

An Introduction to Machine Learning

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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 Networks: longstanding models

Unsupervised / Generative models

Two success stories

AlphaGo (Silver et al. 2016)

AlphaFold (Jumper et al, Nature 2021)

Conclusion

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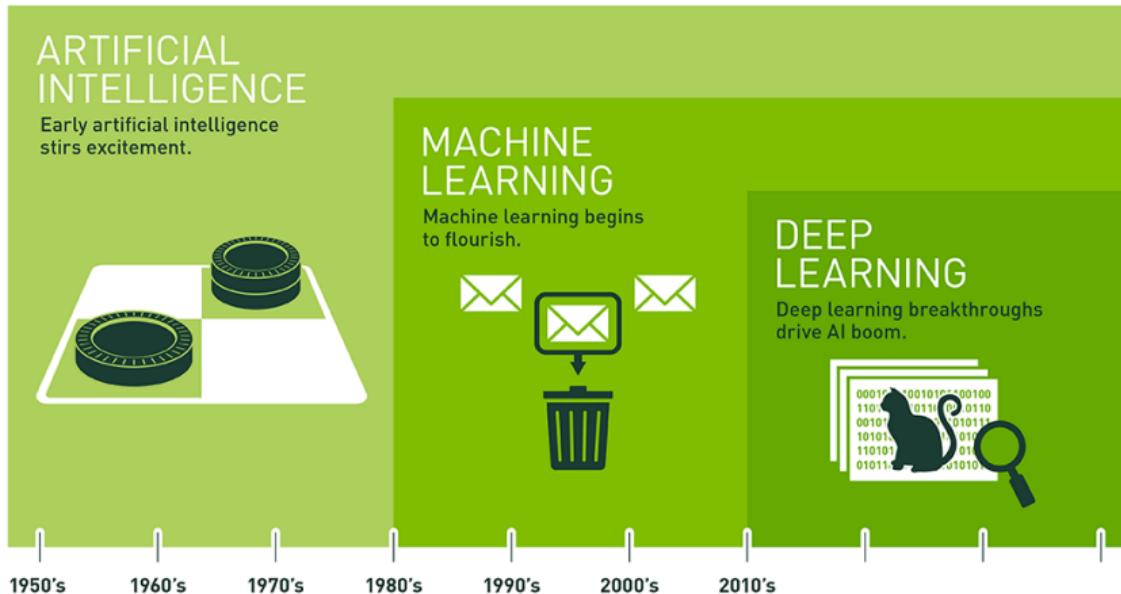
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AlphaFold (Jumper et al, Nature 2021)

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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

Sous-titres

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The search results page displays 10 news items:

- Global Mobile Artificial Intelligence Market Research Report** (businessstandardnews.com) - Il y a 17 heures
- Podcast: The future of artificial intelligence with Ian Bremmer** (gzeromedia.com) - Il y a 1 jour
- Trending news: Researchers make breakthrough in AI** (hindustannewshub.com) - Il y a 42 minutes
- Why Intel is Beating Everyone in Artificial Intelligence** (youtube.com) - Il y a 15 heures
- Holomedicine-Association: LEADERS A...** (holomedicine-association.org) - Il y a 1 jour
- Precision Medicine's Little Helper: Artificial Intelligence** (linkedin.com) - Il y a 22 minutes
- Why Social Networking Algorithms Are Increasingly Unethical** (playcrazygame.com) - Il y a 5 heures
- Artificial Intelligence (AI) in Media and Entertainment Market** (todayssxm.com) - Il y a 1 jour
- White House proposes tech 'bill of rights'** (wbbtv.com) - Il y a 22 heures
- Top Machine Learning Project Ideas for Profes...** (analyticsinsight.net) - Il y a 1 jour

Annotation/Image decoding



(from Farabet et al, 2013)

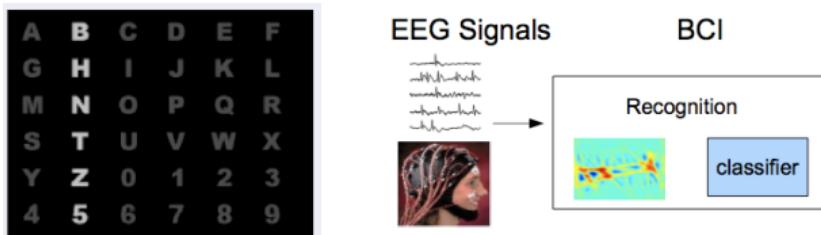
P300 Speller

Vintage P300 Speller

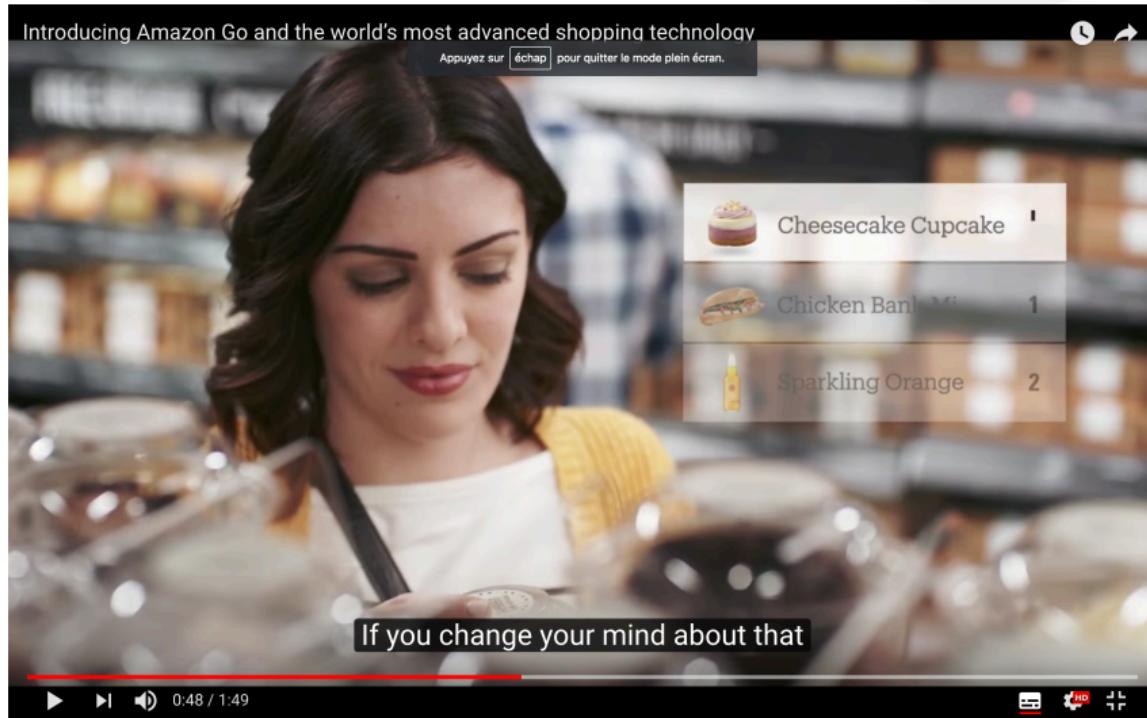


(from Breaking bad)

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

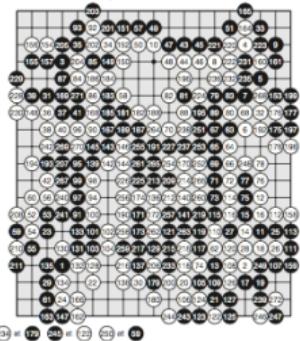


ML-cashing Amazon shops

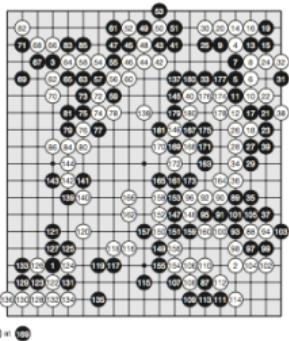


AlphaGo (Silver et al. 2016)

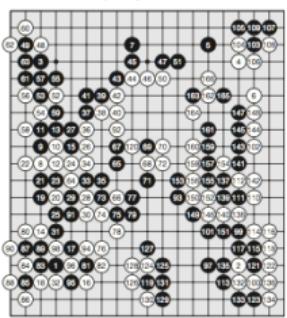
Game 1
Fan Hui (Black), AlphaGo (White)
AlphaGo wins by 2.5 points



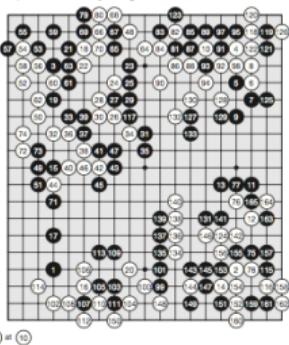
Game 2
AlphaGo (Black), Fan Hui (White)
AlphaGo wins by resignation



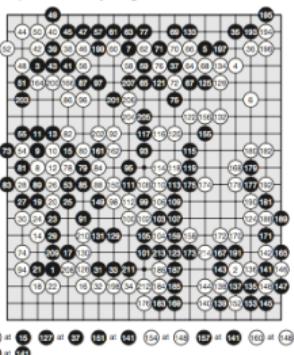
Game 3
Fan Hui (Black), AlphaGo (White)
AlphaGo wins by resignation



