Machine Learning and Data Mining

Maxim Borisyak

National Research University Higher School of Economics (HSE)

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Machine Learning

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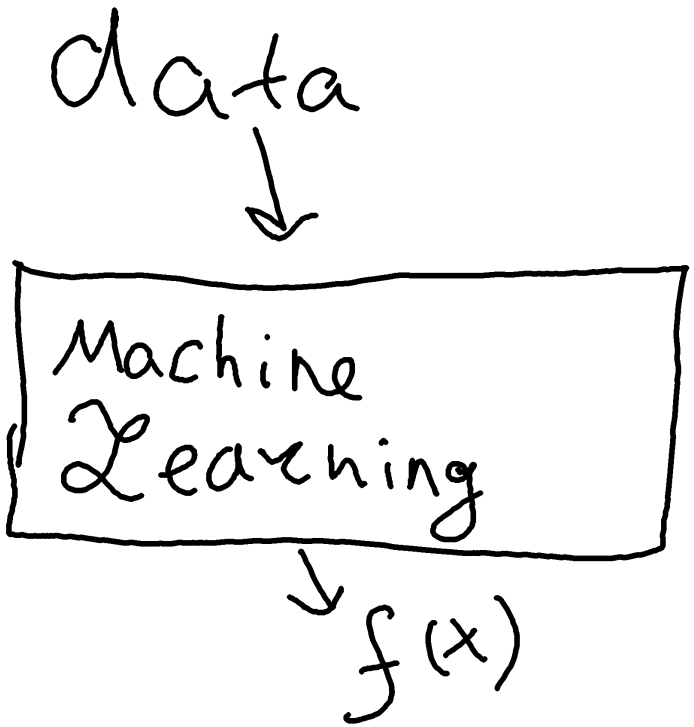


- data comes in;
- an algorithm (decision function) comes out.

Typical learning algorithm structure

- model :

$$\text{model} = \{f_\theta : \text{inputs} \to \text{predictions} \mid \theta \in \text{parameters}\};$$

- solver :

$$\text{solver} : \text{data} \to \text{model};$$

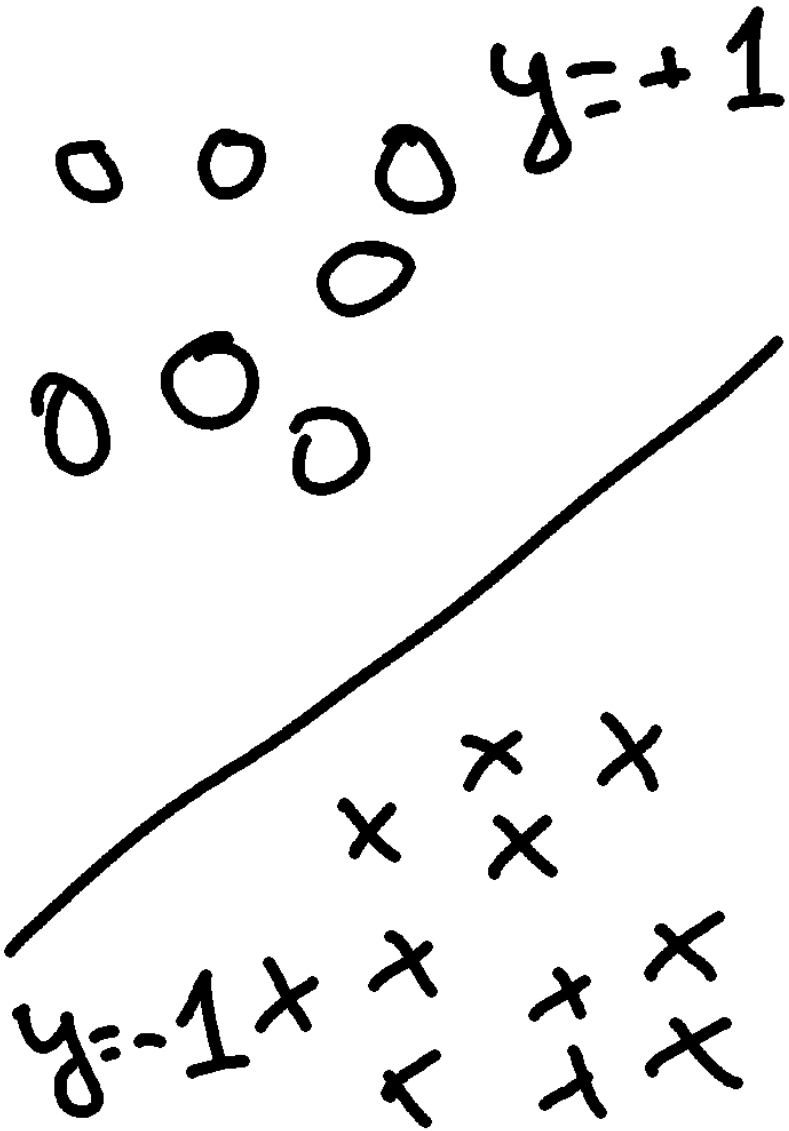
  - loss function:

$$\mathcal{L}(f, \text{data}) = \sum_{x,y \in \text{data}} \text{error}(f(x), y);$$

  - optimizer: gradient descent, genetic algorithms etc.

- quality metric: shows how good algorithm is.

