AI Research – Criteo AI Lab

An Introduction to Machine Learning

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INRAE Jan. 31st, 2022

CRITEO

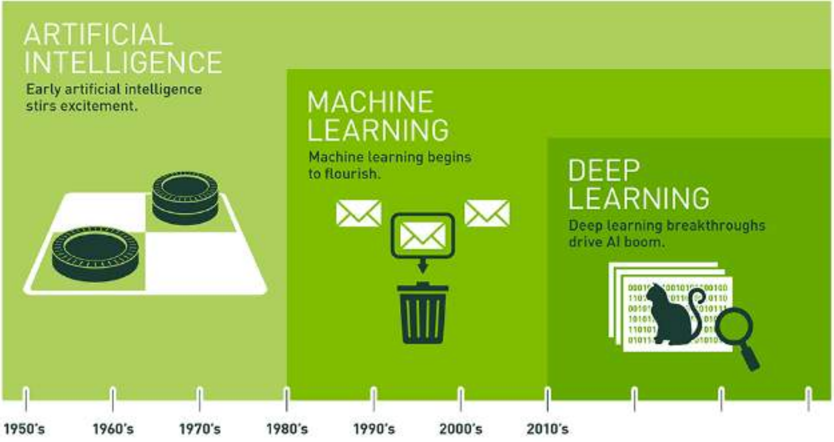
Outline

- Exordium -- captatio benevolentiae
  - AI, Machine Learning, Deep Learning
  - Machine Learning in our everyday life
  - Core goal in supervised learning: generalization
- Pivotal Advances (non Deep things)
  - Positioning
  - Warm-up: a first handcrafted classifier
  - Kernel methods: graceful methods
  - Adaboost: combining weak learners
  - Bandits: exploration vs. exploitation dilemma
- Pivotal advances (deep stuff)
  - Perceptron: travelling in time (1958--)
  - Multilayer Perceptron, Feedforward Neural Netwokrs: longstanding models
  - Unsupervised / Generative models
- Two success stories
  - AlphaGo (Silver et al. 2016)
  - AlphaFold (Jumper et al, Nature 2021)
- Conclusion

Outline

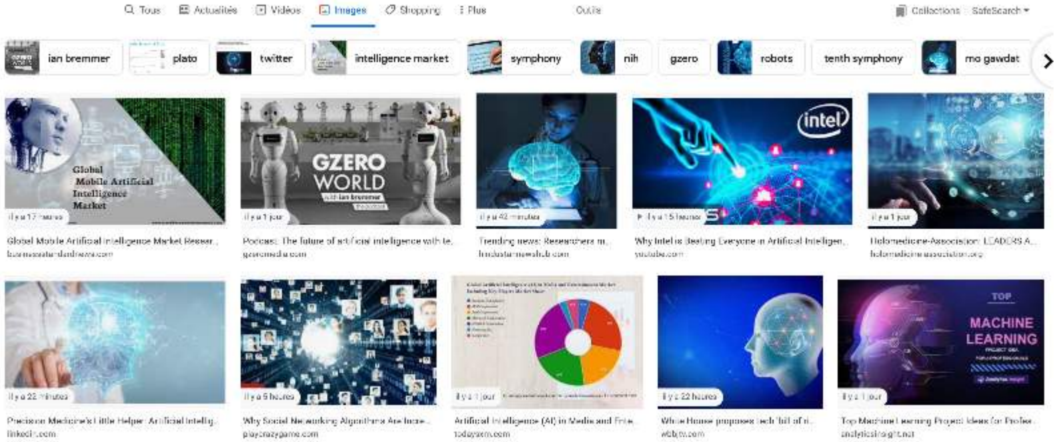
AI, Machine Learning, Deep Learning

Today: data, software, computing power



Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

In the news... as of Oct. 10th, 2021



Annotation/Image decoding

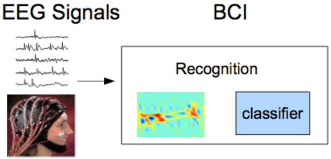
(from Farabet et al, 2013)

P300 Speller

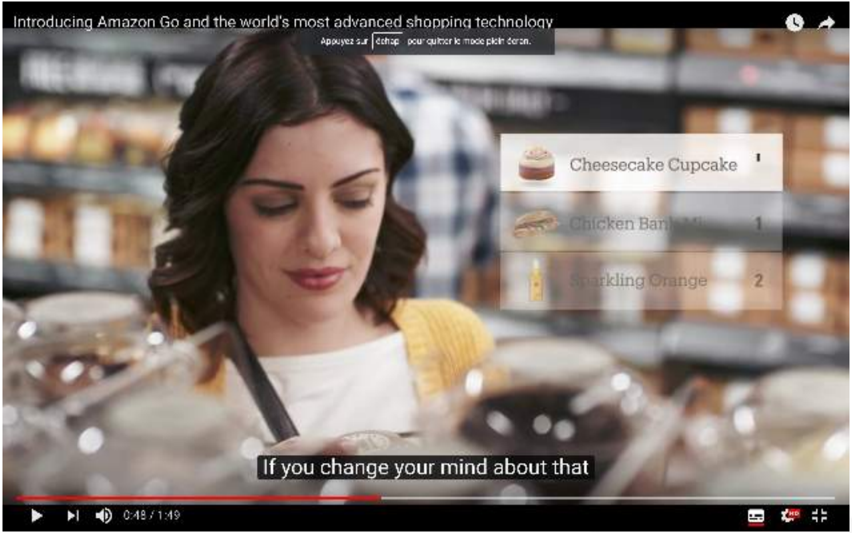
Vintage P300 Speller

(from Breaking bad)

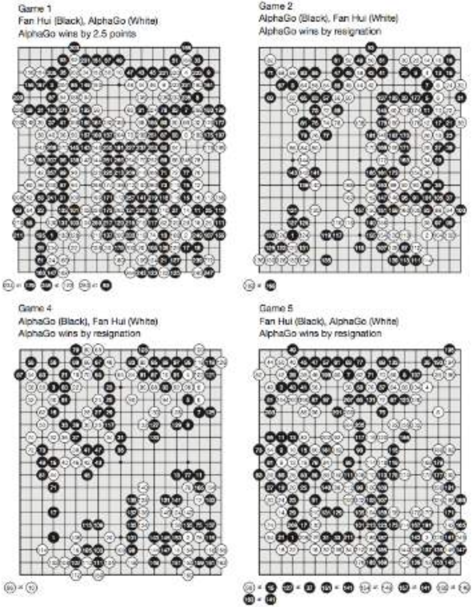
Modern P300 Speller (pictures from A. Rakotomamonjy, video from Robo Doc)