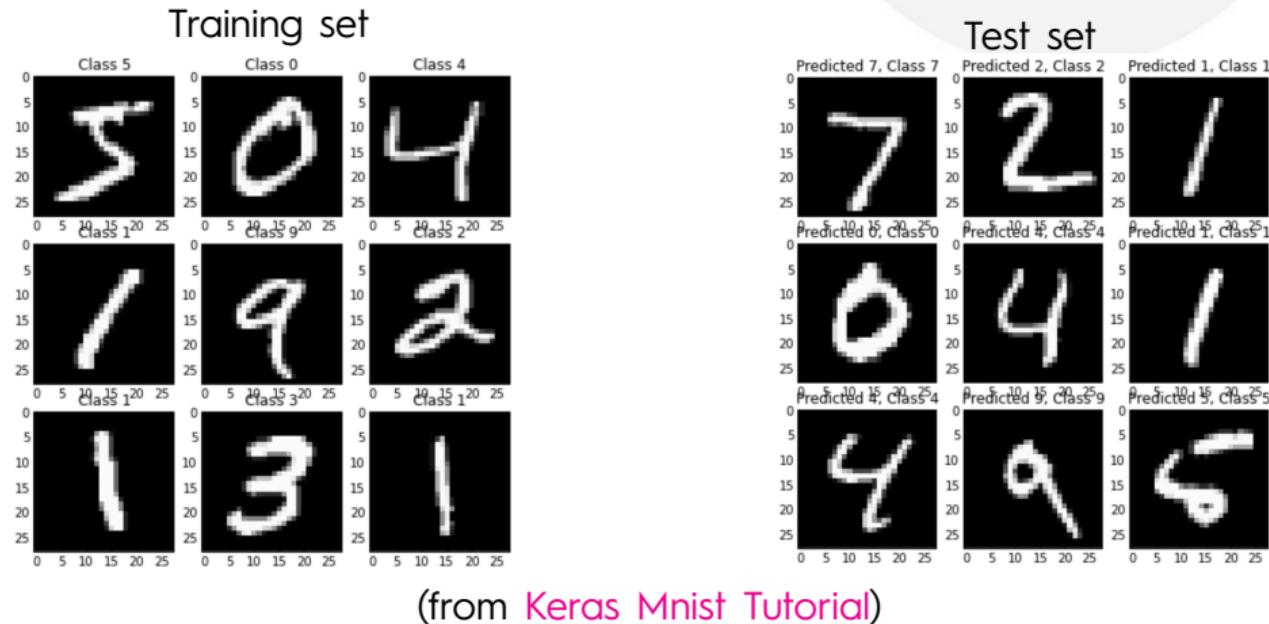
Game 4
AlphaGo (Black), Fan Hui (White)
AlphaGo wins by resignation



Game 5
Fan Hui (Black), AlphaGo (White)
AlphaGo wins by resignation



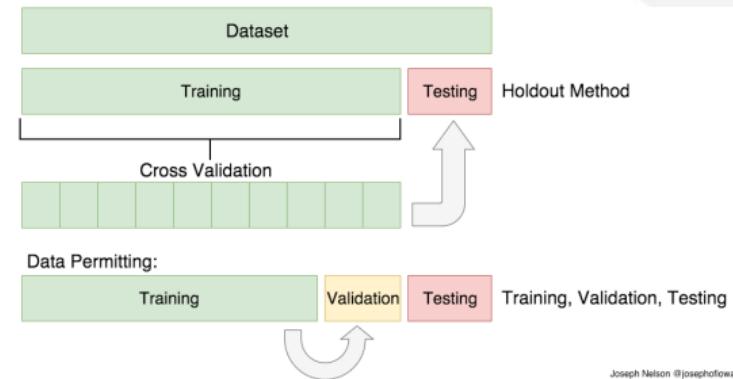
Core goal in supervised learning: generalization



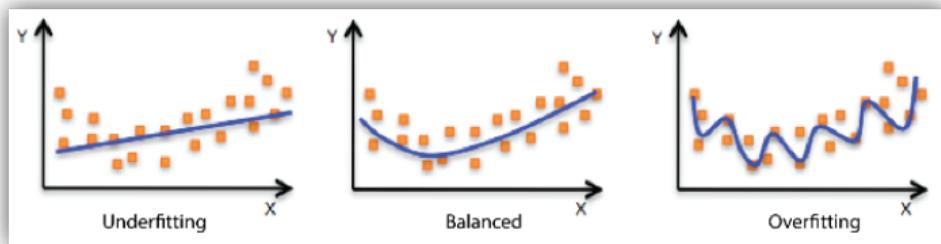
Generalization: from the training set to beyond

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)

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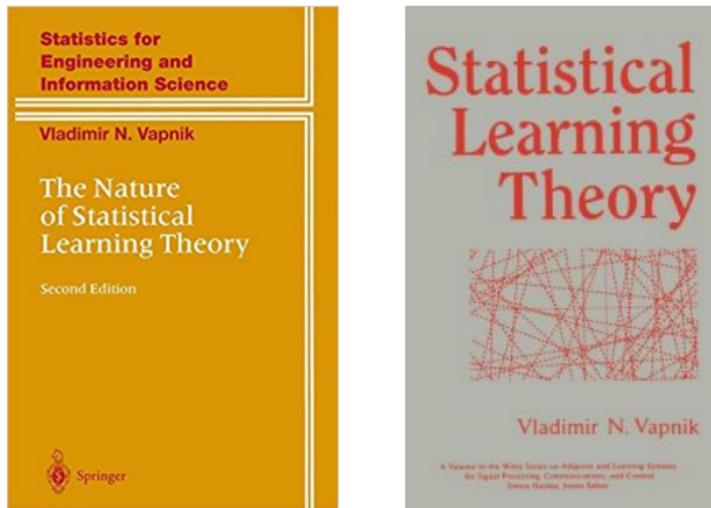
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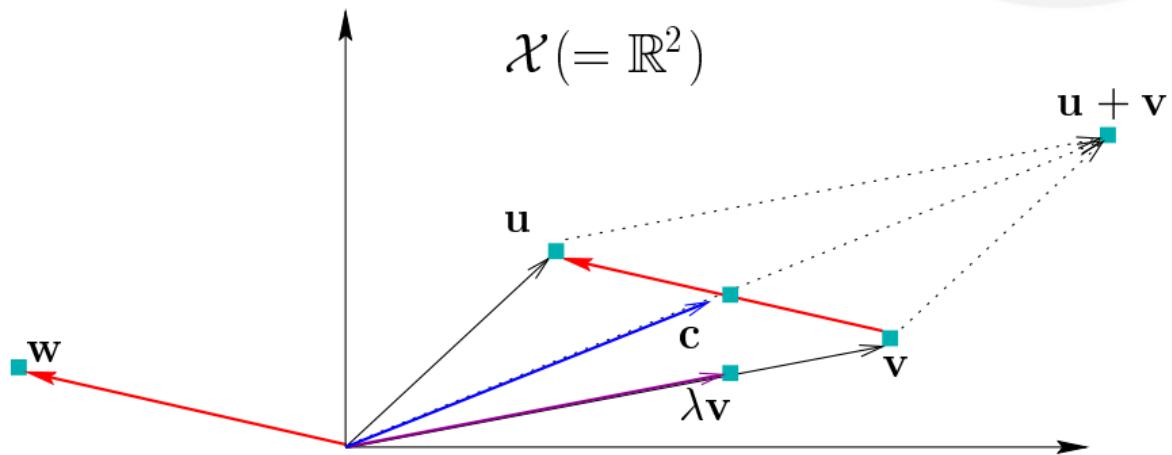
V. Vapnik sets, at the end of the 70's, the mathematical basis of **machine/statistical learning**, at the intersection of computer science, statistics, and optimization



"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 $\langle \cdot, \cdot \rangle : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$

- ▶ 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: $\langle \mathbf{u}, \mathbf{u} \rangle = 0 \Rightarrow \mathbf{u} = 0$

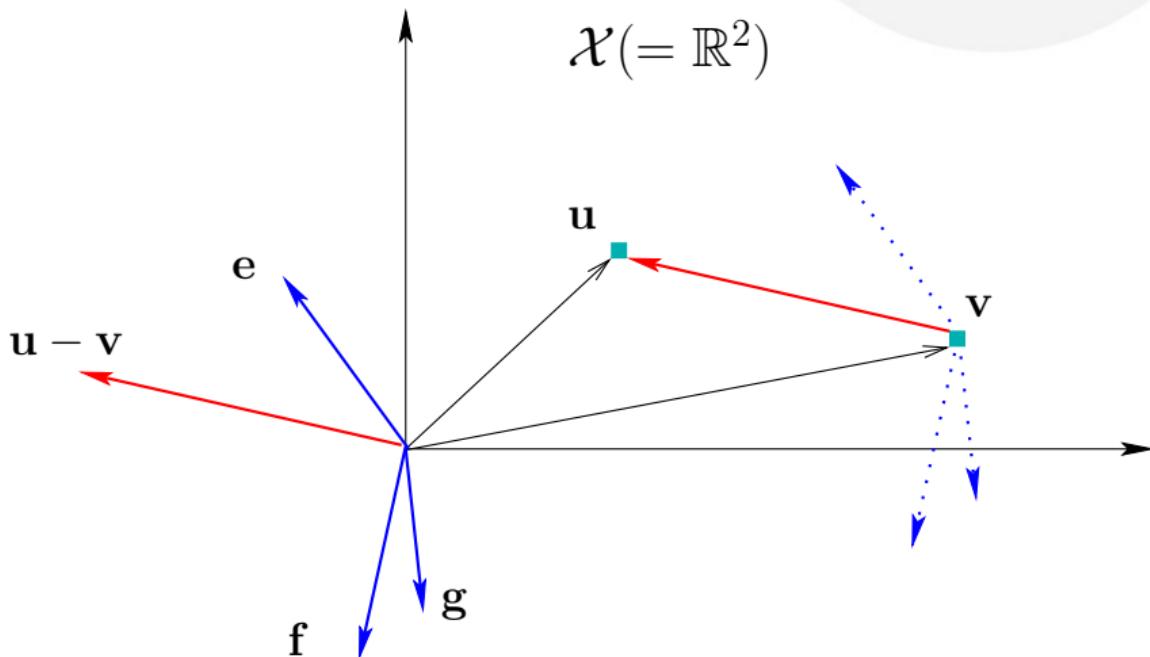
Inner product

- ▶ 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

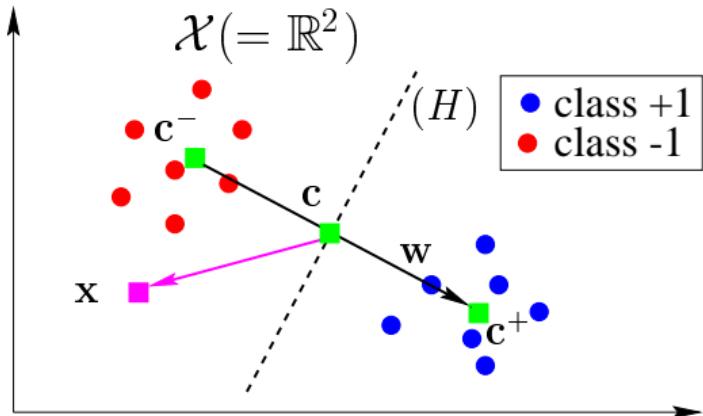
- ▶ $\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}: \langle \mathbf{u}, \mathbf{v} \rangle = u_1 v_1 + u_2 v_2$