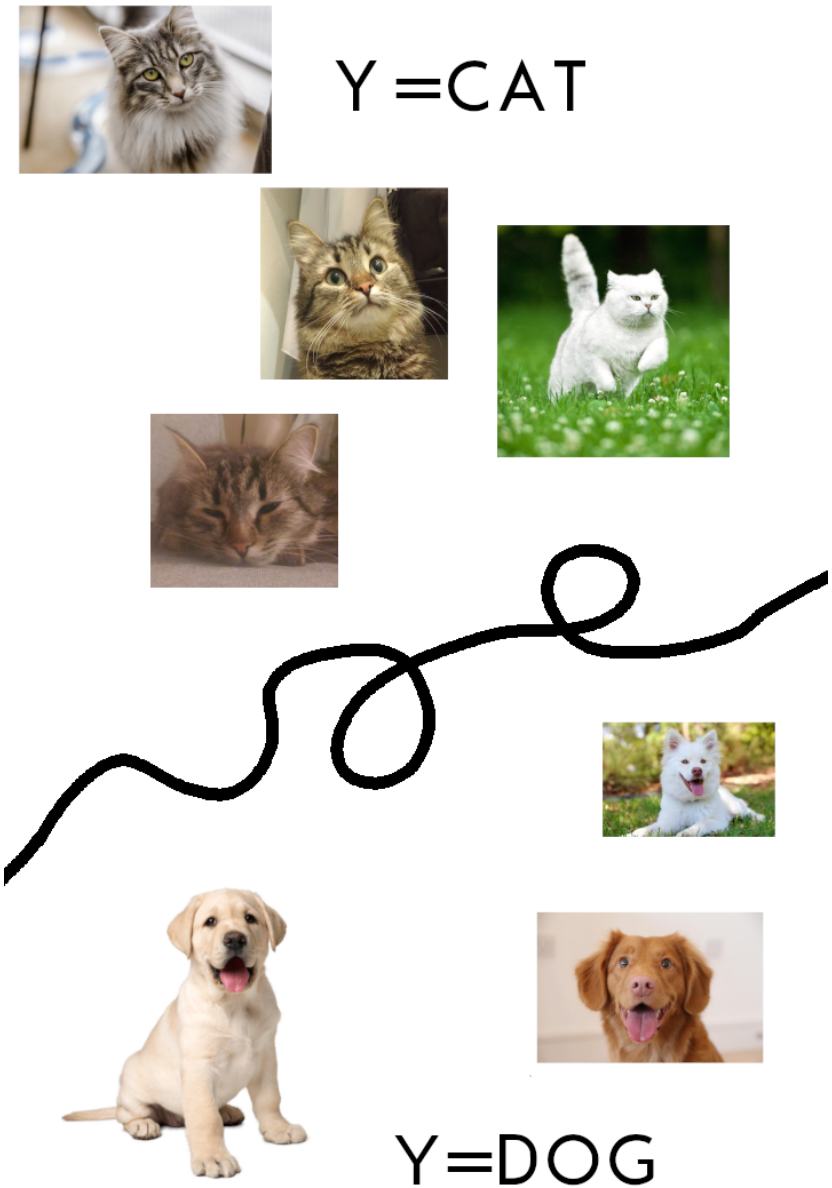
Linear models

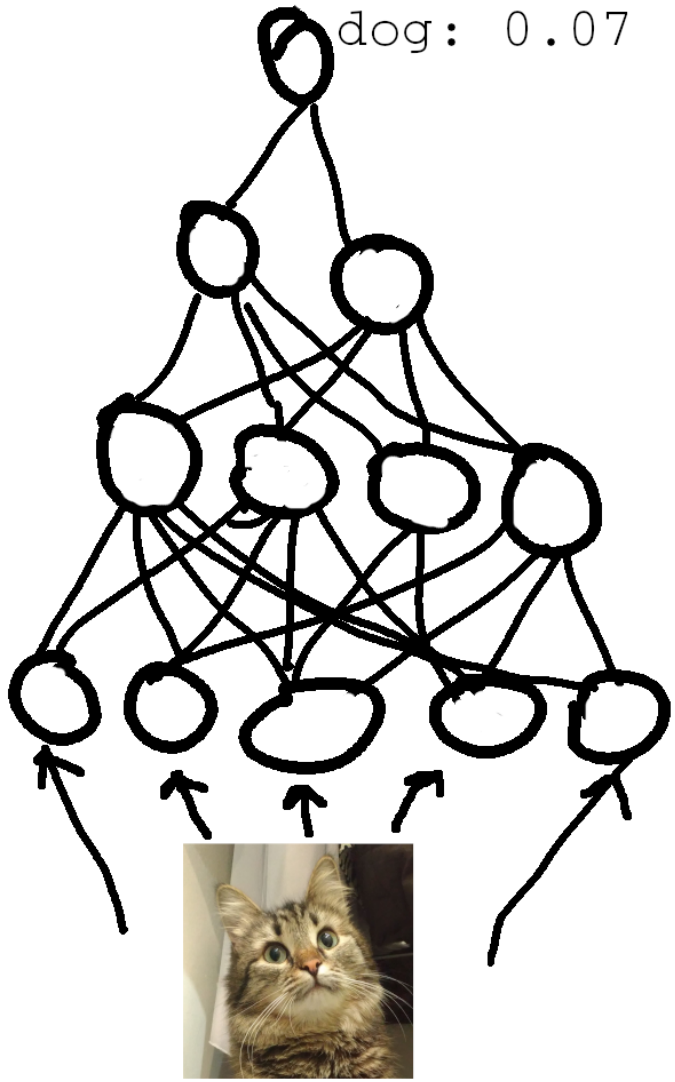


$$f(x) = w \cdot x + b;$$
$$w \in \mathrm{R}^2, b \in \mathrm{R}$$

$$\mathcal{L}(f) = \sum_i \log(1+\exp(y_i f(x_i)))$$

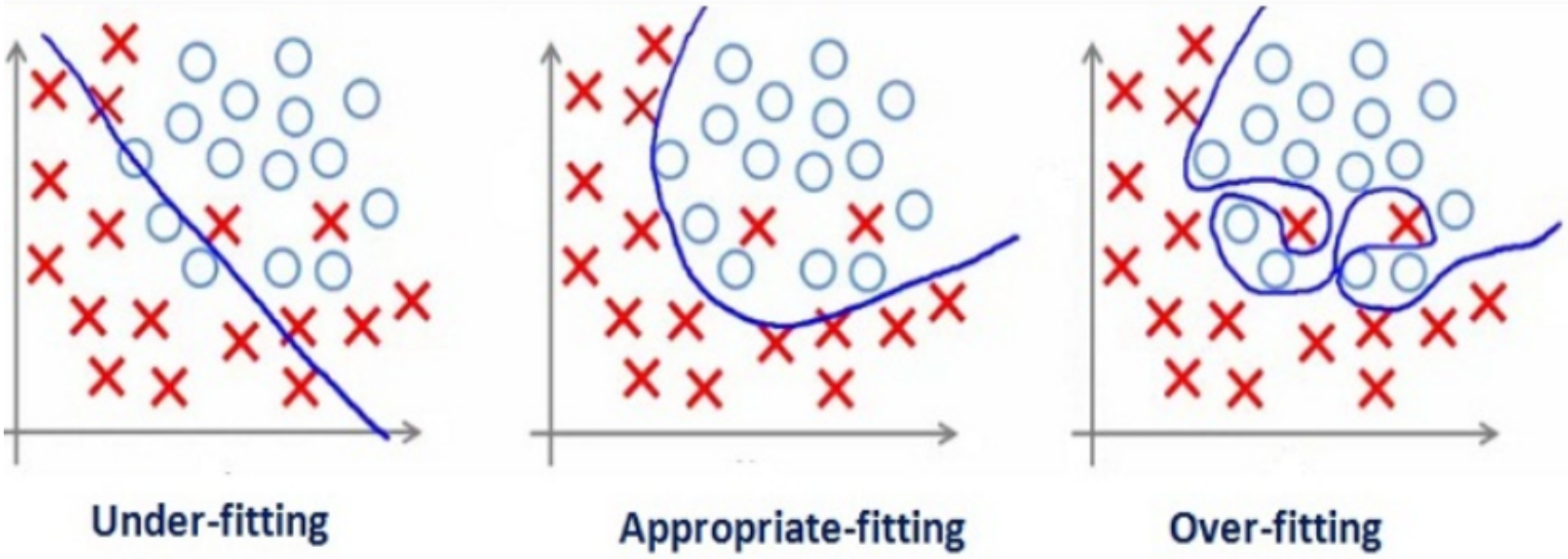
Non-linear models





Over/under-fitting

Over/under-fitting

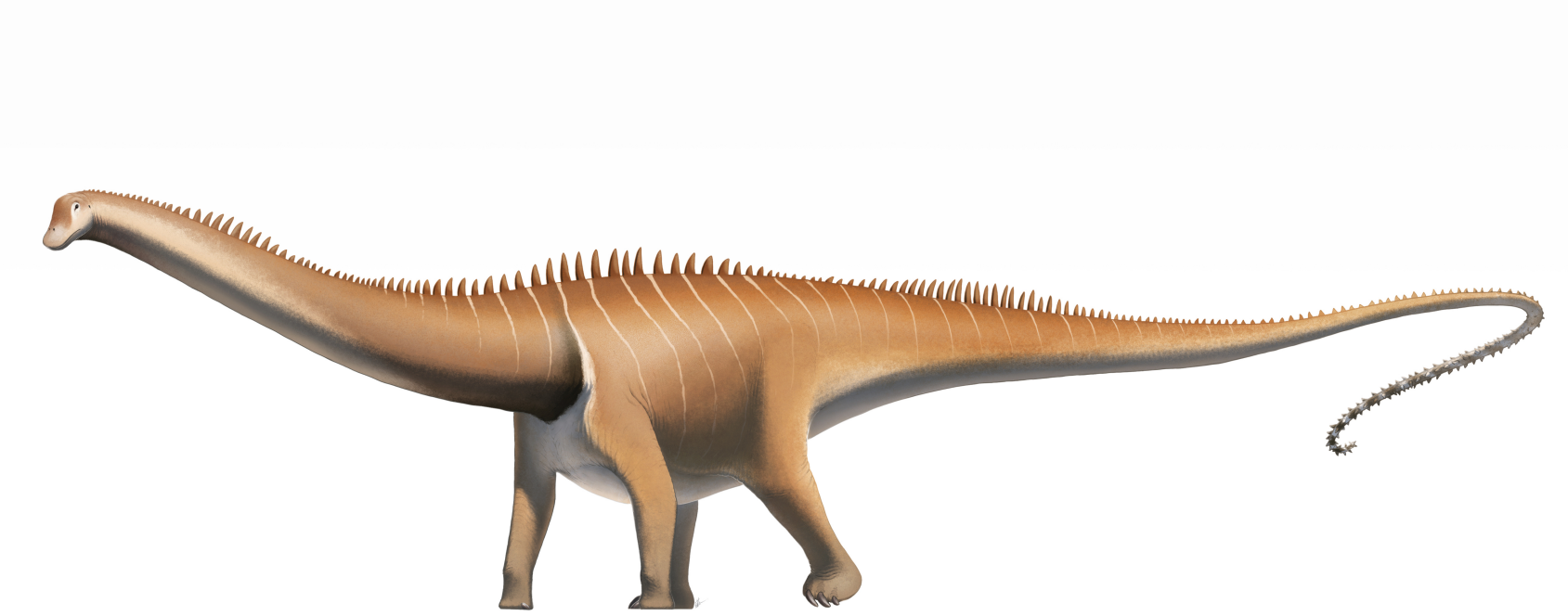


Put yourself into network shoes.