ML-cashing Amazon shops

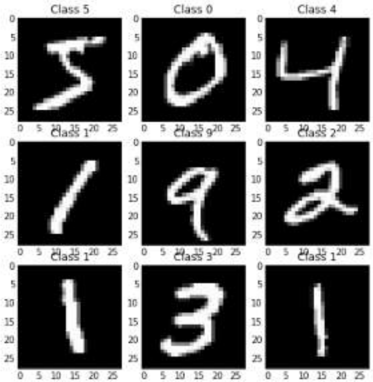


AlphaGo (Silver et al. 2016)

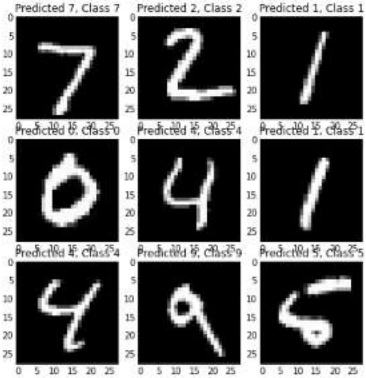


Core goal in supervised learning: generalization

Training set



Test set

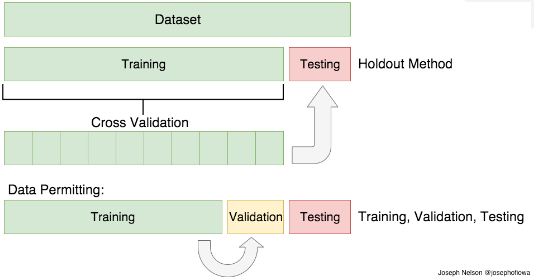


(from Keras Mnist Tutorial)

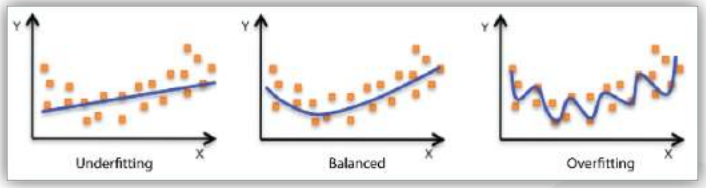
Generalization: from the training set to beyond

Design algorithms capable from pairs (measure, target), to create a predictors which, given a measure, estimates the corresponding target

Core goal in supervised learning: generalization... in practice



(from Train/Test Split and Cross Validation in Python)

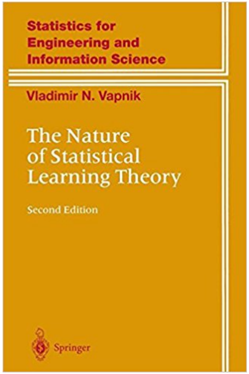


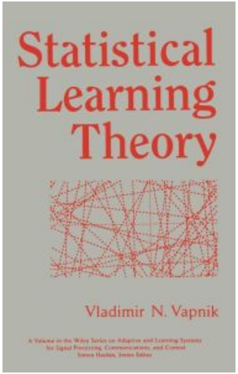
(from Amazon AWS)

Outline

Positioning

V. Vapnik sets, at the end of the 70's, the mathematical basis of machine/statistical learning, at the intersection of computer science, statistics, and optimization

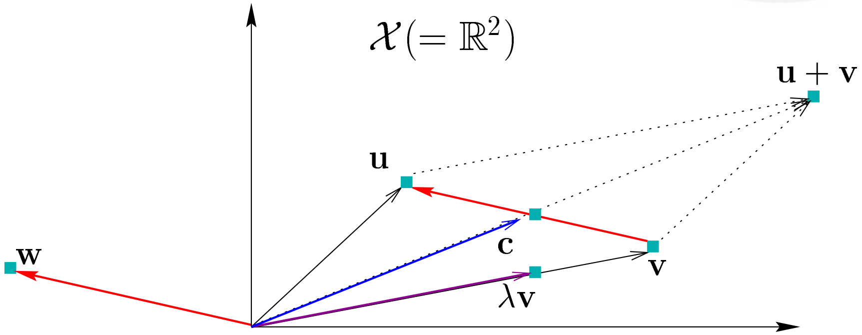




"ML is the study of computer algorithms that improve automatically through experience."

T. Mitchell, 1997

Warm-up: a first handcrafted classifier



- $\mathbf{u}, \mathbf{v}, \mathbf{w}, \mathbf{c}$ are vectors
- $\mathbf{w} = \mathbf{u} - \mathbf{v}$ (red arrows)
- $\mathbf{c} = \frac{1}{2}(\mathbf{u}+\mathbf{v})$
- Here: $0 < \lambda < 1$

Warm-up: a first handcrafted classifier

Inner product $\langle \cdot, \cdot \rangle : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$

- symmetric: $\langle \mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle$
- bilinear: $\langle \lambda \mathbf{u}_1 + \gamma \mathbf{u}_2, \mathbf{v} \rangle = \lambda \langle \mathbf{u}_1, \mathbf{v} \rangle + \gamma \langle \mathbf{u}_2, \mathbf{v} \rangle$
- positive: $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0$
- definite: $\langle \mathbf{u}, \mathbf{u} \rangle = 0 \Rightarrow \mathbf{u} = 0$

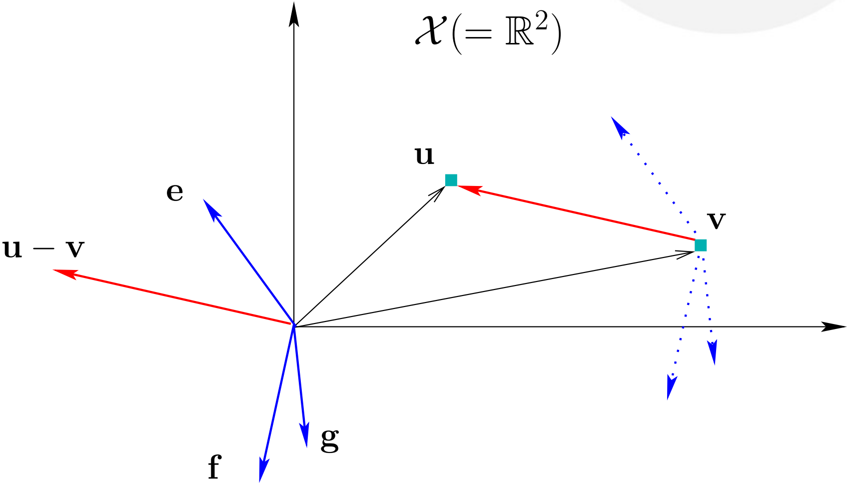
Inner product

- provides $\mathcal{X}$ with a structure
- can be viewed as a 'similarity'
- defines a norm $\| \cdot \|$ on $\mathcal{X}$: $\|\mathbf{u}\| = \sqrt{\langle \mathbf{u}, \mathbf{u} \rangle}$

