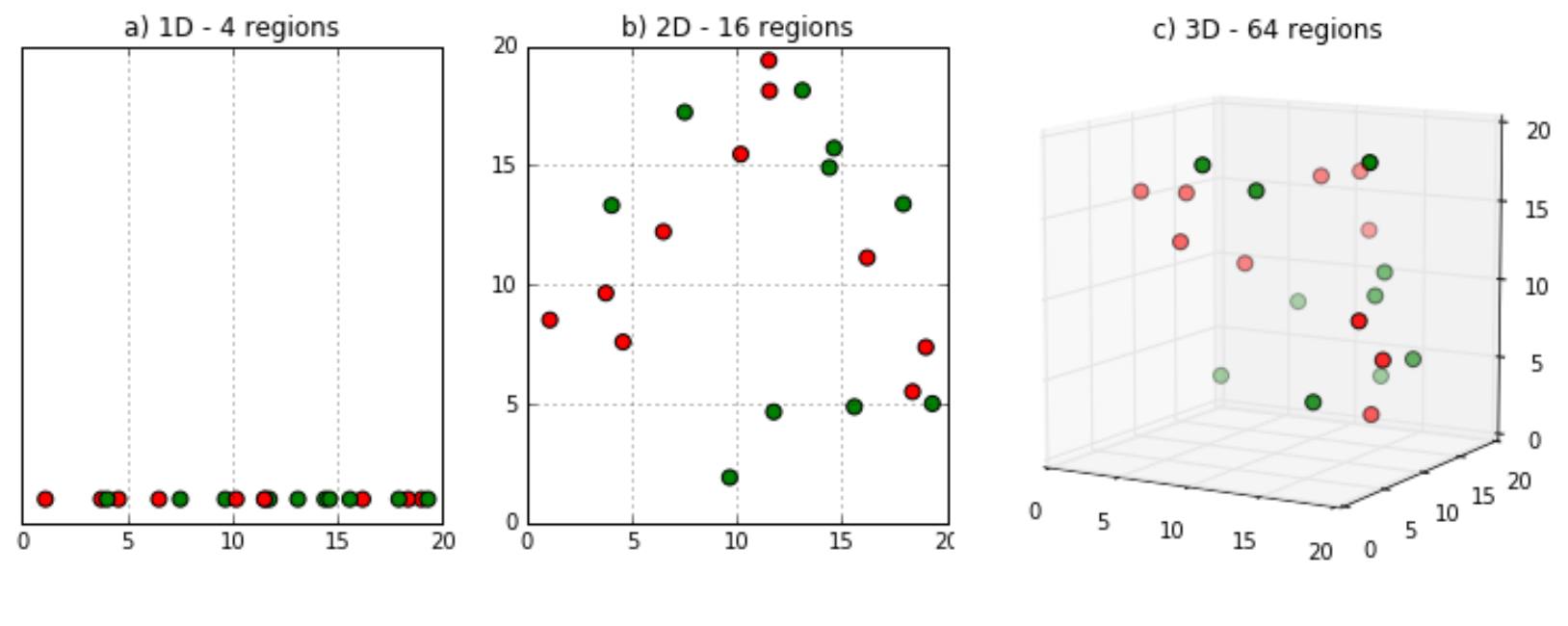
1. Perceptron (Rosenblatt, 1958, 1962)
2. Adaptive linear element (Widrow and Hoff, 1960)
3. Neocognitron (Fukushima, 1980)
4. Early back-propagation network (Rumelhart et al., 1986b)
5. Recurrent neural network for speech recognition (Robinson and Fallside, 1991)
6. Multilayer perceptron for speech recognition (Bengio et al., 1991)
7. Mean field sigmoid belief network (Saul et al., 1996)
8. LeNet-5 (LeCun et al., 1998b)
9. Echo state network (Jaeger and Haas, 2004)
10. Deep belief network (Hinton et al., 2006)
11. GPU-accelerated convolutional network (Chellapilla et al., 2006)
12. Deep Boltzmann machine (Salakhutdinov and Hinton, 2009a)
13. GPU-accelerated deep belief network (Raina et al., 2009)
14. Unsupervised convolutional network (Jarrett et al., 2009)
15. GPU-accelerated multilayer perceptron (Ciresan et al., 2010)
16. OMP-1 network (Coates and Ng, 2011)
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)

Limitations and difficulties

Deep learning algorithms are very efficient in many domains (in particular image recognition), but they require **a lot of data to train** because of large number of **dimensions** and high number of **hyperparameters.**

Illustration: the “curse of dimensionality

Simple example: classify each region depending on majority of labels



As dimensions grows, dimensions space increases exponentially.
Classification ok for ~2 variables, but fails at higher dimensions !