It is a Diplodocus:

Put yourself into network shoes.

It is a Diplodocus:



Put yourself into network shoes.

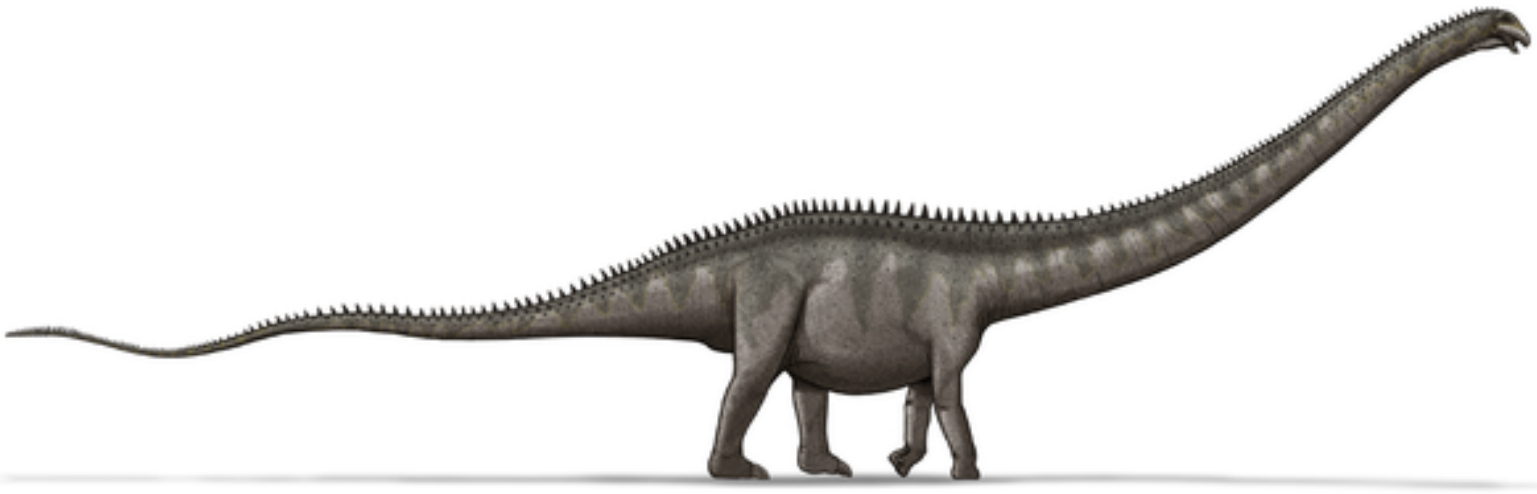
It is not a Diplodocus:

Put yourself into network shoes.

It is not a Diplodocus:

Put yourself into network shoes.

Is it a Diplodocus?



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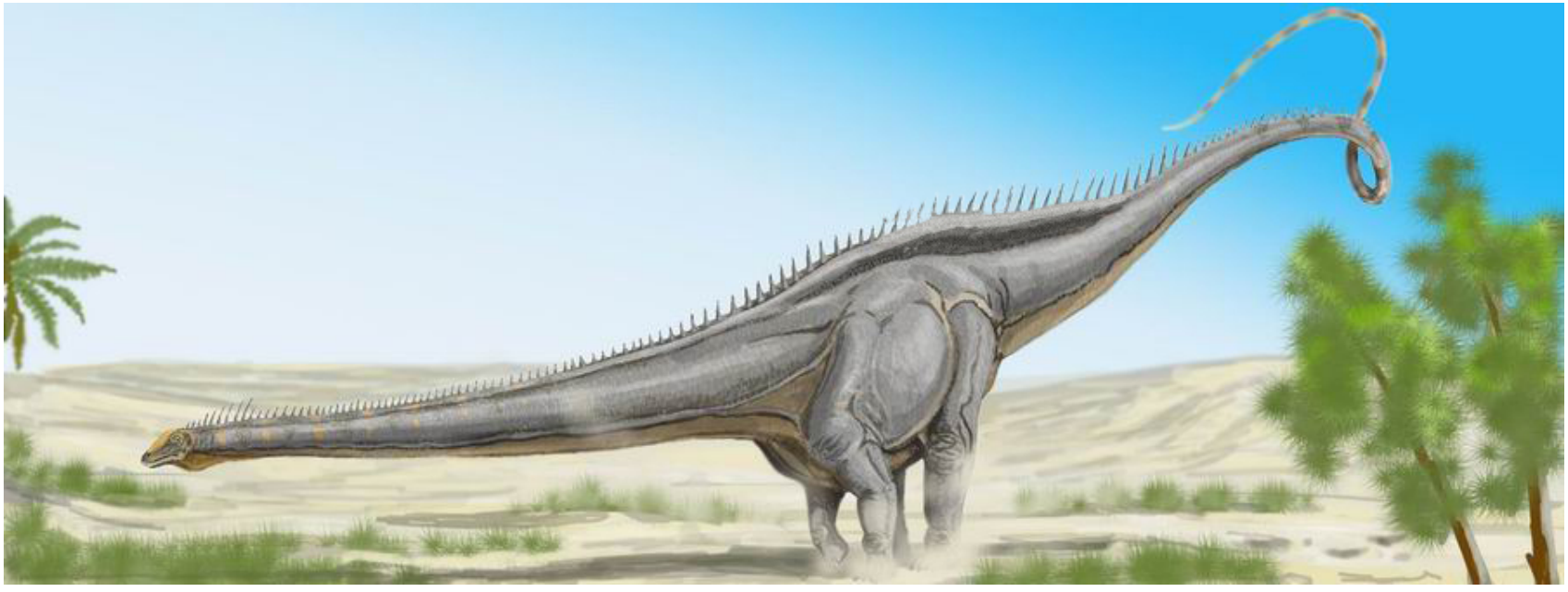


How to detect

- split dataset into two:
  - training set — for selecting decision function;
  - validation set — for **independent** quality metric evaluation.

- $Q_{\text{validation}} \approx Q_{\text{train}}$ and both low — probably underfitting;
- $Q_{\text{validation}} \approx Q_{\text{train}}$ and both high — just right;
- $Q_{\text{validation}} < Q_{\text{train}}$ — overfitting;

Which ML algorithms are the best?

IQ test: try to learn yourself!

First question from MENSA website:
Following the pattern shown in the number sequence below, what is the missing number?

$$1, 8, 27, ?, 125, 216$$

Possible answers:

- 36
- 45
- 46
- 64
- 99

IQ test: try to learn yourself!

First question from MENSA website:
Following the pattern shown in the number sequence below, what is the missing number?

X_{train}	1	2	3	5	6
y_{train}	1	8	27	125	216

$$X_{\text{test}} = (4,)$$

IQ test: try to learn yourself!

My solution:

$$y = \frac{1}{12}(91x^5 - 1519x^4 + 9449x^3 - 26705x^2 + 33588x - 14940)$$

- fits perfectly!

My answer:

- 99

IQ test

Why solution:

$$y = x^3$$

seems much more suitable than

$$y = \frac{1}{12}(91x^5 - 1519x^4 + 9449x^3 - 26705x^2 + 33588x - 14940)?$$

No Free Lunch theorem

Given:

- binary classification;
- metric: off-training set accuracy;
- **uniform prior over problems**.