In $\mathbb{R}^2$

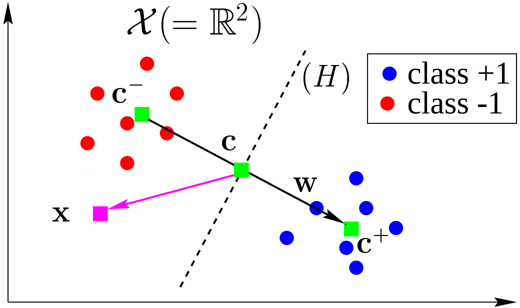
- $\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$, $\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$: $\langle \mathbf{u}, \mathbf{v} \rangle = u_1 v_1 + u_2 v_2$

Warm-up: a first handcrafted classifier



- $\langle \mathbf{u}-\mathbf{v}, \mathbf{e}\rangle > 0$: $\mathbf{u}-\mathbf{v}$ and $\mathbf{e}$ point to the 'same direction'
- $\langle \mathbf{u}-\mathbf{v}, \mathbf{f}\rangle = 0$: $\mathbf{u}-\mathbf{v}$ and $\mathbf{f}$ are orthogonal
- $\langle \mathbf{u}-\mathbf{v}, \mathbf{g}\rangle < 0$: $\mathbf{u}-\mathbf{v}$ and $\mathbf{g}$ point to 'opposite directions'

Warm-up: a first handcrafted classifier



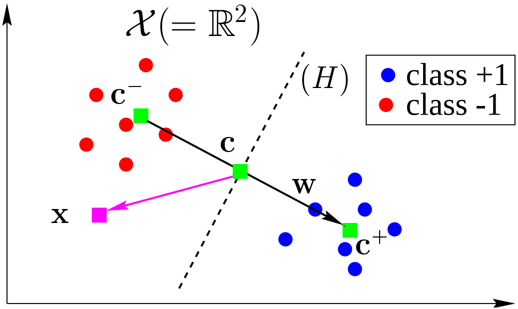
- $\mathbf{c}^+ = \frac{1}{n^+} \sum_{\{i: y_i = +1\}} \mathbf{x}_i$
- $\mathbf{c}^- = \frac{1}{n^-} \sum_{\{i: y_i = -1\}} \mathbf{x}_i$
- $\mathbf{c} = \frac{1}{2}(c^+ + c^-)$
- $\mathbf{w} = c^+ - c^-$

Decision function

Classify points $\mathbf{x}$ according to which of the two class means $\mathbf{c}^+$ or $\mathbf{c}^-$ is closer:

- for $\mathbf{x} \in \mathcal{X}$, it is sufficient to take the sign of the inner product between $\mathbf{w}$ and $\mathbf{x} - \mathbf{c}$
- if $h(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} - \mathbf{c} \rangle$, we have the classifier $f(\mathbf{x}) = \text{sign}(h(\mathbf{x}))$
- the (dotted) hyperplane (H), of normal vector $\mathbf{w}$, is the decision surface

Warm-up: a first handcrafted classifier



- $\mathbf{c}^+ = \frac{1}{n^+} \sum_{\{i: y_i = +1\}} \mathbf{x}_i$
- $\mathbf{c}^- = \frac{1}{n^-} \sum_{\{i: y_i = -1\}} \mathbf{x}_i$
- $\mathbf{c} = \frac{1}{2}(c^+ + c^-)$
- $\mathbf{w} = c^+ - c^-$

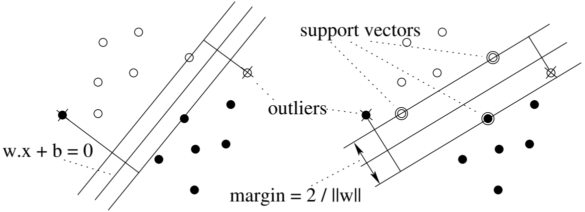
On evaluating $h(\mathbf{x})$

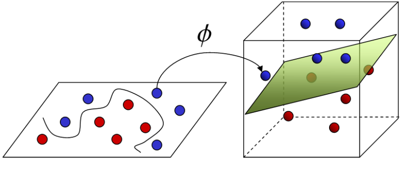
$$h(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} - \mathbf{c} \rangle = \langle \mathbf{w}, \mathbf{x} \rangle - \langle \mathbf{w}, \mathbf{c} \rangle = \ldots$$

$$= \sum_{i=1,\ldots,m} \alpha_i \langle \mathbf{x}_i, \mathbf{x} \rangle + b, \quad \text{with } b \text{ a real constant}$$

Inner products are sufficient (remember that)

Kernel methods: graceful methods

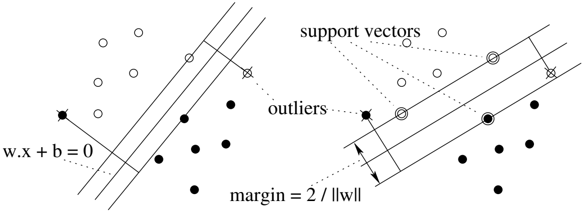


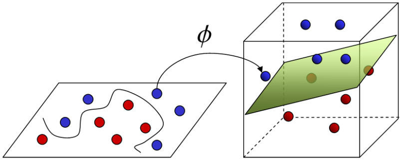


Silk methods

- Thereotical guarantees
- Convex optimization
- Nonlinearity handled through the kernel trick
- Success stories: structured data classification, ranking, scoring, theory

Kernel methods: graceful methods





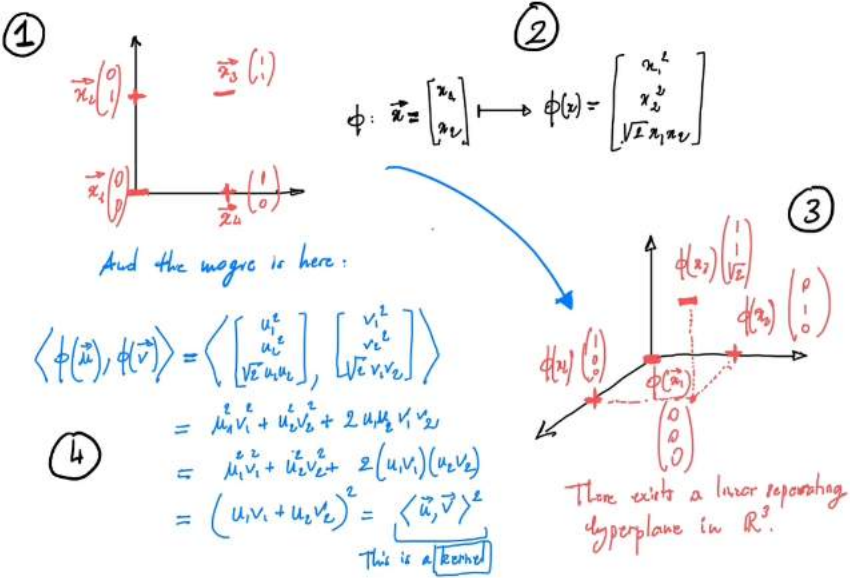
Kernelizing the handcrafted classifier

$h(\cdot) = \sum_{i=1,\ldots,m} \alpha_i \langle \mathbf{x}_i, \cdot \rangle + b$ simply turns into

$$h(\mathbf{x}) = \sum_{i=1,\ldots,m} \alpha_i \mathbf{k}(\mathbf{x}_i, \mathbf{x}) + b, \quad \text{with } b \text{ a real constant}$$

where $k(\cdot,\cdot)$ has replaced $\langle \cdot, \cdot \rangle$ and computes an inner product on the nonlinear embedding of its arguments