Limitations and difficulties

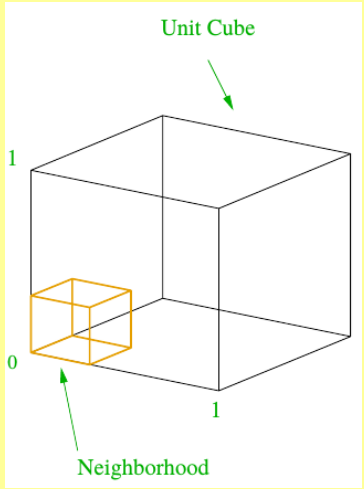
Deep learning algorithms are very efficient in many domains (in particular image recognition), but they require **a lot of data to train** because of large number of **dimensions** and high number of **hyperparameters.**

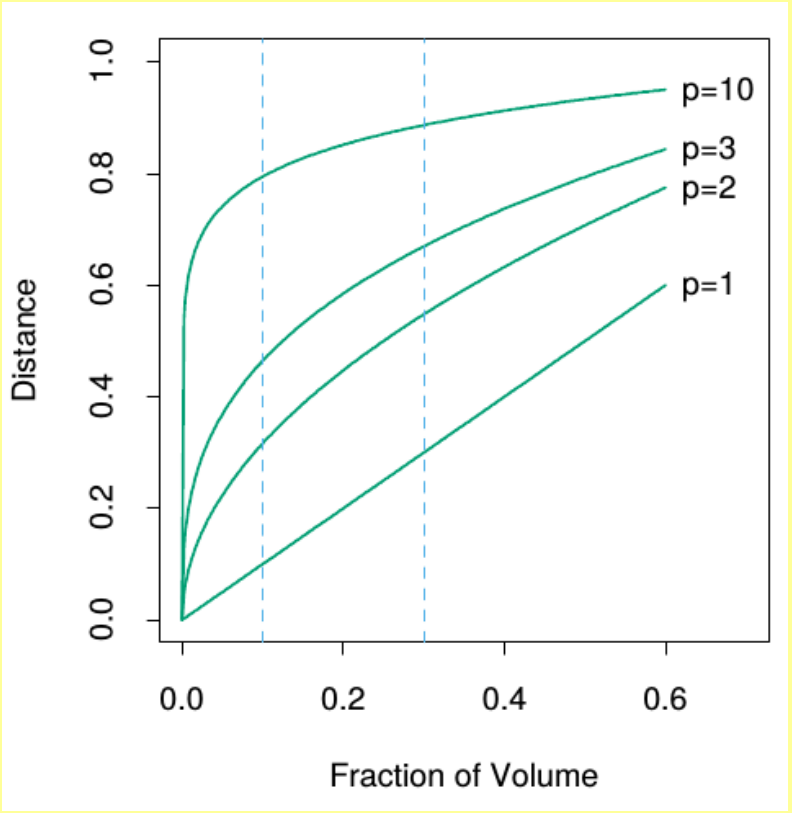
Illustration: the “curse of dimensionality

In a hypercube of length 1 and dimension **p** a fraction **r** of the volume corresponds to an edge length $\mathbf{e_p(r) = r^{1/p}}$

- p=10 and r=1%: $e_{10}(0.01)=0.63$
- p=10 and r=10%: $e_{10}(0.1)=0.80$

To contain 1% or 10% of the volume we must cover 63% or 80%, respectively, of the range of each input variable !





Limitations and difficulties

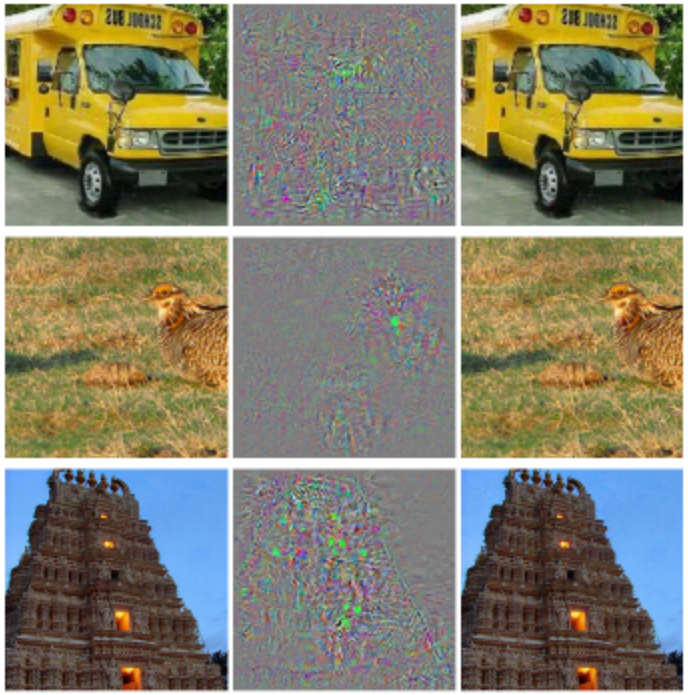
Algorithms get so **complex** that it is difficult to **interpret** what they really do !