Any two learning algorithms **on average** perform equally.

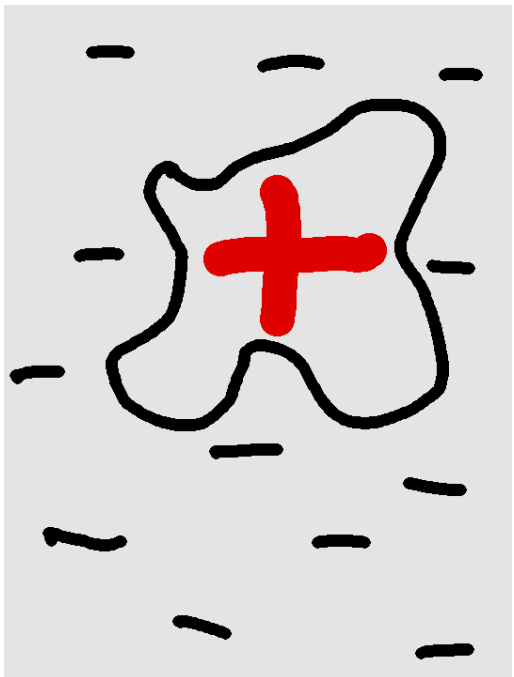
No Free Lunch theorem

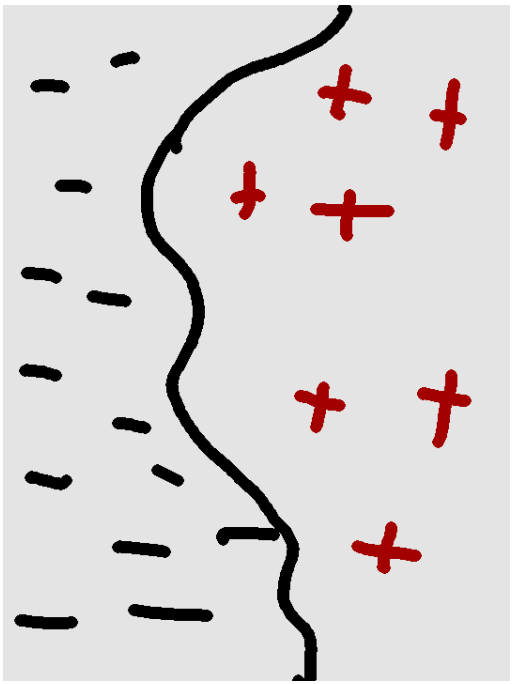
Given:

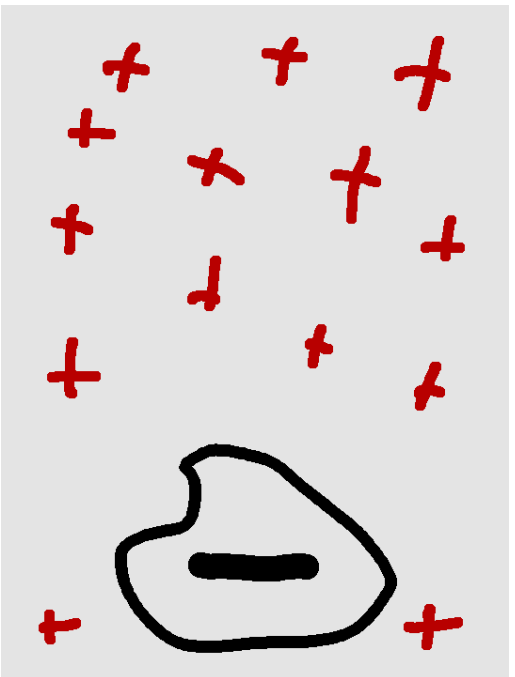
- binary classification;
- metric: off-training set accuracy;

Any increase in performance on one set of problems **must** be accompanied by equivalent decrease on another.