Warm-up: a first handcrafted classifier



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

Warm-up: a first handcrafted classifier



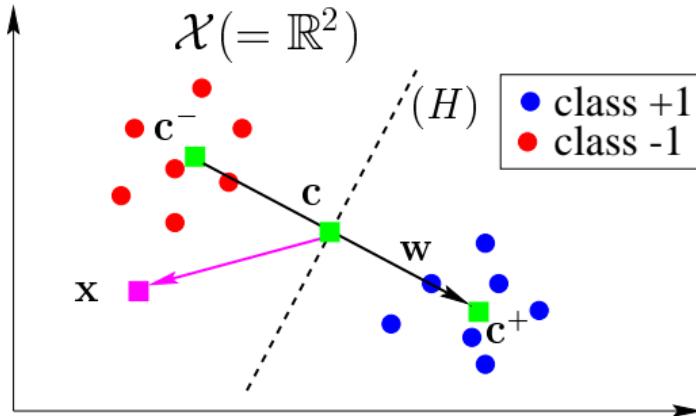
- $c^+ = \frac{1}{n^+} \sum_{\{i:y_i=+1\}} \mathbf{x}_i$
- $c^- = \frac{1}{n^-} \sum_{\{i:y_i=-1\}} \mathbf{x}_i$
- $\mathbf{c} = \frac{1}{2}(c^+ + c^-)$
- $\mathbf{w} = c^+ - c^-$

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



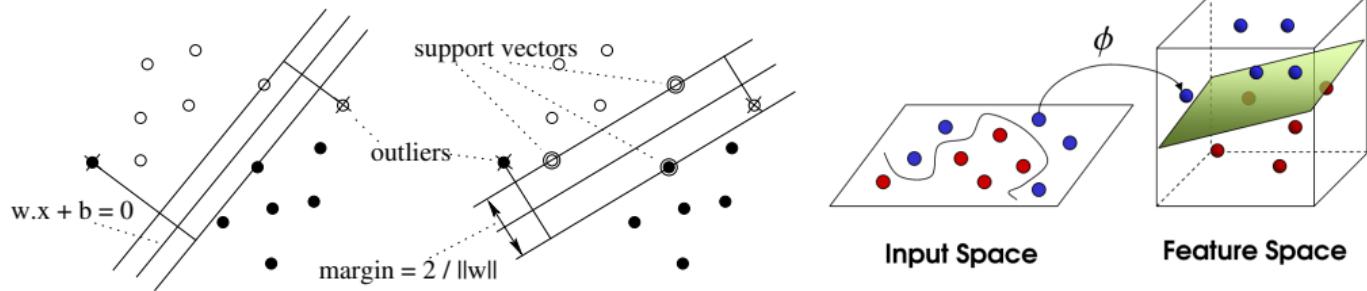
- $c^+ = \frac{1}{n^+} \sum_{\{i:y_i=+1\}} x_i$
- $c^- = \frac{1}{n^-} \sum_{\{i:y_i=-1\}} x_i$
- $c = \frac{1}{2}(c^+ + c^-)$
- $w = c^+ - c^-$

On evaluating $h(x)$

$$\begin{aligned} h(x) &= \langle w, x - c \rangle = \langle w, x \rangle - \langle w, c \rangle = \dots \\ &= \sum_{i=1, \dots, m} \alpha_i \langle x_i, x \rangle + b, \quad \text{with } b \text{ a real constant} \end{aligned}$$

Inner products are sufficient (remember that)

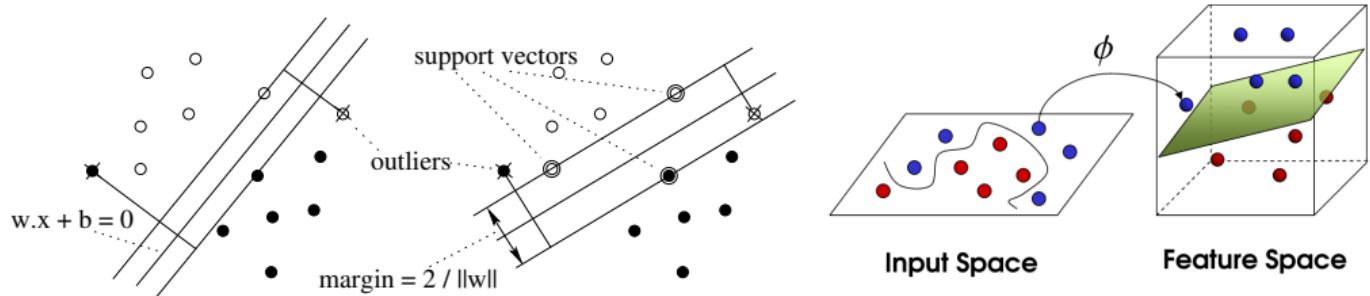
Kernel methods: graceful methods



Silk methods

- ▶ Theoretical 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

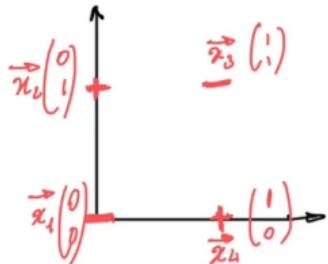
$h(\cdot) = \sum_{i=1,\dots,m} \alpha_i \langle \mathbf{x}_i, \cdot \rangle + b$ simply turns into

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

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

Example: 2nd degree polynomial kernel

①



②

$$\phi: \vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \longmapsto \phi(x) = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{bmatrix}$$

And the magic is here:

$$\langle \phi(\vec{u}), \phi(\vec{v}) \rangle = \left\langle \begin{bmatrix} u_1^2 \\ u_2^2 \\ \sqrt{2}u_1u_2 \end{bmatrix}, \begin{bmatrix} v_1^2 \\ v_2^2 \\ \sqrt{2}v_1v_2 \end{bmatrix} \right\rangle$$

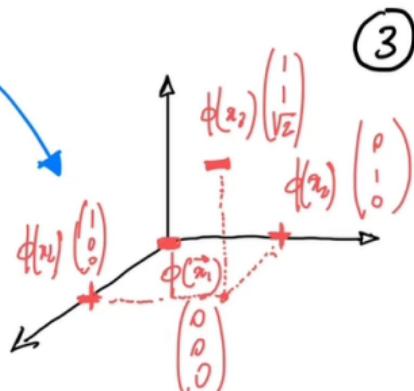
$$= u_1^2 v_1^2 + u_2^2 v_2^2 + 2u_1 u_2 v_1 v_2$$

$$= u_1^2 v_1^2 + u_2^2 v_2^2 + 2(u_1 v_1)(u_2 v_2)$$

$$= (u_1 v_1 + u_2 v_2)^2 = \langle \vec{u}, \vec{v} \rangle^2$$

This is a kernel

④



There exists a linear separating hyperplane in \mathbb{R}^3 .

Adaboost: combining weak learners

Given: $(x_1, y_1), \dots, (x_m, y_m)$ where $x_i \in \mathcal{X}, y_i \in \{-1, +1\}$.

Initialize: $D_1(i) = 1/m$ for $i = 1, \dots, m$.