Example: 2nd degree polynomial kernel



Adaboost: combining weak learners

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in \mathscr{X}$, $y_i \in \{-1, +1\}$.
Initialize: $D_1(i) = 1/m$ for $i = 1, \ldots, m$.
For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.
- Get weak hypothesis $h_t : \mathscr{X} \to \{-1, +1\}$.
- Aim: select h_t with low weighted error:

$$\varepsilon_t = \Pr_{i \sim D_t}[h_t(x_i) \neq y_i].$$

- Choose $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\varepsilon_t}{\varepsilon_t}\right)$.
- Update, for $i = 1, \ldots, m$:

$$D_{t+1}(i) = \frac{D_t(i)\exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

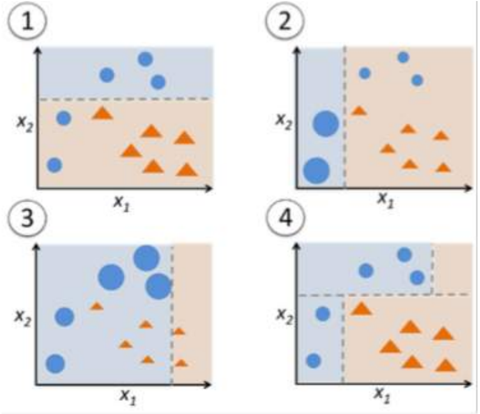
where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

Output the final hypothesis:

$$H(x) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right).$$

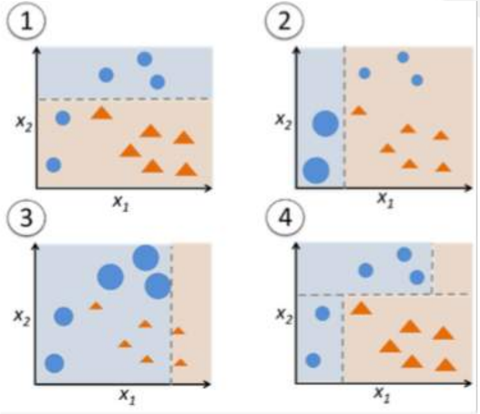
(from Freund and Schapire, 1997, 2012)

Adaboost: combining weak learners



(from Raschka, https://sebastianraschka.com/faq/docs/bagging-boosting-rf.html)

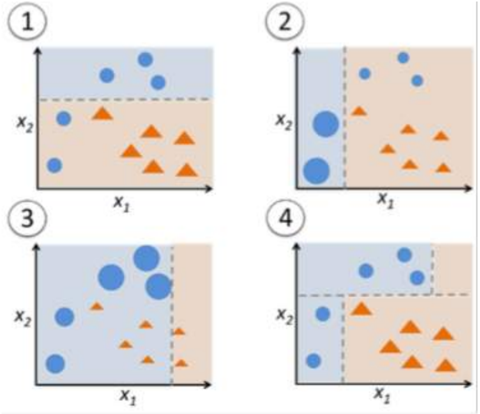
Adaboost: combining weak learners



(from Raschka, `https://sebastianraschka.com/faq/docs/bagging-boosting-rf.html`)

- Algorithmic simplicity, effectiveness
- Theoretical results
- Gödel price 2003

Adaboost: combining weak learners



(from Raschka, https://sebastianraschka.com/faq/docs/bagging-boosting-rf.html)

Find an illustrative example of Adaboost running

Bandits: exploration vs. exploitation dilemma

How to make the best use of your budget and bet?

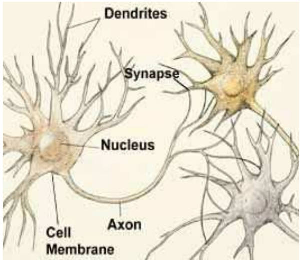
Features

- Problem easy to pose, many variations
- Exploration/exploitation dilemma
- Success stories: ad placement, recommendation, Go

Outline

Perceptron, binary case (Rosenblatt, 1958)

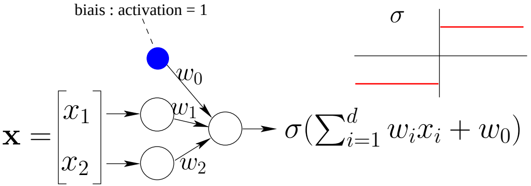
Inspiration: (real) neural networks



Biological motivations

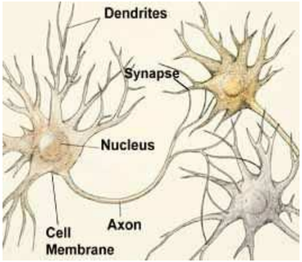
- Learning systems made of several simple computational units connected to each other
- Memory capacity / plasticity of these systems

Perceptron: a linear classifier, $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \{-1, +1\}$



Perceptron, binary case (Rosenblatt, 1958)

Inspiration: (real) neural networks



Biological motivations

- Learning systems made of several simple computational units connected to each other
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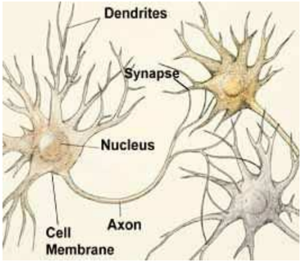
Perceptron: a linear classifier, $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \{-1, +1\}$

- Classifier parameters: $\mathbf{w} \in \mathbb{R}^d$
- Prediction of the classifier: $f(\mathbf{x}) = \text{sign}\langle \mathbf{w}, \mathbf{x} \rangle$
- Question: how to learn $\mathbf{w}$ from observations?