Example

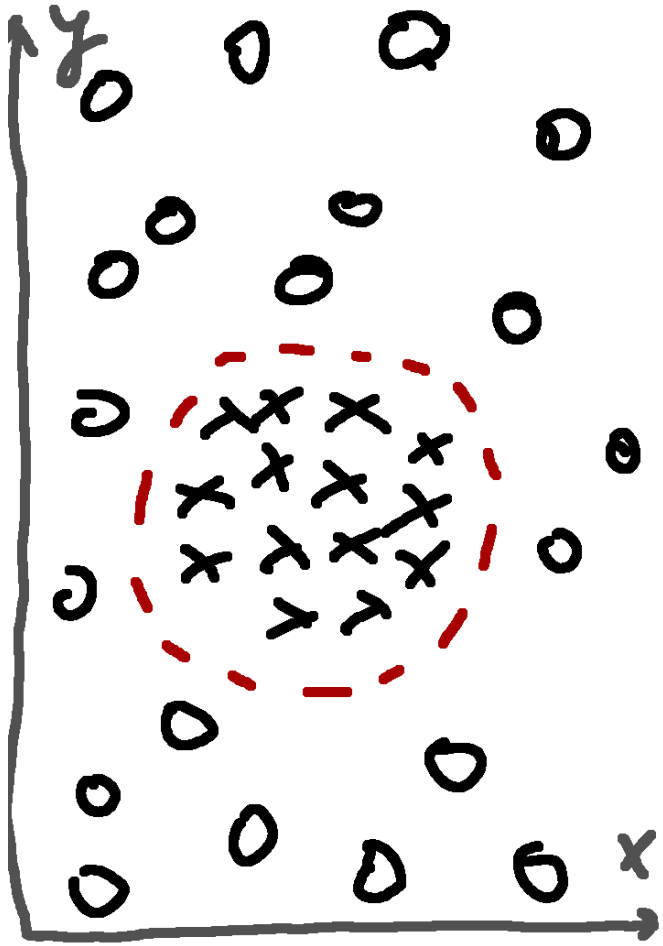




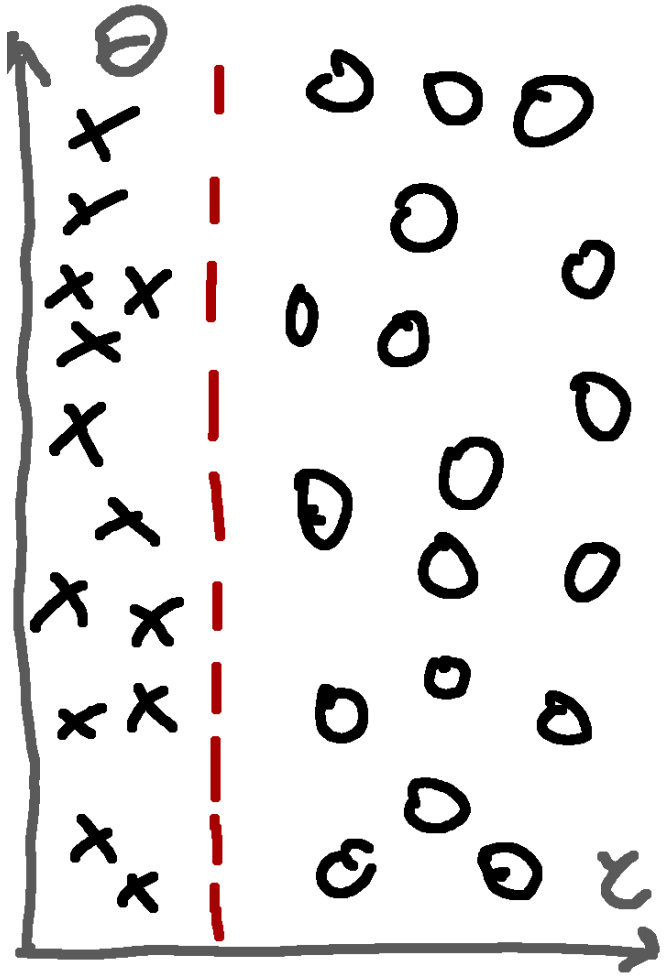


Example

Cartesian

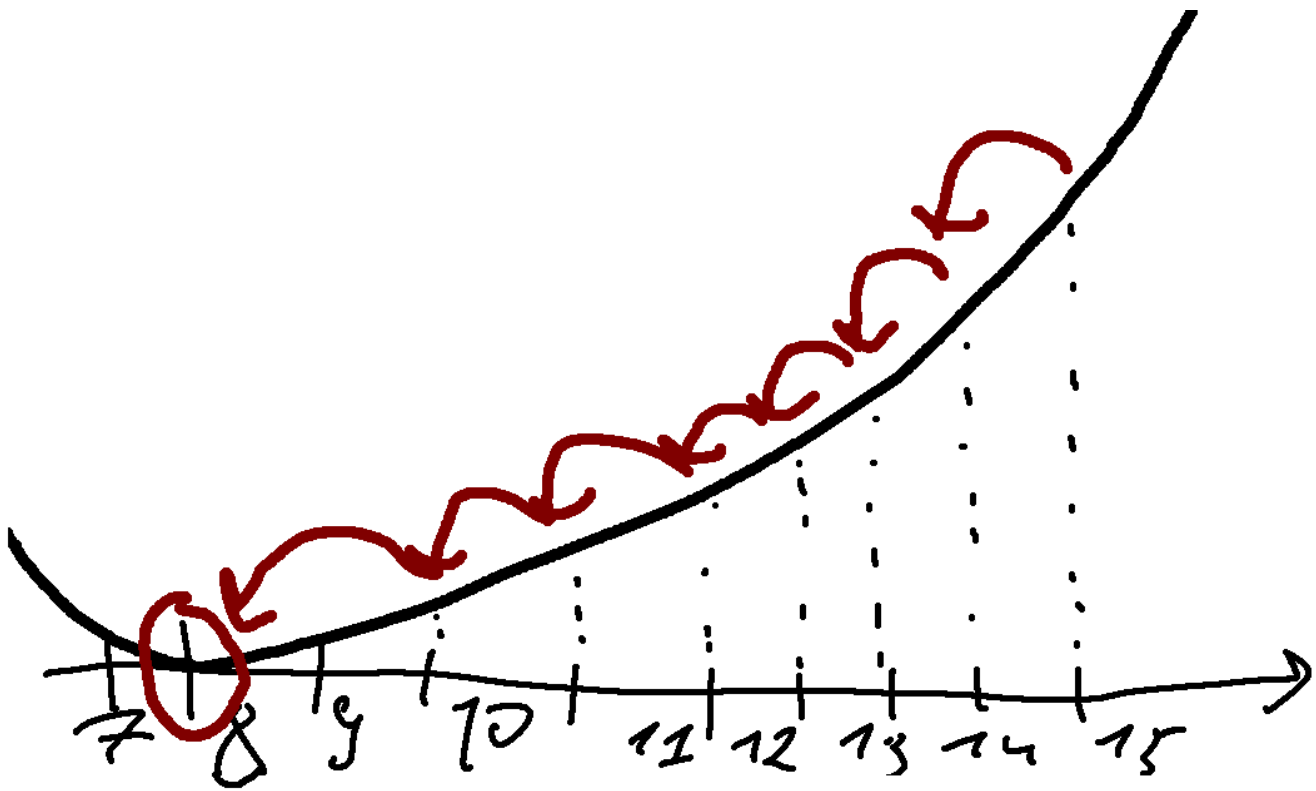


Polar



Example

$$\min_{x \in \{0,\ldots,15\}} (x-8)^2$$



Example

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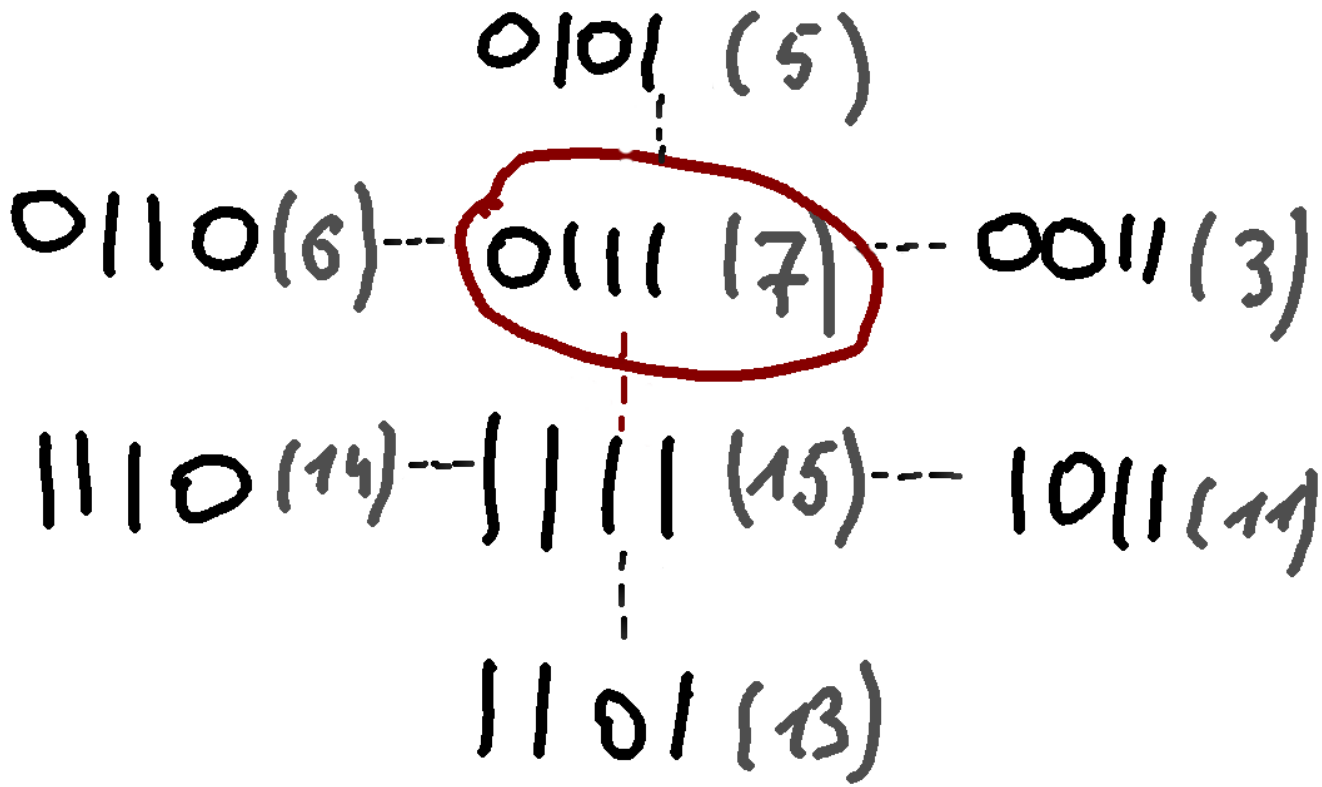


Neural Networks

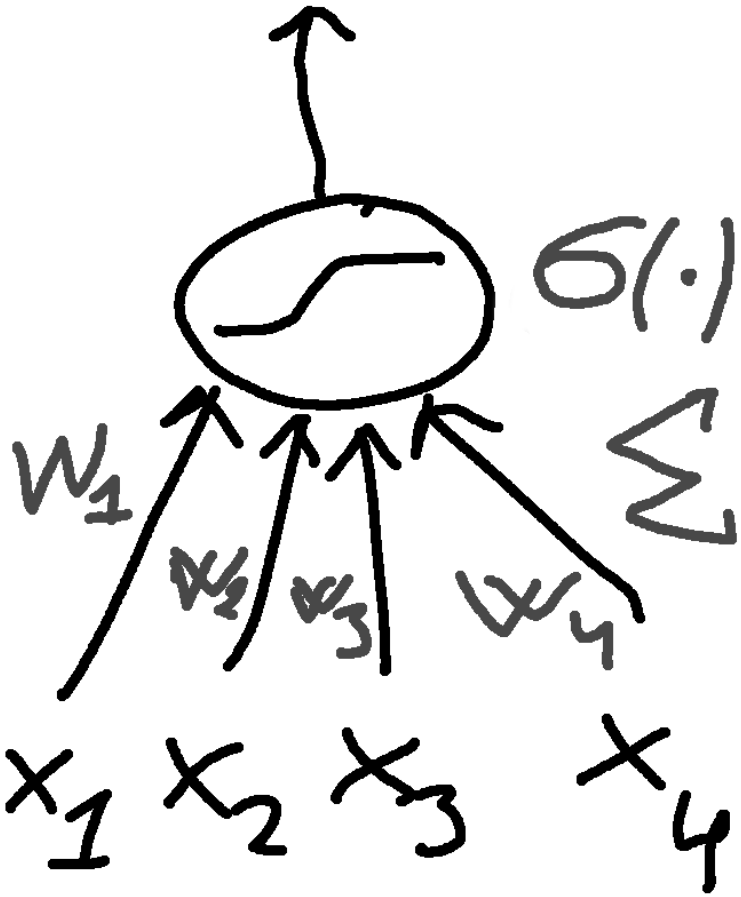
NFL vs humans

One learning algorithm can not be better than others[1].

