Machine Learning and Data Mining

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February 4, 2019

Machine Learning

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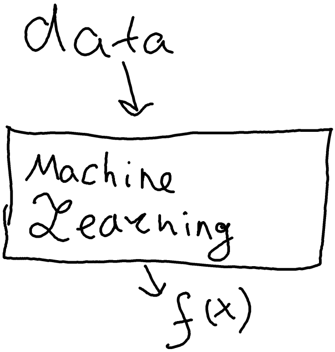


- data comes in;
- an algorithm (decision function) comes out.

Typical learning algorithm structure

- model :

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

- solver :

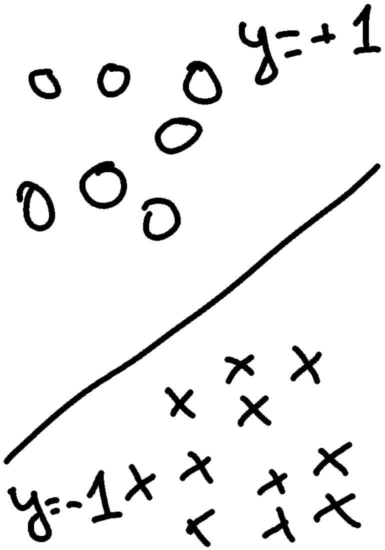
$$\text{solver} : \text{data} \to \text{model};$$

  - 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.

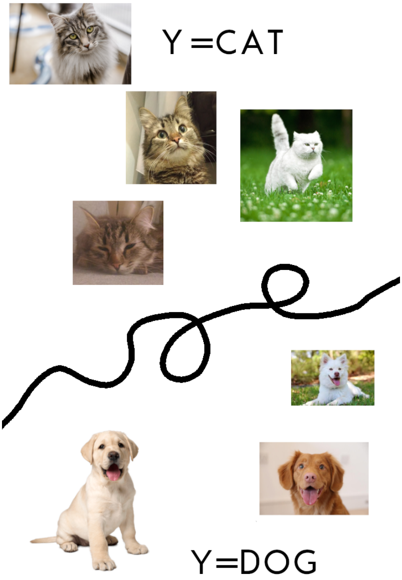
Linear models

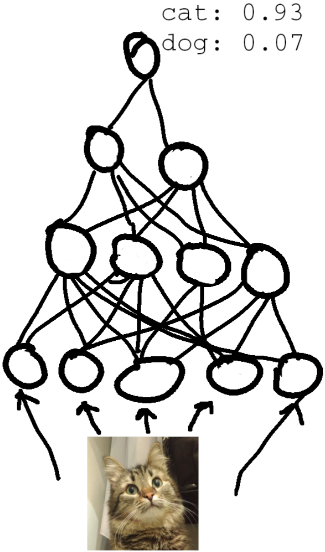


$$
\begin{aligned}
f(x) &= w \cdot x + b; \\
w &\in \mathrm{R}^2, b \in \mathrm{R}
\end{aligned}
$$