Perceptron, binary case (Rosenblatt, 1958)

Inspiration: (real) neural networks



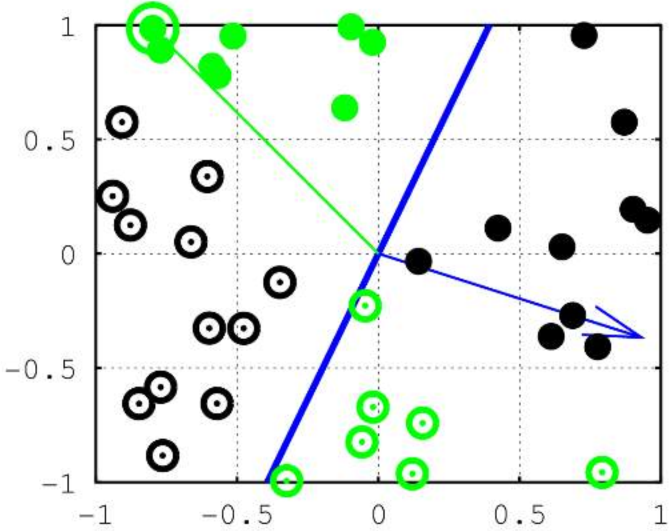
Biological motivations

- Learning systems made of several simple computational units connected to each other
- Memory capacity / plasticity of these systems

Algorithm: $\mathcal{D} = \{(X_n, Y_n)\}_{n=1}^{N}$

$\mathbf{w} \leftarrow \mathbf{0}$
while there exists (X_n, Y_n): $Y_n \langle \mathbf{w}, X_n \rangle \leq 0$ **do**
  $\mathbf{w} \leftarrow \mathbf{w} + Y_n X_n$
end while

Perceptron learning in action



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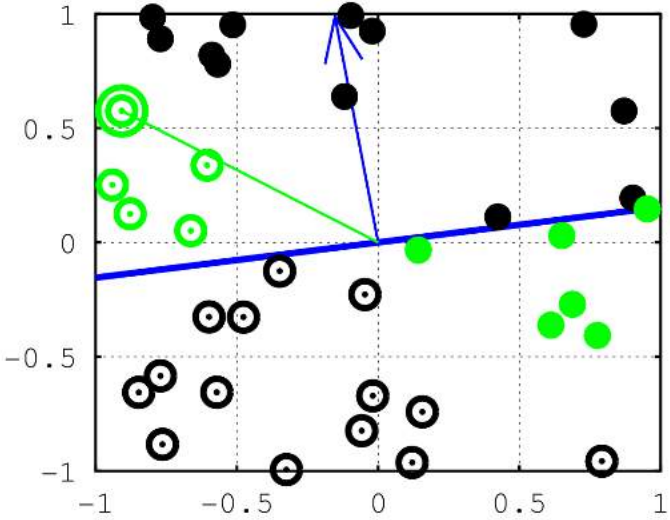

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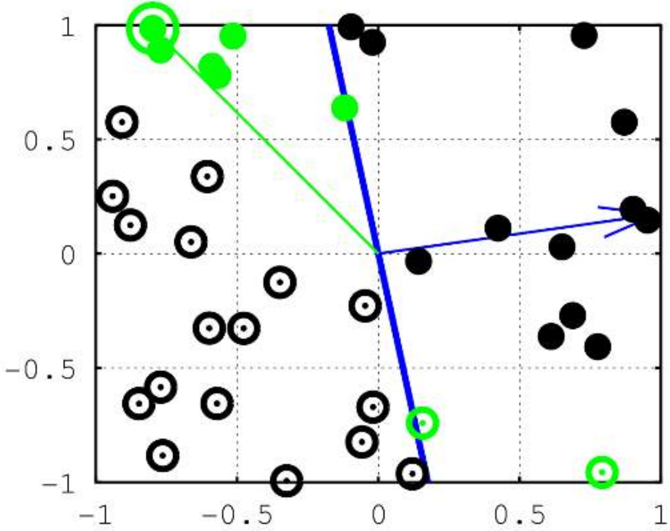

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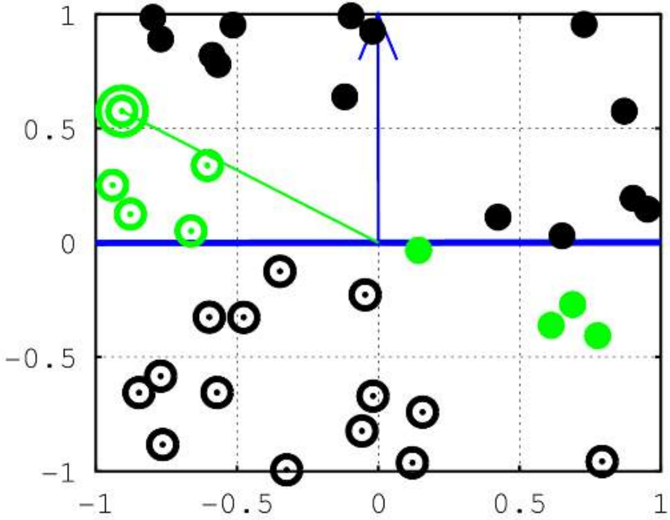

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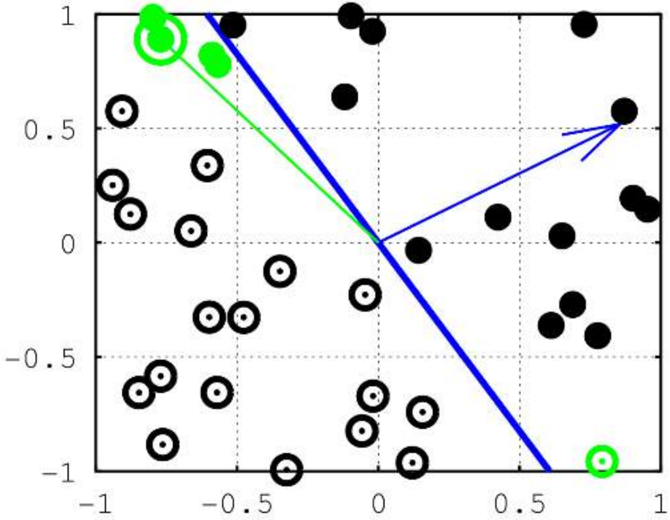

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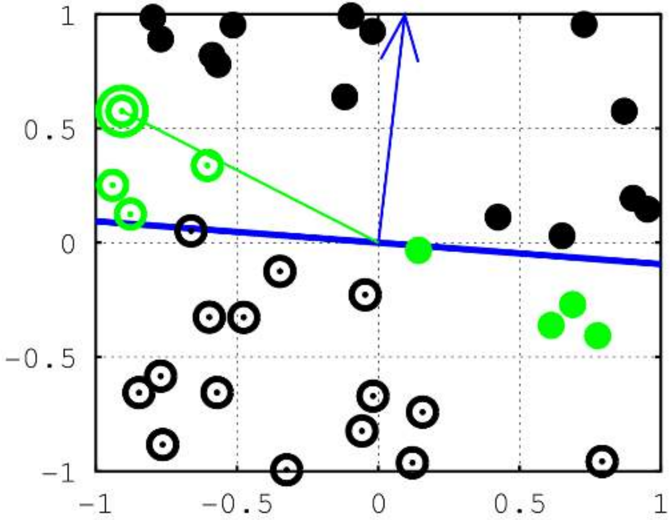