Family of algorithms can.

[1] assuming uniform prior over problems

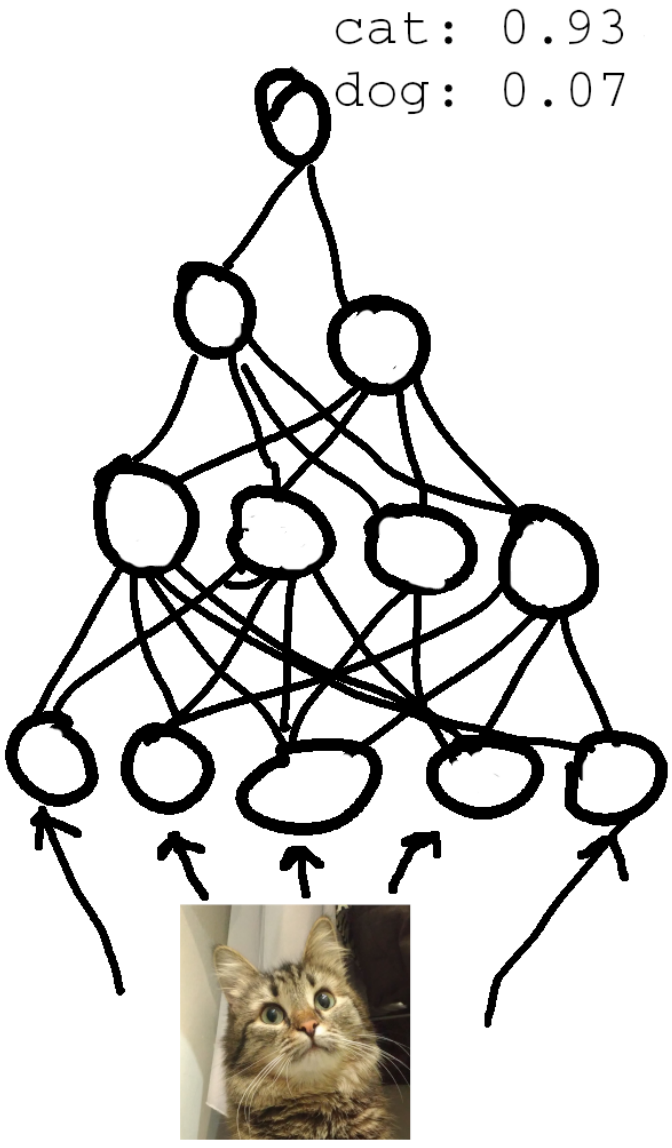
"Neuron"



$$\text{output} = \sigma(b + \sum_i w_i x_i)$$

- sum of all inputs with weights;
- non-linearity.