For $t = 1, \dots, T$:

- Train weak learner using distribution D_t .
- Get weak hypothesis $h_t : \mathcal{X} \rightarrow \{-1, +1\}$.
- 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 $i = 1, \dots, m$:

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

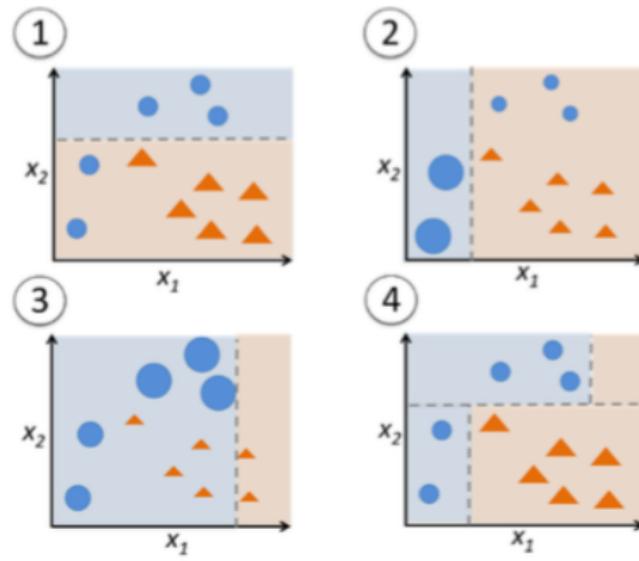
where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

Output the final hypothesis:

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

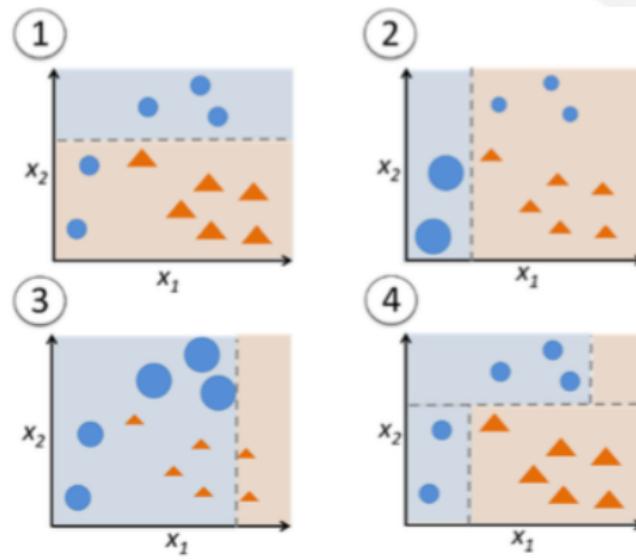
(from Freund and Schapire, 1997, 2012)

Adaboost: combining weak learners



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

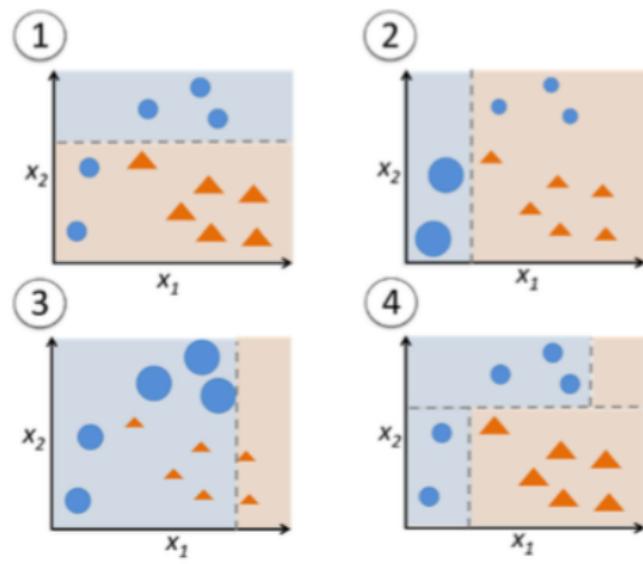
Adaboost: combining weak learners



(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

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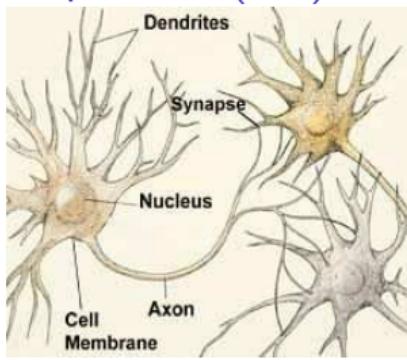
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AlphaFold (Jumper et al, Nature 2021)

Conclusion

Perceptron, binary case (Rosenblatt, 1958)

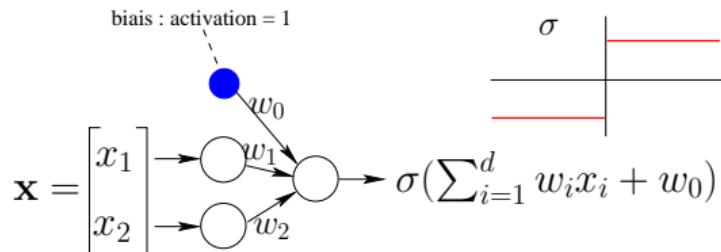
Inspiration: (real) neural networks



Biological motivations

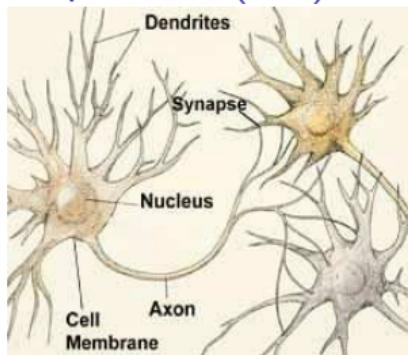
- ▶ Learning systems made of several simple computational units connected to each other
- ▶ Memory capacity / plasticity of these systems

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



Perceptron, binary case (Rosenblatt, 1958)

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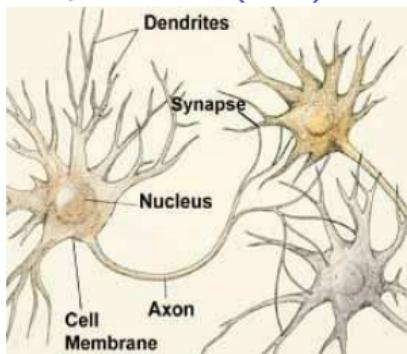
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Perceptron: a linear classifier, $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \{-1, +1\}$

- ▶ 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



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- ▶ Learning systems made of several simple computational units connected to each other
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Algorithm: $\mathcal{D} = \{(X_n, Y_n)\}_{n=1}^N$