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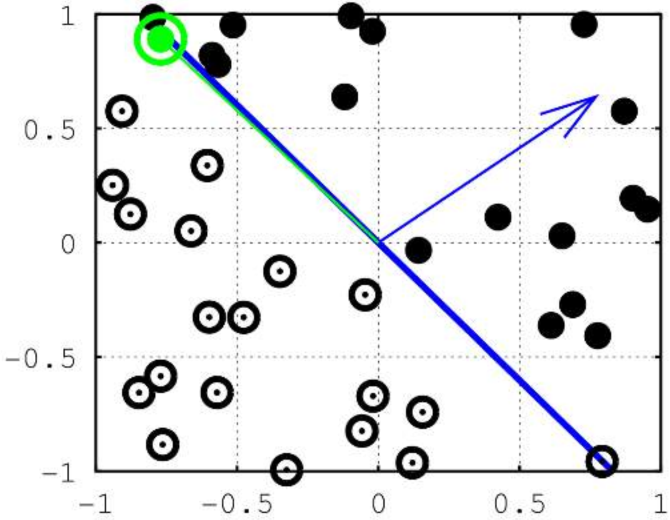

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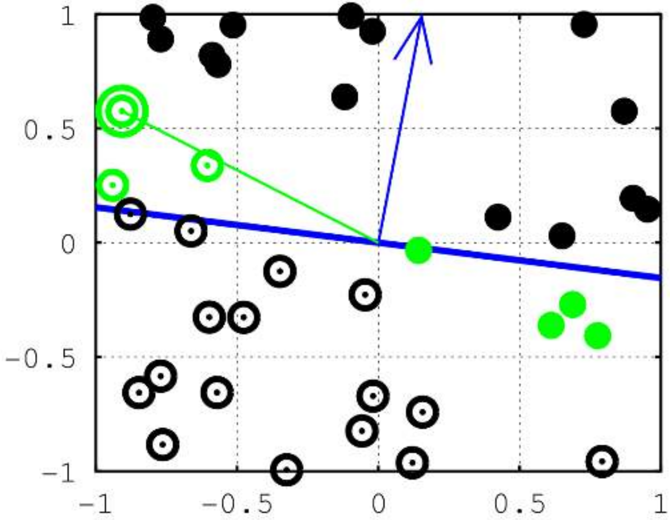

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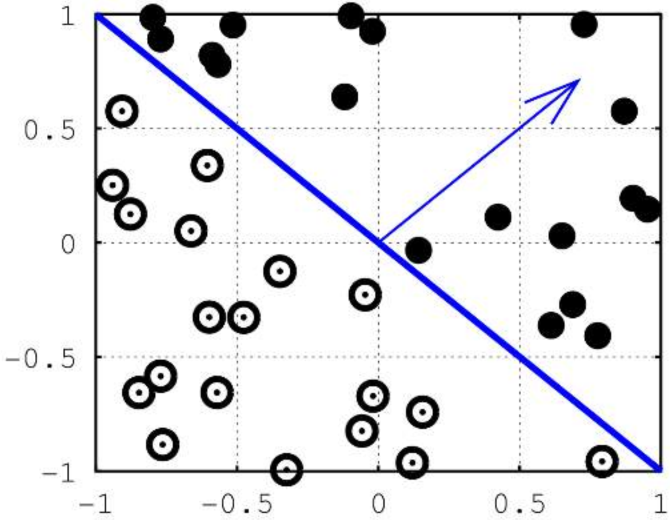


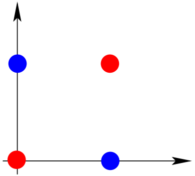
Perceptron: a few results

Theorem (Bound on the number of updates, Novikoff, 1962)

If there exist $\gamma > 0$, $\mathbf{w}^*$, $\|\mathbf{w}^*\| = 1$, $\|X_n\| \leq R, \forall n = 1, \ldots, N$, et $Y_n \langle \mathbf{w}^*, X_n \rangle \geq \gamma$ then the Perceptron algorithm converges in less than R^2/γ^2 updates

Theorem (XOR, Minsky, Papert, 1969)

The Perceptron (algorithm) cannot solve the XOR problem

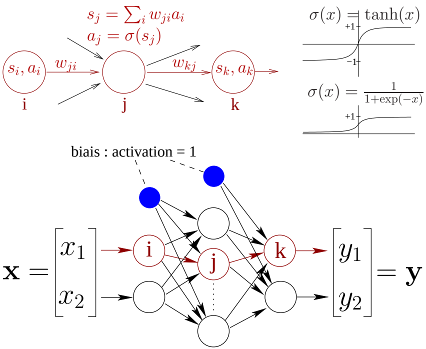


Theorem (Generalization error, Vapnik et Chevonenkis, 1979)

$\forall \mathbf{w} \in \mathbb{R}^d$: *with high probability*

$$R(w) \leq \hat{R}(\mathbf{w}, \mathcal{D}) + \tilde{O}\left(\sqrt{\frac{d}{n}}\right)$$

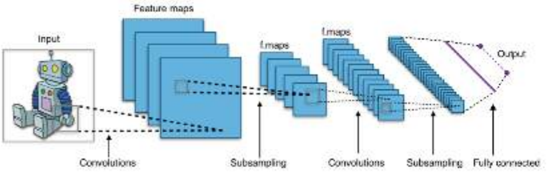
Multilayer Perceptron, Convolutional Networks



Up until the 90's

- Feedforward networks
- Gradient backpropagation (Rumelhart et al. 86)
- Preferred task: multiclass classification

Multilayer Perceptron, Convolutional Networks



(By Aphex34 - Own work, CC BY-SA 4.0, Wikimedia CNN)

Since 2005

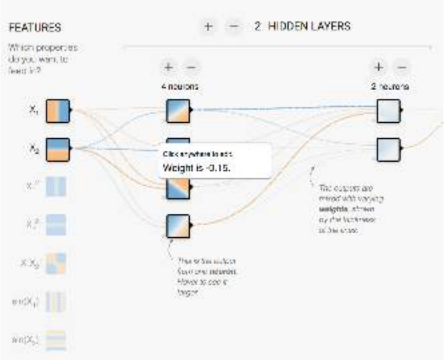
- Feedforward networks, recurrent networks
- Backpropagation (and autodiff), layerwise learning, computational power
- Tasks: almost everything (provided there is data)

But, more importantly

- Libraries: Tensorflow, Theano, Keras, Torch, Caffe (see là)
- Hardware: GPU, TPU (Tensor Processing Units)
- Data...