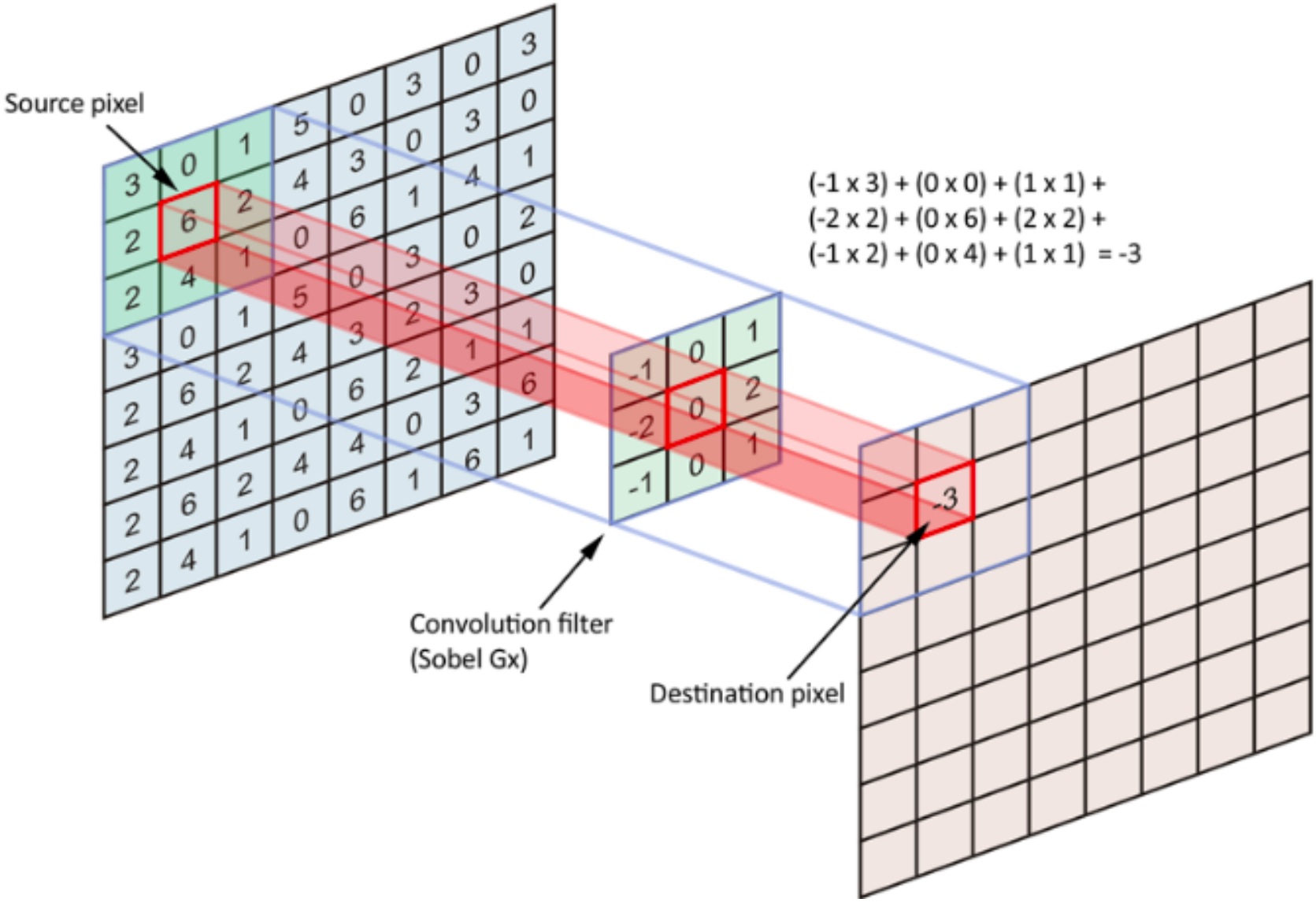
Deep learning



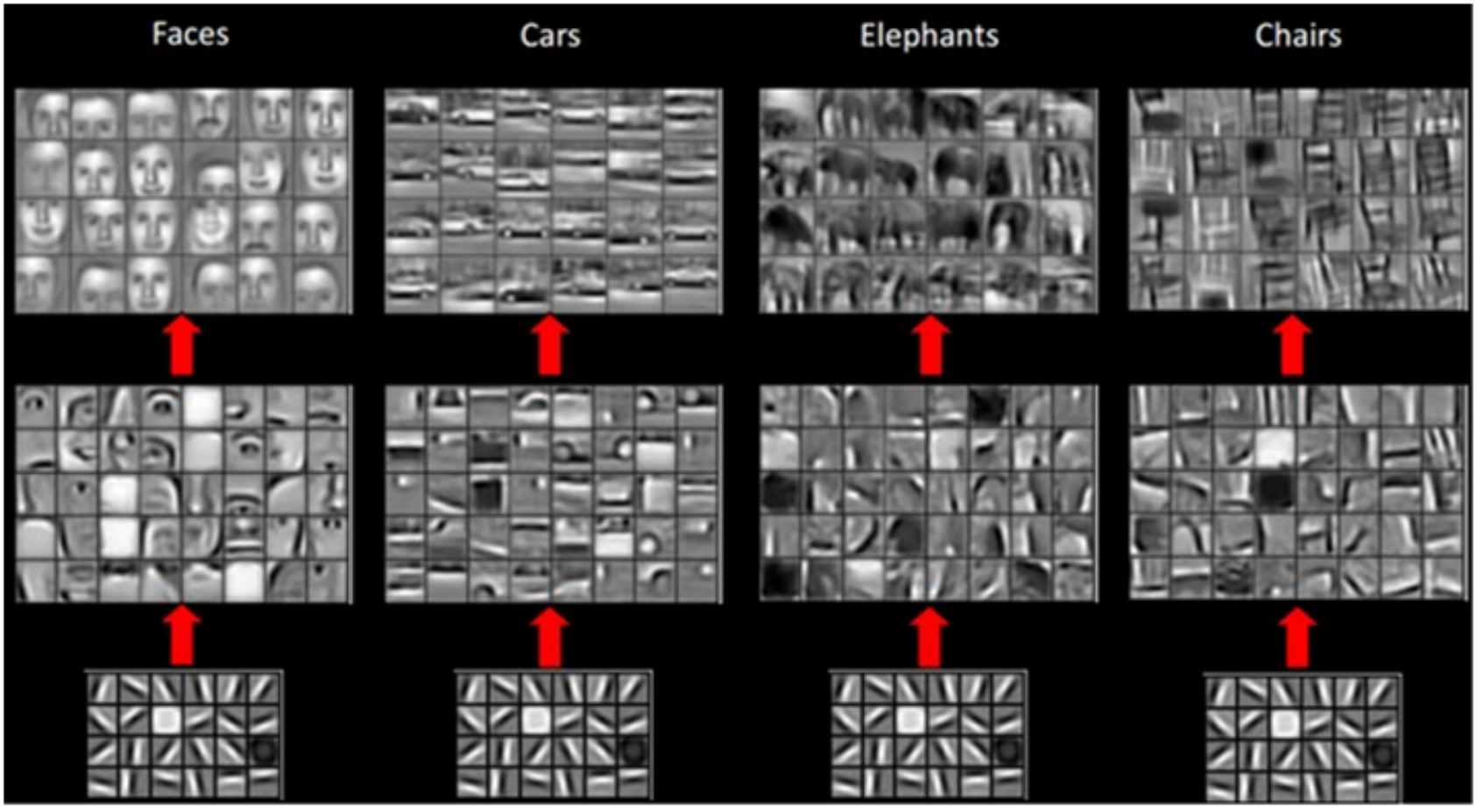
- neurons are organized into layer;
- layer are typically connected sequentially.

Convolutional Networks

Convolutional Networks

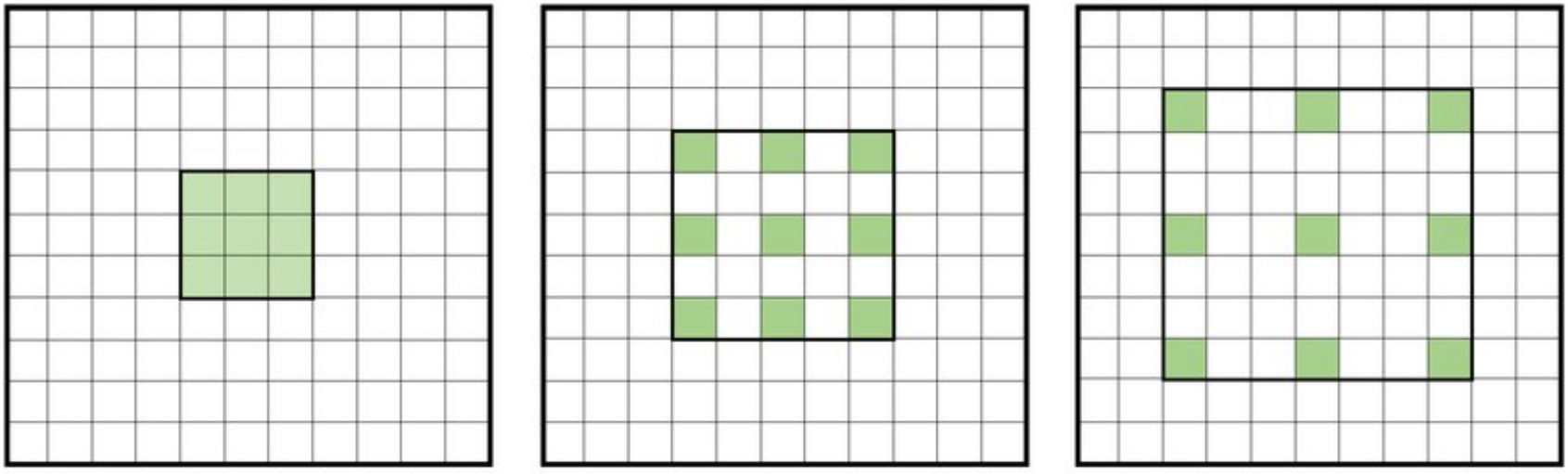


Convolutional Networks



Types of convolution

- ordinary / atrous / strided;
- size of the window: 1x1 / 3x3 / 5x5;
- ordinary / depthwise / separable / ...

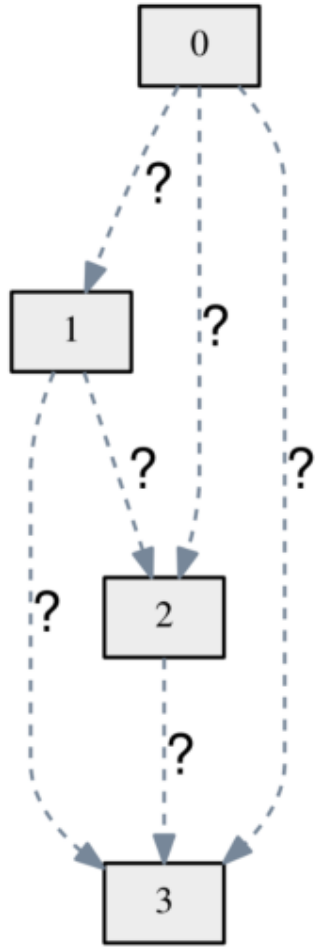


Which one to choose?

Which one to choose?