Also their complexity can become a **weakness/threat**:

School bus

Bird
(partridge)

Temple



[arxiv:1312.6199]

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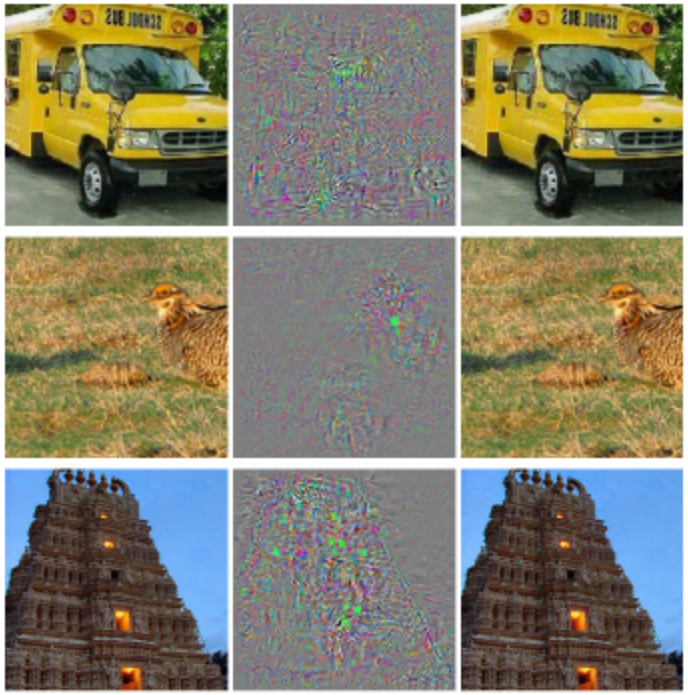
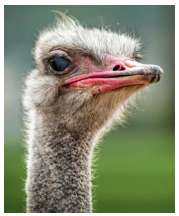


Ostrich !

Ostrich !

Ostrich !



?!

Perturbation

[arxiv:1312.6199]

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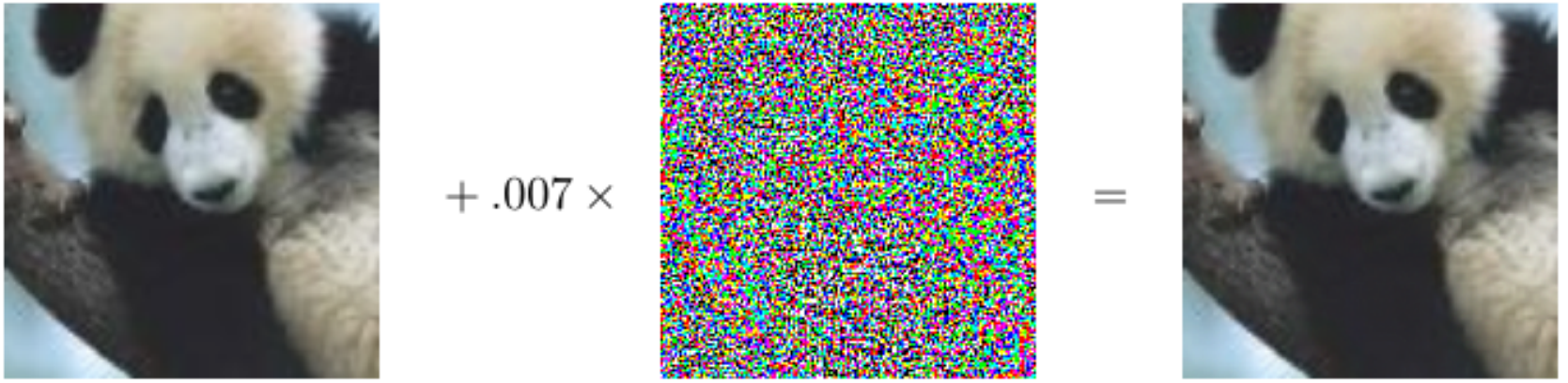

[arxiv:1412.6572]

Summary

Machine Learning is based on statistics and computing (and lots of data !)

Not new (‘40s) but field in **exponential evolution** since 10 years

Today: huge amount of **resources and tools** on the web

However real **understanding** of ML requires some efforts

Worth it because ML is becoming evermore present in our life’s