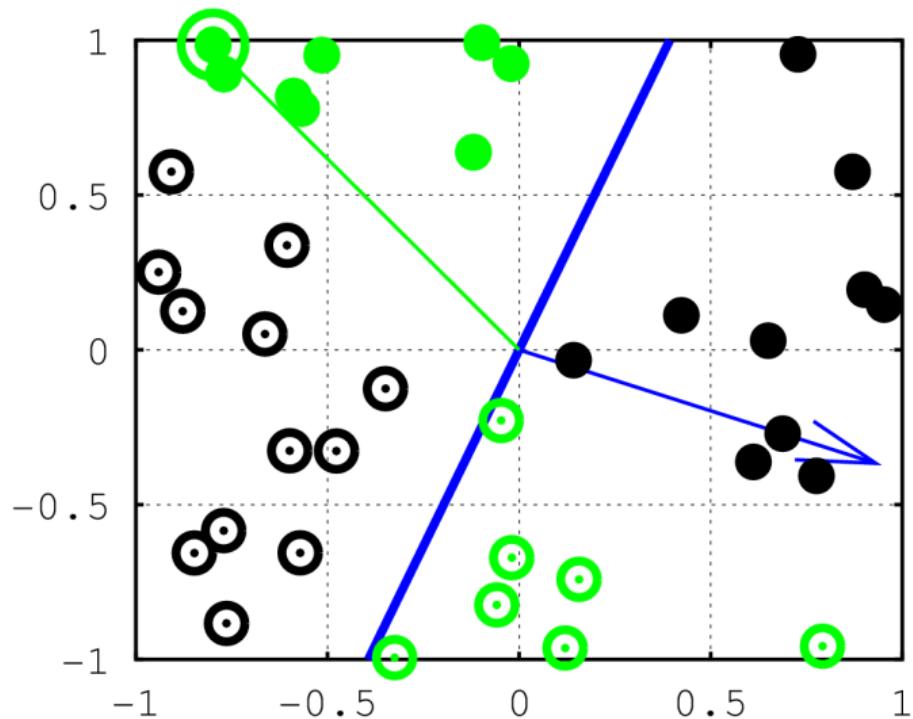
$w \leftarrow 0$

while there exists (X_n, Y_n) : $Y_n \langle w, X_n \rangle \leq 0$ **do**

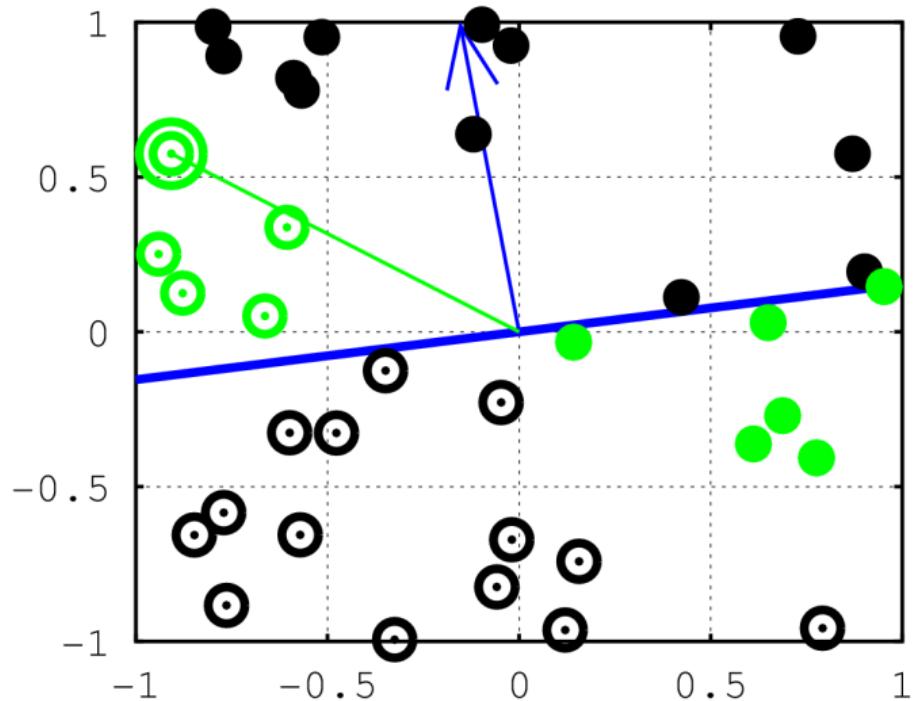
$w \leftarrow w + Y_n X_n$

end while

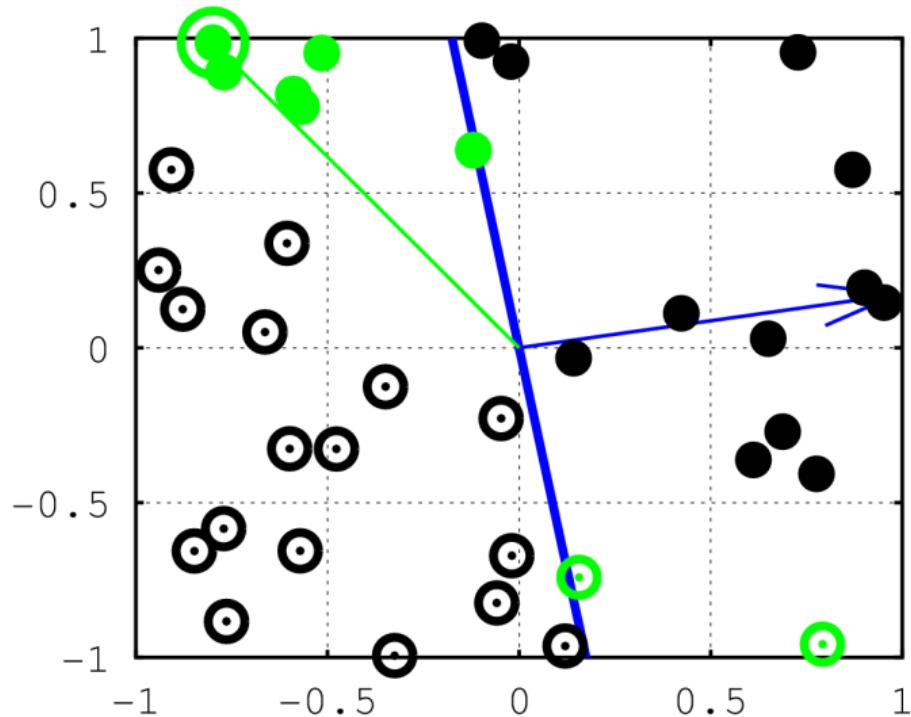
Perceptron learning in action



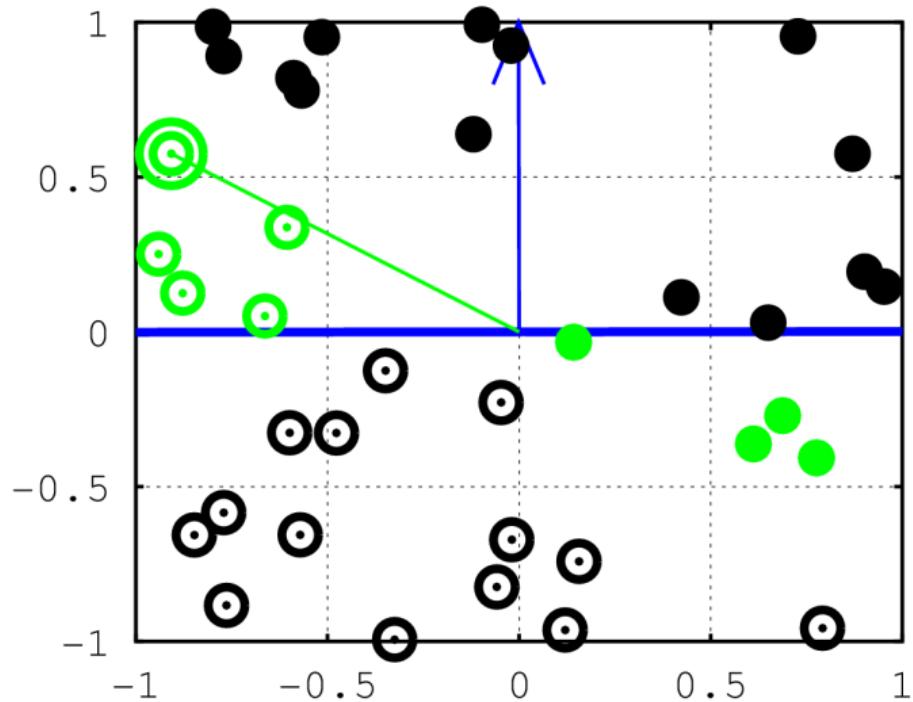
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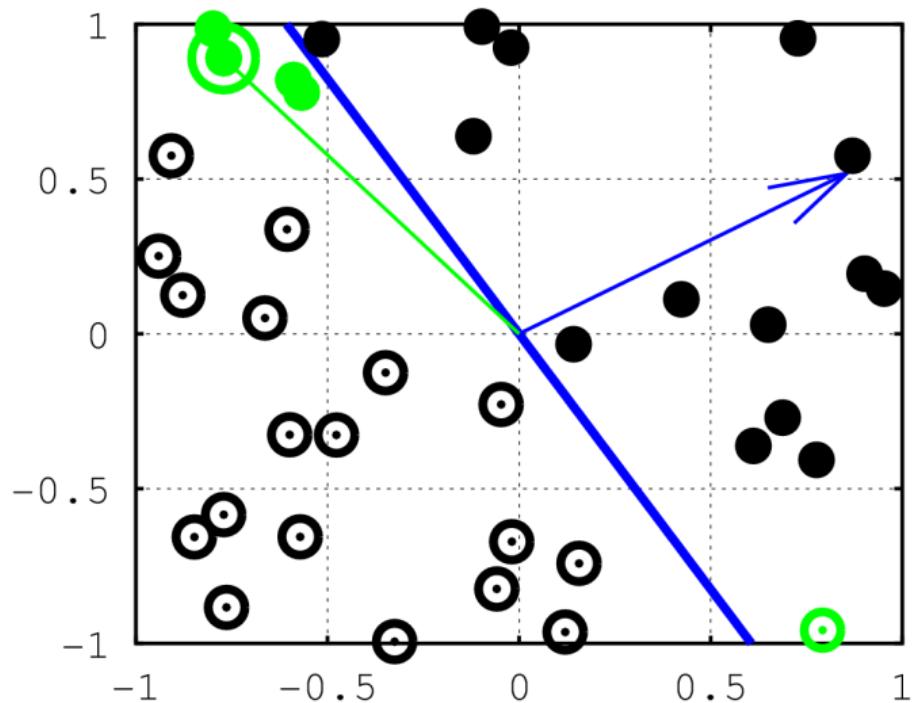
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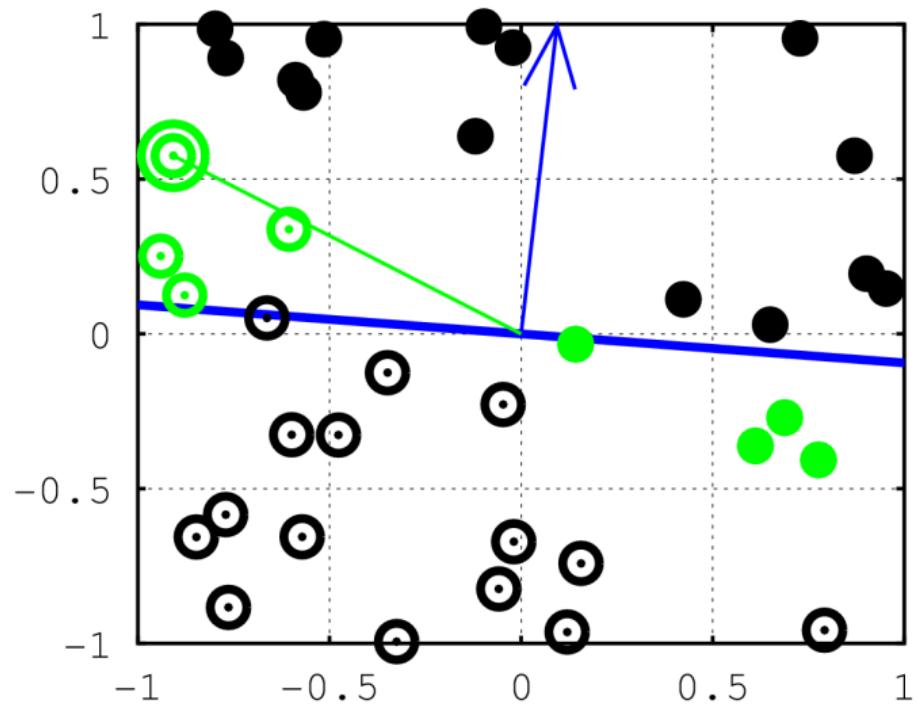
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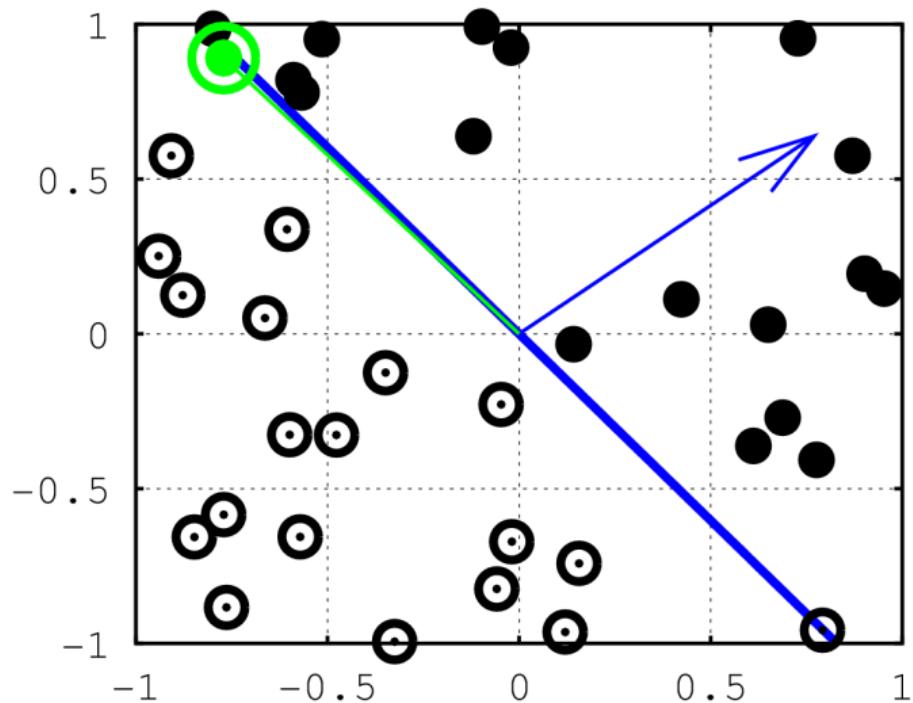
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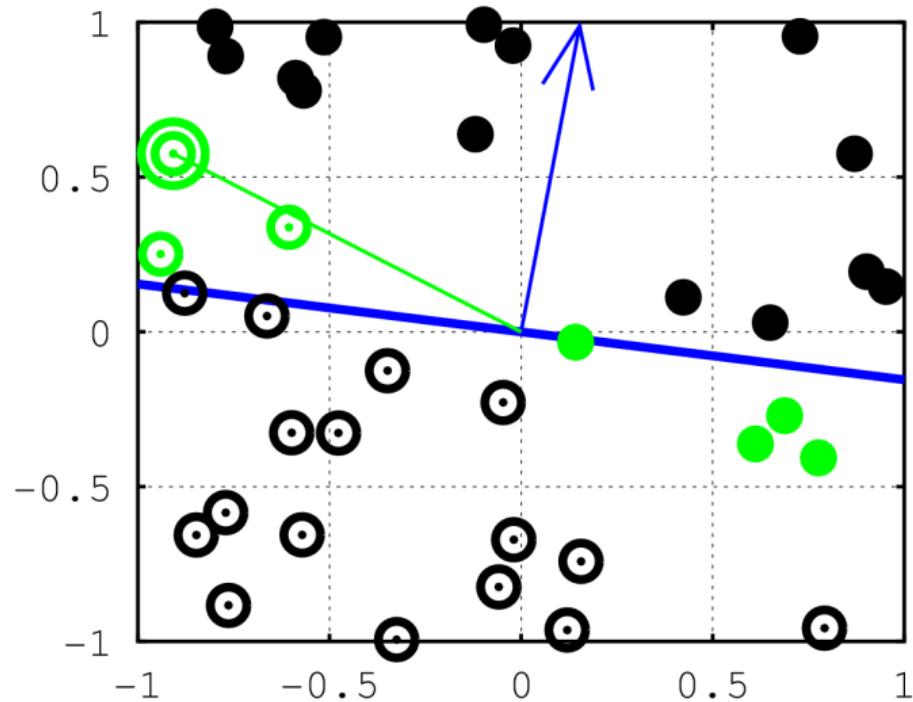
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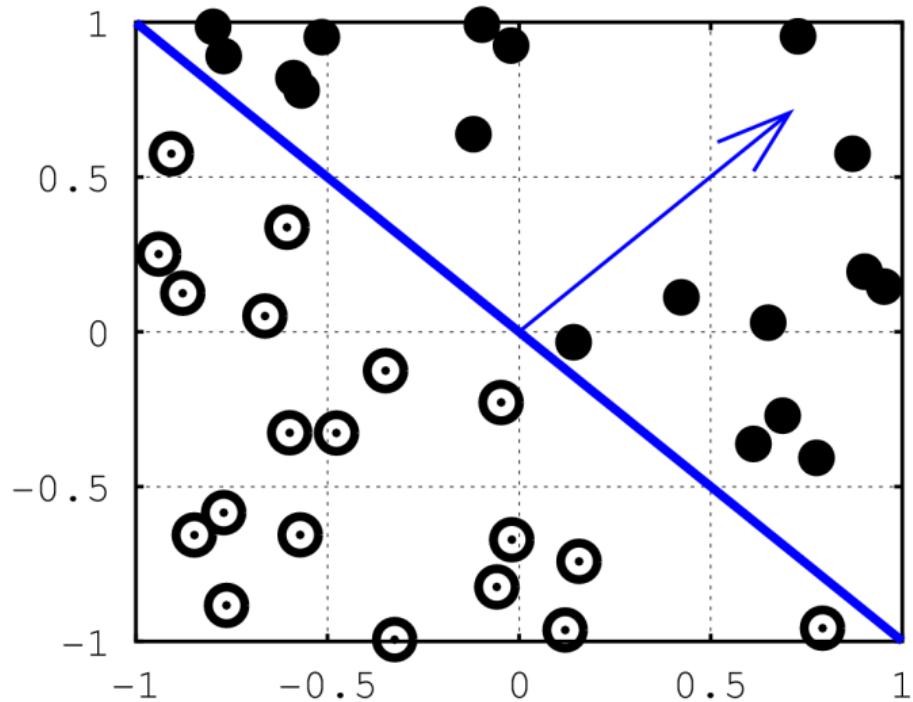
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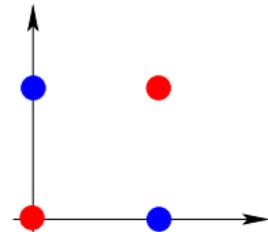
Perceptron: a few results