- people are bad at fine tuning;
  - even data scientists;
- checking all possible combinations:
  - 5 layer network with 3 options for each layer:
    - 243 options ($\sim$ 1 year).
- evolutionary algorithms;
- Bayesian Optimization;

DARTS



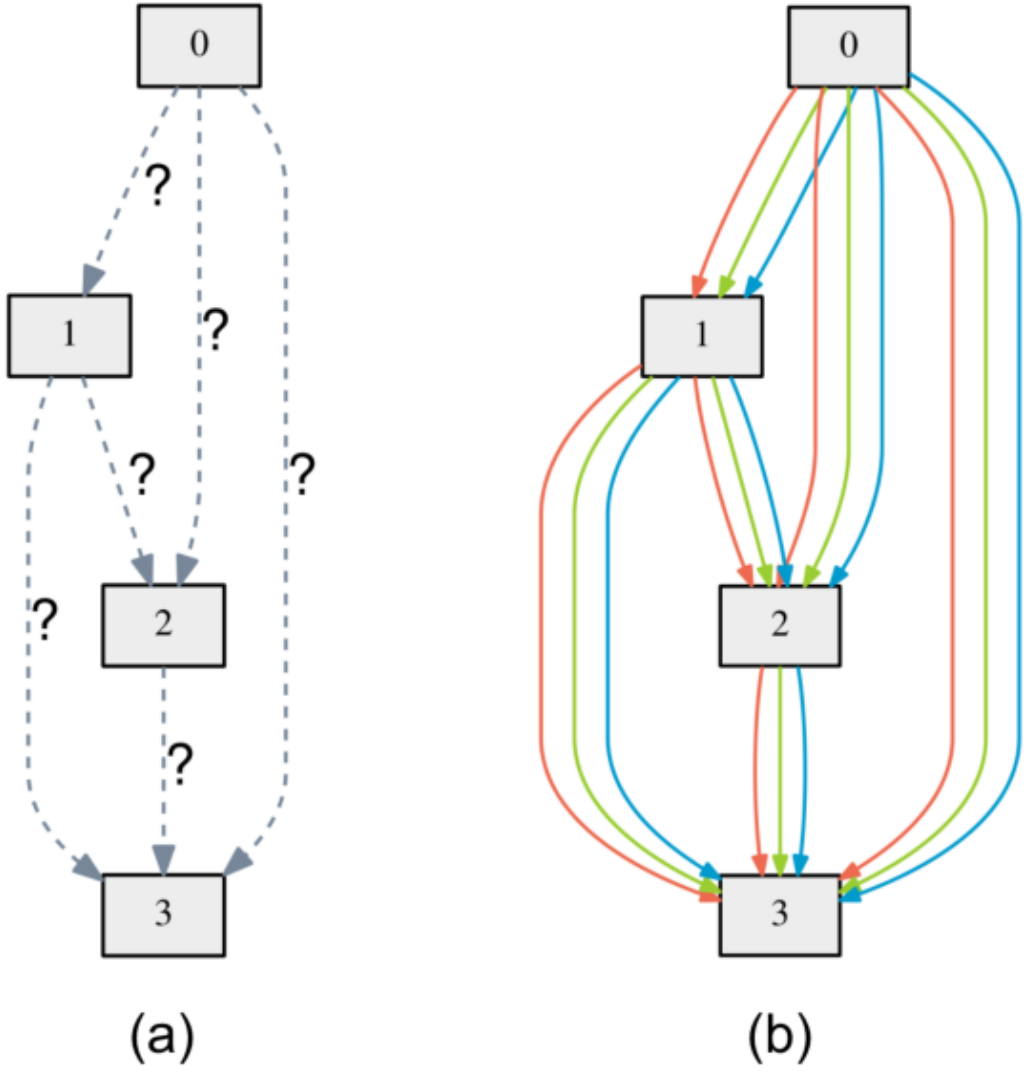
(a)

DARTS

- $O_i(x)$ — i-th candidate operation:
  - e.g. $O_1(x)$ - convolution 1x1, $O_2(x)$ - convolution 3x3, etc

$$O(x) = \sum_i \frac{\exp(\alpha_i)}{\sum_k \exp(\alpha_k)} O_i(x)$$

DARTS



DARTS

- X_{train} — data for training;
- $X_{\text{validation}}$ — data for validation;

$$\begin{aligned} \min_{\alpha} \quad & \mathcal{L}_{\text{val}}(w^*(\alpha), \alpha) \\ \text{s.t.} \quad & w^*(\alpha) = \arg\min_w \mathcal{L}_{\text{train}}(w, \alpha) \end{aligned}$$

DARTS

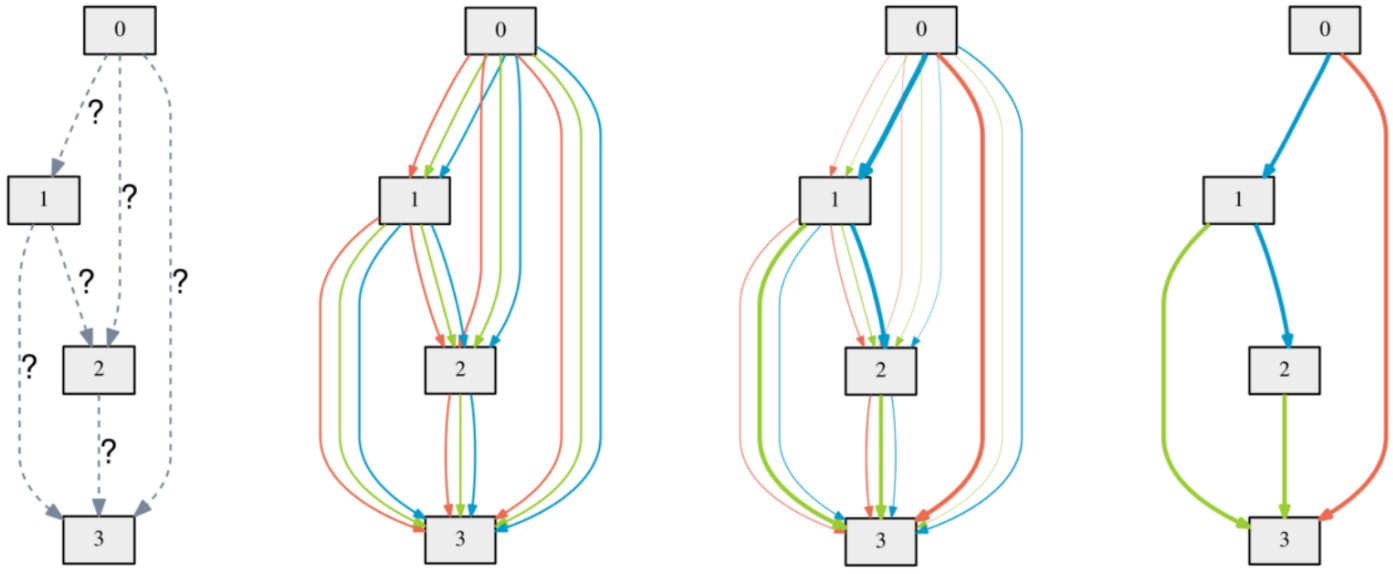


Figure 1: An overview of DARTS: (a) Operations on the edges are initially unknown. (b) Continuous relaxation of the search space by placing a mixture of candidate operations on each edge. (c) Joint optimization of the mixing probabilities and the network weights by solving a bilevel optimization problem. (d) Inducing the final architecture from the learned mixing probabilities.

Machine Learning and Data Mining

Machine Learning and Data Mining

1. a little bit of theory:
    - No Free Lunch theorem;
    - bias-variance decomposition;
2. meta-algorithms:
    - boosting;
    - bagging;
    - stacking;
3. optimization:
    - gradient optimization;
    - black-box optimization (incl. Bayesian Optimization);
4. Deep Learning:
    - overview, methods and tricks;
    - generative models (incl. RBM, VAE, GAN);
5. Meta Learning:
    - model selection (incl. DARTS);
    - learning to learn; concept learning.

Summary

Summary

1. Structure of a Machine Learning Algorithm.
2. No Free Lunch Theorem.
3. Neural Networks and Deep Learning.
4. Convolutional Neural Network.
5. Optimal Architecture Search.
6. The course syllabus.

References

- Wolpert DH. The supervised learning no-free-lunch theorems. InSoft computing and industry 2002 (pp. 25-42). Springer, London.
- Liu H, Simonyan K, Yang Y. Darts: Differentiable architecture search. arXiv preprint arXiv:1806.09055. 2018 Jun 24.
- Sermanet P, Chintala S, LeCun Y. Convolutional neural networks applied to house numbers digit classification. InPattern Recognition (ICPR), 2012 21st International Conference on 2012 Nov 11 (pp. 3288-3291). IEEE.
- Moscato P. On evolution, search, optimization, genetic algorithms and martial arts: Towards memetic algorithms. Caltech concurrent computation program, C3P Report. 1989 Sep;826:1989.