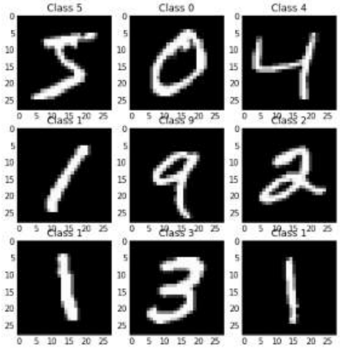
Deep Learning: Hands-on

Visualization



https://tinyurl.com/ydclvgas

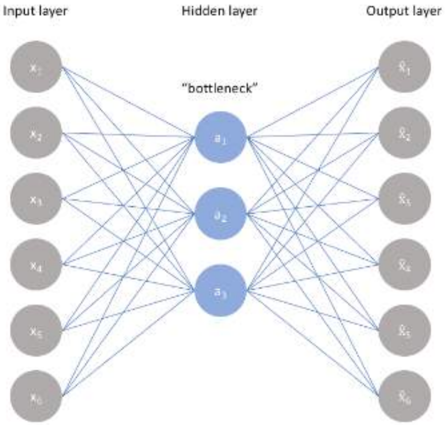
Keras Mnist Tutorial



https://tinyurl.com/ydzypus4

Dozens of examples can be found on Keras code examples page

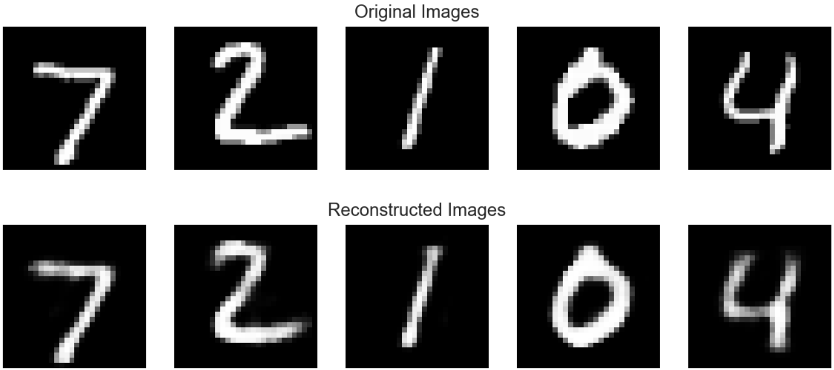
Unsupervised Deep Learning: auto-encoders



(From An introduction to Autoencoders)

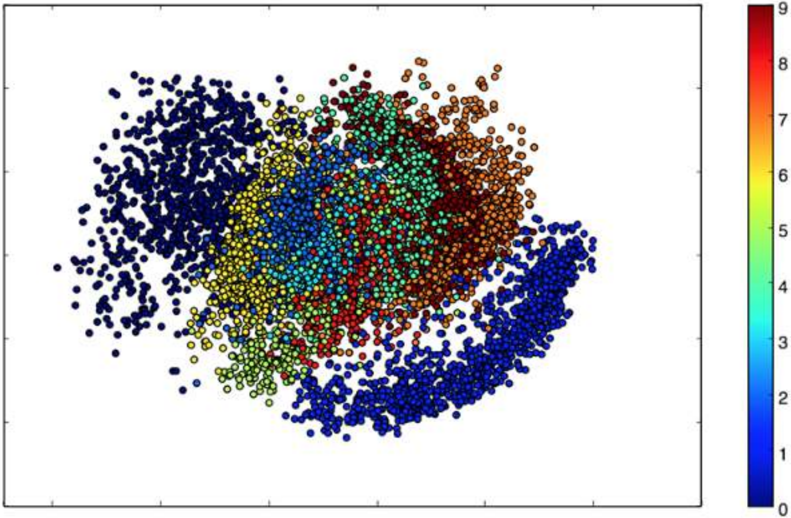
Code: `https://www.tensorflow.org/tutorials/generative/autoencoder`

Unsupervised Deep Learning: auto-encoders



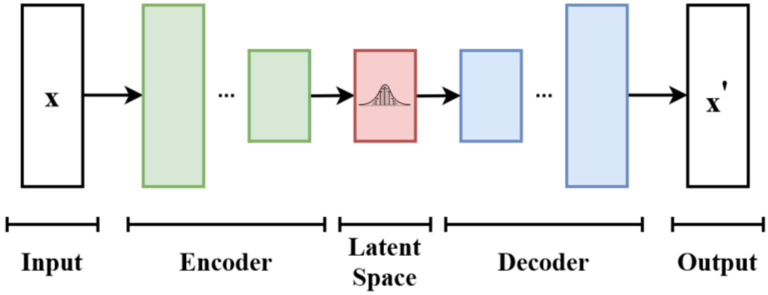
(From Applied Deep Learning - Part 3: Autoencoders)

Unsupervised Deep Learning: auto-encoders



(From Building Autoencoders in Keras)

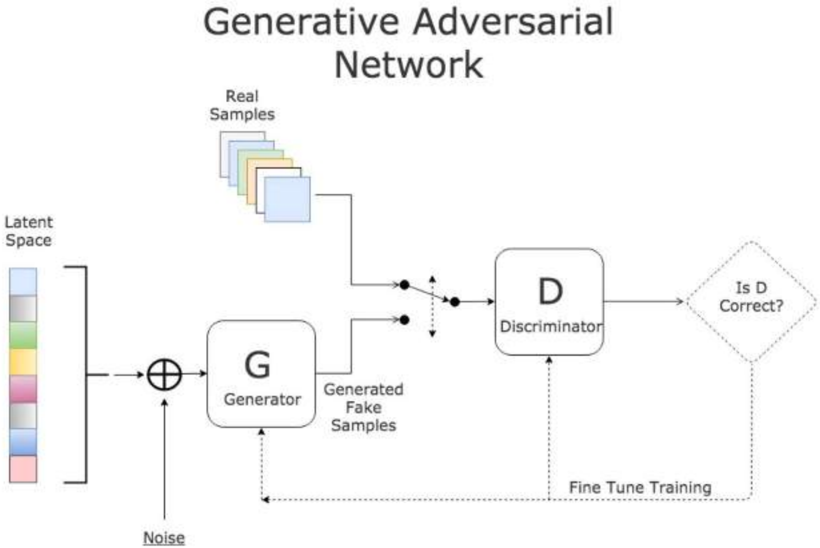
Unsupervised/Generative Deep Learning: Variational Auto-Encoders (Kingma and Welling, 2014)



(From Wikipedia VAE page)

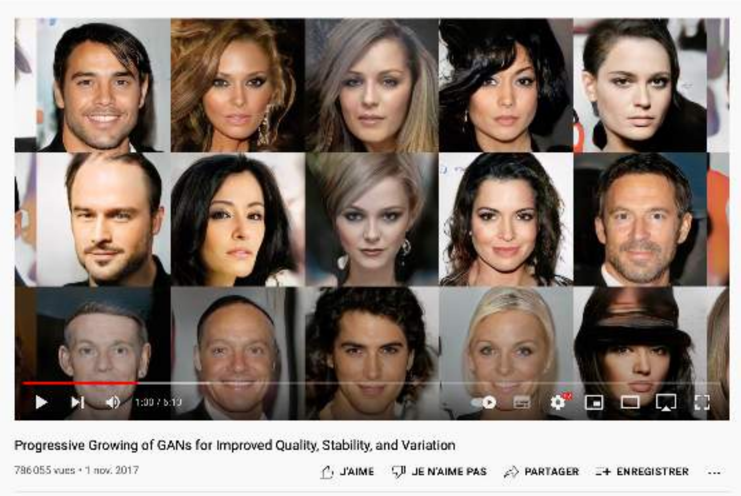
Code: https://deeplearning.neuromatch.io/tutorials/W2D5_GenerativeModels/student/W2D5_Tutorial1.html