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

If there exist $\gamma > 0$, \mathbf{w}^* , $\|\mathbf{w}^*\| = 1$, $\|X_n\| \leq R$, $\forall n = 1, \dots, N$, 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

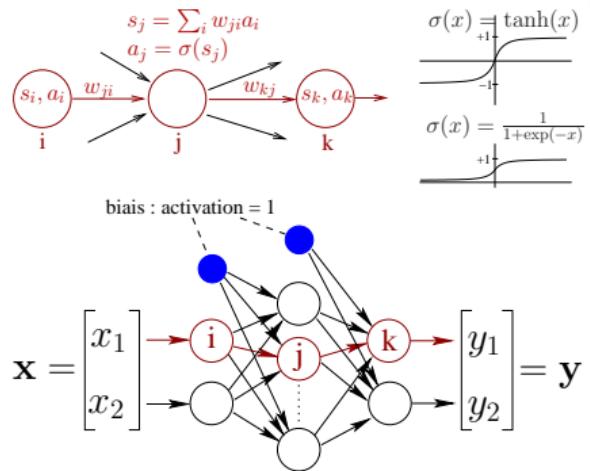


Theorem (Generalization error, Vapnik et Chevonenkis, 1979)

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

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

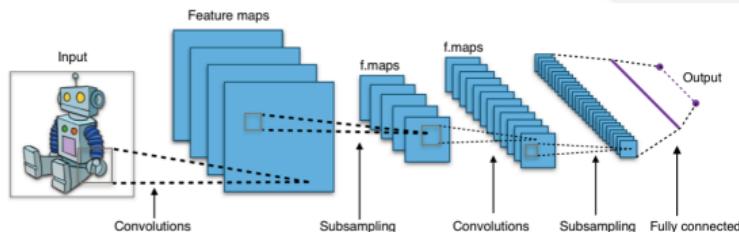
Multilayer Perceptron, Convolutional Networks



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

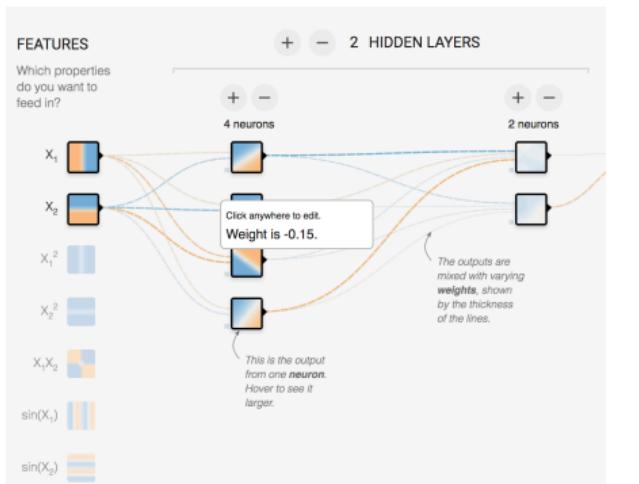
- ▶ Feedforward networks, recurrent networks
- ▶ Backpropagation (and autodiff), layerwise learning, computational power
- ▶ Tasks: almost everything (provided there is data)

But, more importantly

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

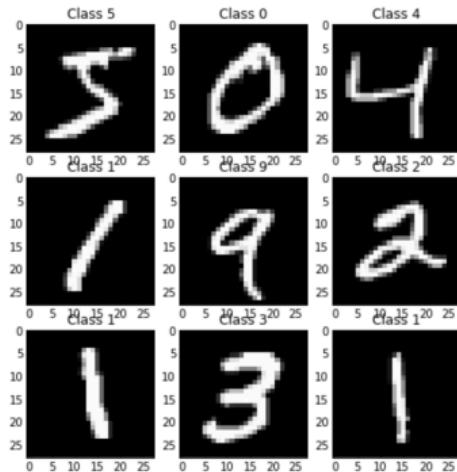
Deep Learning: Hands-on

Visualization



<https://tinyurl.com/ydclvgas>

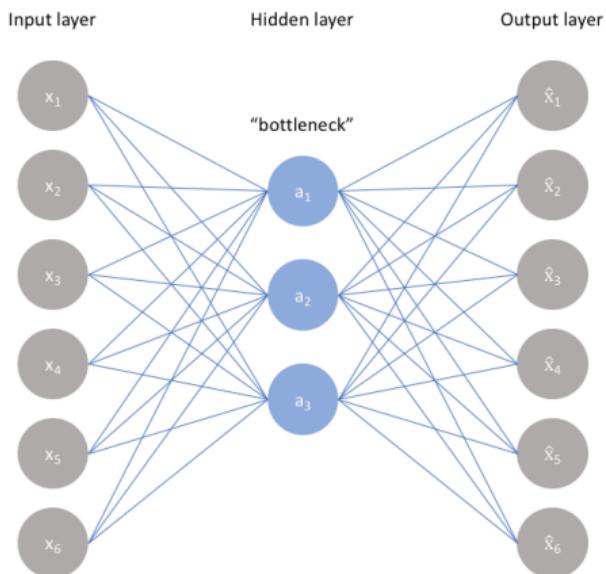
Keras Mnist Tutorial



<https://tinyurl.com/ydzypus4>

Dozens of examples can be found on [Keras code examples page](#)

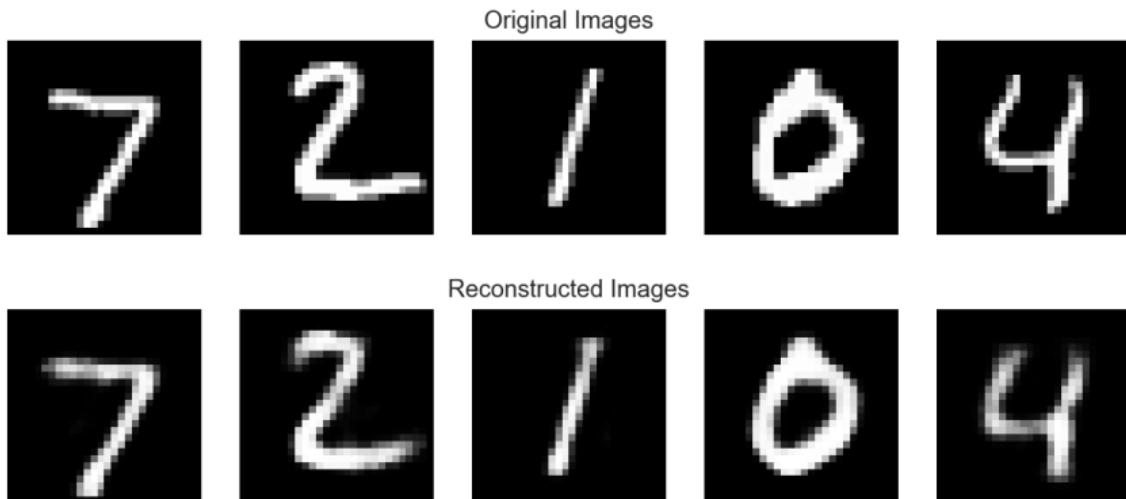
Unsupervised Deep Learning: auto-encoders



(From An introduction to Autoencoders)

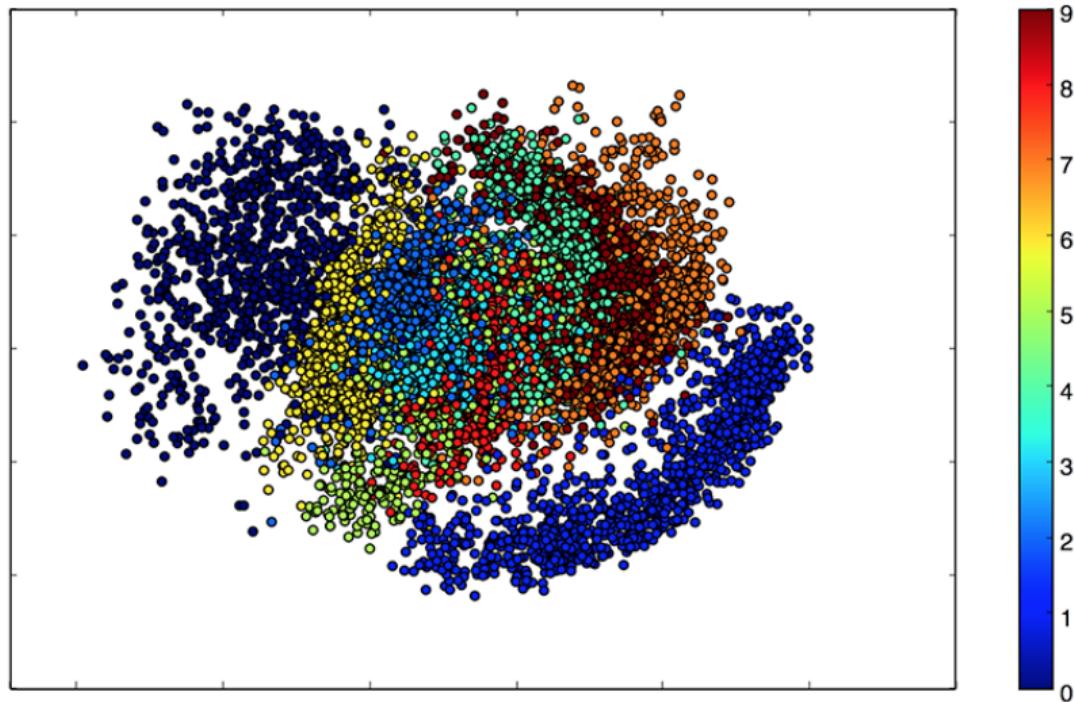
Code: <https://www.tensorflow.org/tutorials/generative/autoencoder>

Unsupervised Deep Learning: auto-encoders



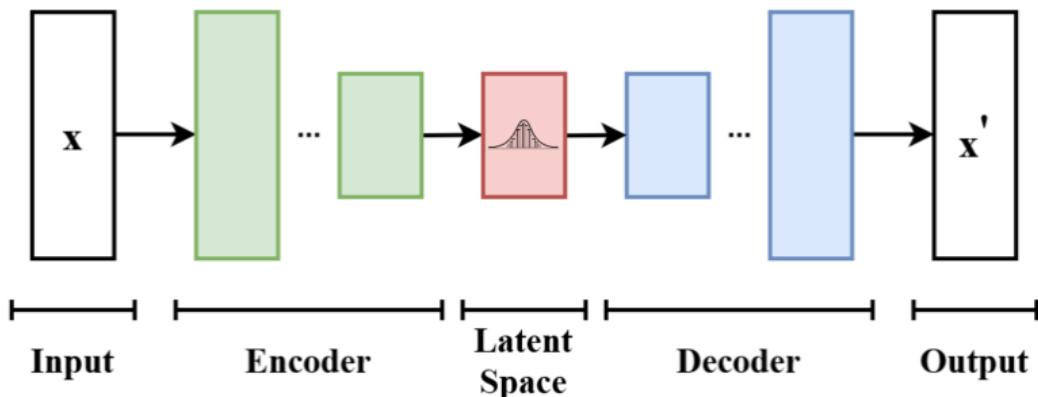
(From Applied Deep Learning - Part 3: Autoencoders)

Unsupervised Deep Learning: auto-encoders



(From [Building Autoencoders in Keras](#))

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

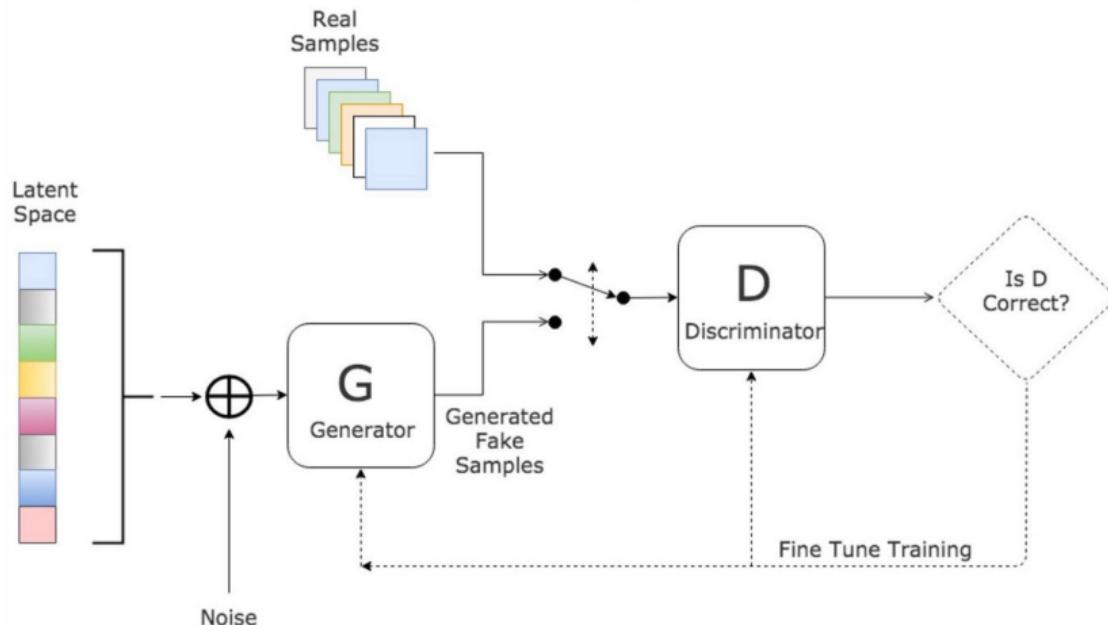


(From Wikipedia VAE page)