Generative Deep Learning: GANs, (Goodfellow and al, 2014



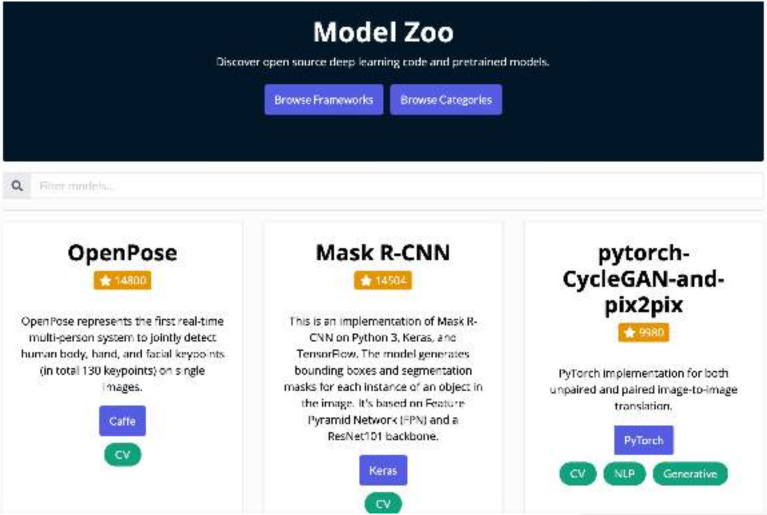
(From GANs from Scracth)

Generative Deep Learning: GANs, (Goodfellow and al, 2014



(From NVidia Video)

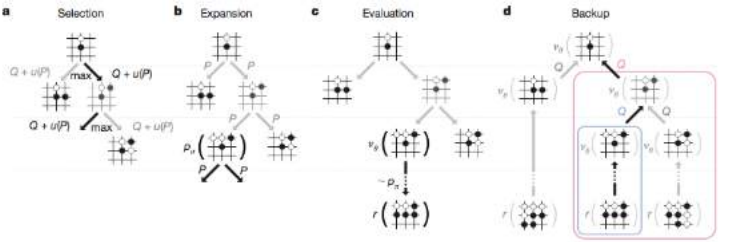
Models Zoo

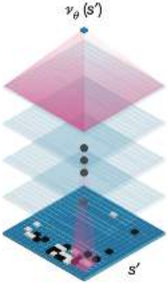


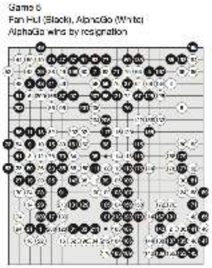
https://modelzoo.co

Outline

AlphaGo (Silver et al. 2016)





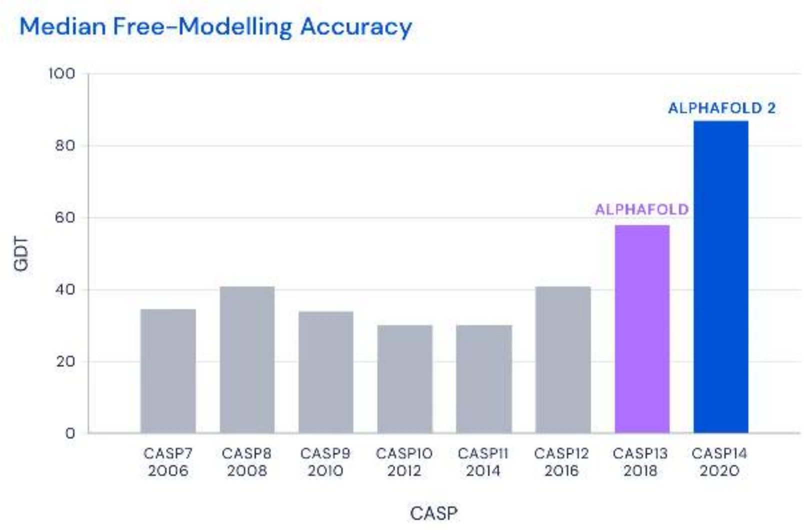


https://deepmind.com/blog/alphago-zero-learning-scratch/

AlphaGo (Silver et al. 2016)

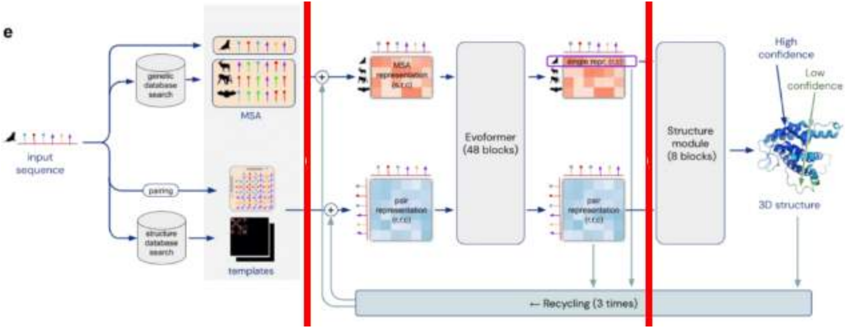
(From AlphaGo Netflix (Deepmind youtube))

AlphaFold (Jumper et al, Nature 2021)



(From AlphaFold: a solution to a 50-year-old grand challenge in biology)

AlphaFold (Jumper et al, Nature 2021)



(From Jumper et al, Nature, 2021)

AlphaFold (Jumper et al, Nature 2021)

A notebook to play around

(From AlphaFold Notebook)

Outline

Machine Learning: a Variety of Problems/Mixes

Many application fields

- Computer vision
- NLP
- Robotics
- Advertising, recommendation systems
- Games (Go, chess, poker)
- Biology
- ...

Many problems

- Algorithmics
- Statistics
- Modelling
- ... and beyond

Conclusion

Machine Learning: a field in itselft

- A vivid branch of AI
- At the crossroads of computer science and mathematics
- Ever-growing community (from applied research to more fundamental one)

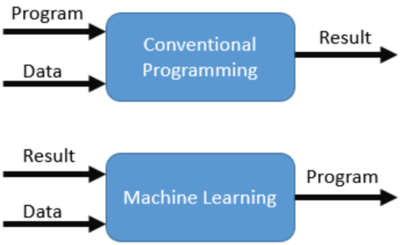
Machine Learning is ubiquituous

- At the heart of data science
- In many real-world applications
- ML at the time of revisiting other well-established fields of research

Example of future problems

- ML and small datasets: prior knowledge, active learning, feature selection
- ML & other fields: game theory, cryptography, biology, physics, law...

Hot AI topics (personal take)



Revisit classical fields from the Machine Learning perspective

- Privacy-Preserving ML: MLize encryption mechanisms, distributed computing
- Repeated Mechanism Design: MLize game theory, deal with coopetitive and competitve agents
- Green ML: hardware-aware methods, communication-sensitive methods...