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

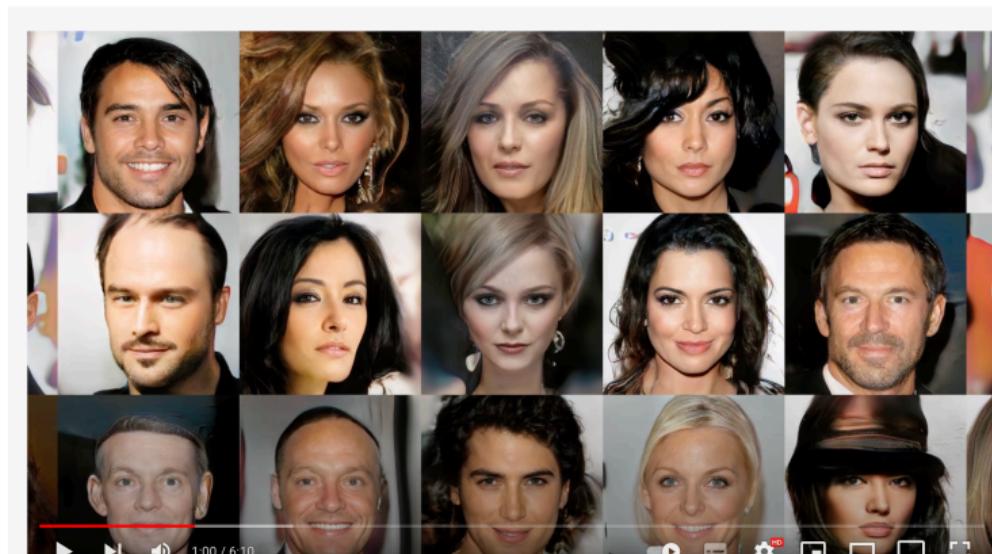
Generative Deep Learning: GANs, (Goodfellow and al, 2014)

Generative Adversarial Network



(From [GANs from Scratch](#))

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



Progressive Growing of GANs for Improved Quality, Stability, and Variation

786 055 vues • 1 nov. 2017

JAIME

JE N'AIME PAS

PARTAGER

ENREGISTRER

...

(From NVidia Video)

Models Zoo

The screenshot shows the homepage of the Model Zoo. At the top center is the title "Model Zoo". Below it is a subtitle "Discover open source deep learning code and pretrained models." Two buttons are visible: "Browse Frameworks" and "Browse Categories". A search bar with a magnifying glass icon and the placeholder "Filter models..." is located below the subtitle. Three model cards are displayed in a grid:

- OpenPose** (★ 14800): Described as the first real-time multi-person system to jointly detect human body, hand, and facial keypoints. It is available in Caffe and CV frameworks.
- Mask R-CNN** (★ 14504): An implementation of Mask R-CNN on Python 3, Keras, and TensorFlow. It generates bounding boxes and segmentation masks. It is based on Feature Pyramid Network (FPN) and a ResNet101 backbone. It is available in Keras and CV frameworks.
- pytorch-CycleGAN-and-pix2pix** (★ 9980): A PyTorch implementation for both unpaired and paired image-to-image translation.

<https://modelzoo.co>

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 Networks: longstanding models

Unsupervised / Generative models

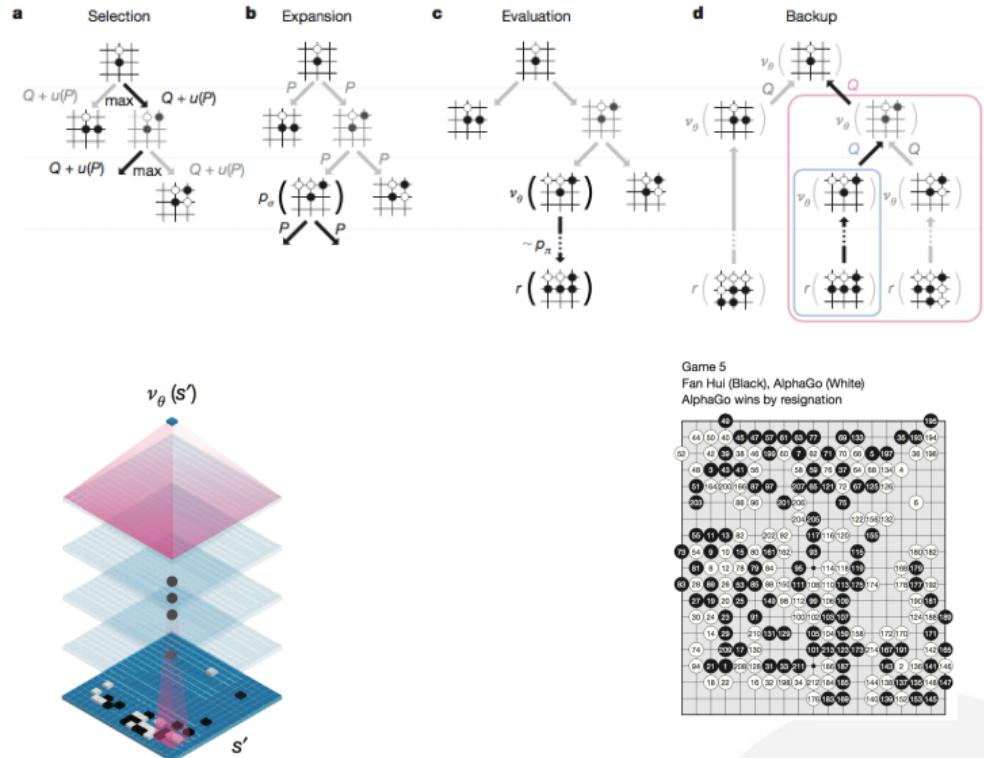
Two success stories

AlphaGo (Silver et al. 2016)

AlphaFold (Jumper et al, Nature 2021)

Conclusion

AlphaGo (Silver et al. 2016)



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

AlphaGo (Silver et al. 2016)



(From AlphaGo Netflix (Deepmind youtube))

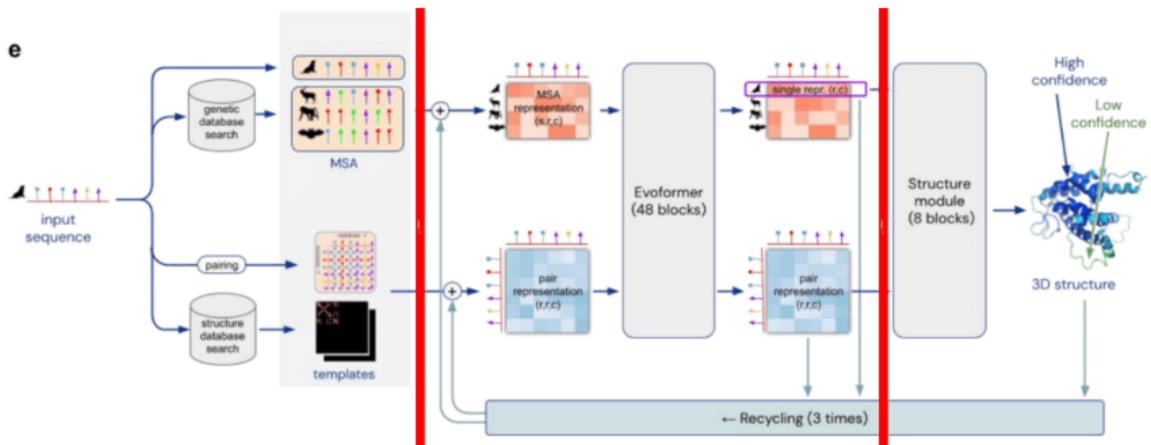
AlphaFold (Jumper et al, Nature 2021)

Median Free-Modelling Accuracy



(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

ColabFold: AlphaFold2 using MMseqs2

Easy to use protein structure and complex prediction using [AlphaFold2](#) and [AlphaFold2-multimer](#). Sequence alignments/templates are generated through [MMseqs2](#) and [HHsearch](#). For more details, see [bottom](#) of the notebook, checkout the [ColabFold GitHub](#) and read our manuscript:

[Mirdita M, Schütze K, Moriwaki Y, Heo L, Ovchinnikov S, Steinegger M. ColabFold - Making protein folding accessible to all. bioRxiv, 2021](#)

Old versions: [v1.0](#), [v1.1](#), [v1.2](#)

Input protein sequence(s), then hit Runtime > Run all

```
query_sequence: "PIAQIHLILEGRSDEQKETLIREVSEAISSRLDAPLTSVRVIITEMAKGHFGIGGELASK"
```

- Use : to specify inter-protein chainbreaks for **modeling complexes** (supports homo- and hetro-oligomers). For example PI...SK:PI...SK for a mono-dimer

```
jobname: "test"
```

```
use_amber: 
```

```
use_templates: 
```

```
save_to_google_drive: 
```

- if the save_to_google_drive option was selected, the result zip will be uploaded to your Google Drive

Advanced settings

(From [AlphaFold Notebook](#))

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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 itself

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

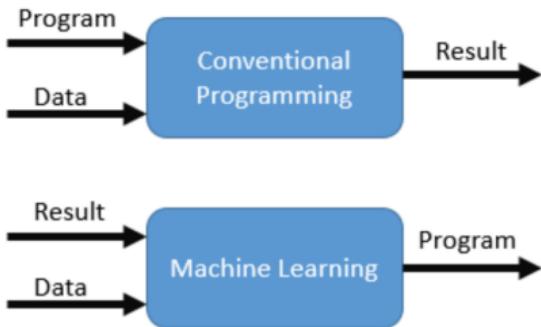
Machine Learning is ubiquitous

- ▶ 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 cooperative and competitive agents
- ▶ Green ML: hardware-aware methods, communication-sensitive methods...