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

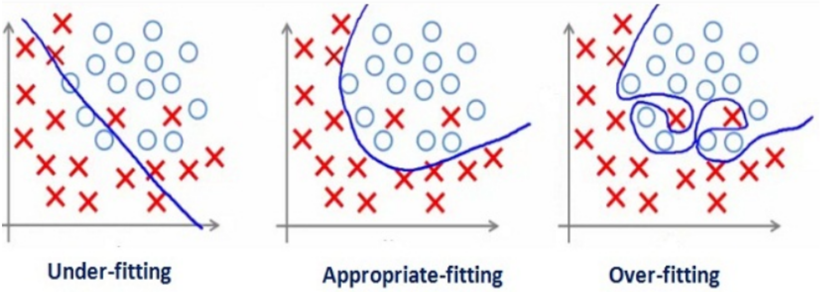
Non-linear models





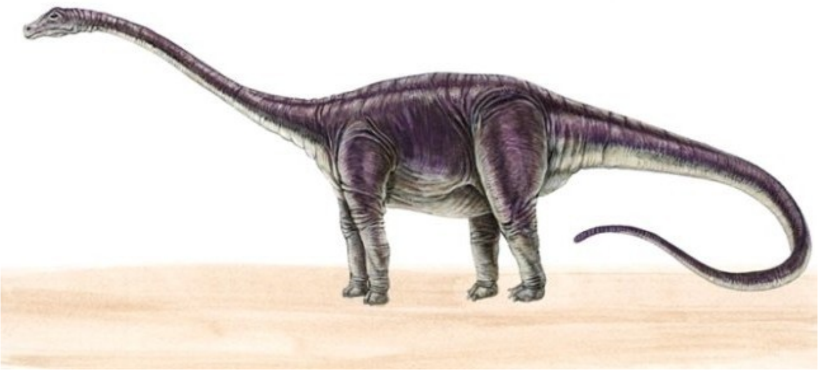
Over/under-fitting

Over/under-fitting



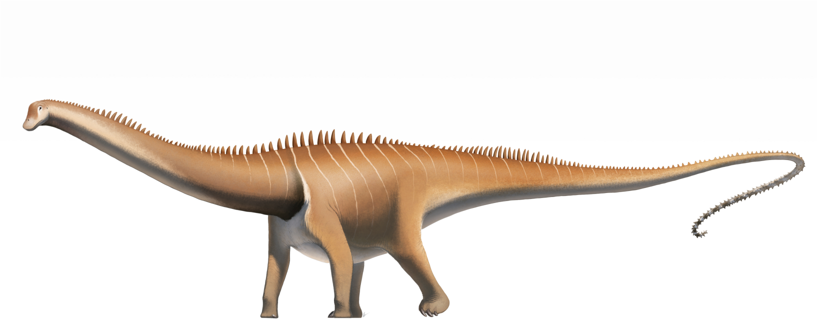
Put yourself into network shoes.

It is a Diplodocus:



Put yourself into network shoes.

It is a Diplodocus:



Put yourself into network shoes.

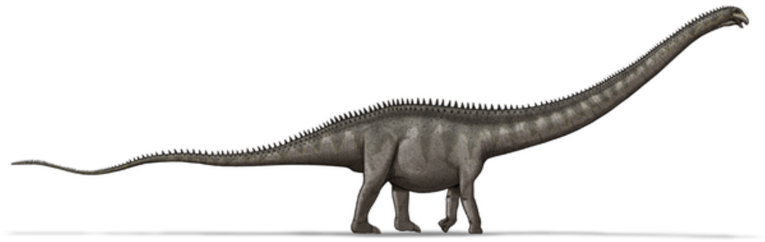
It is not a Diplodocus:

Put yourself into network shoes.

It is not a Diplodocus:

Put yourself into network shoes.

Is it a Diplodocus?



Put yourself into network shoes.

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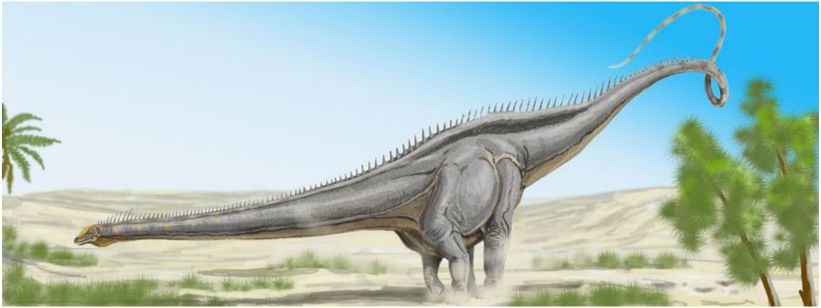
Put yourself into network shoes.

Is it a Diplodocus?



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.

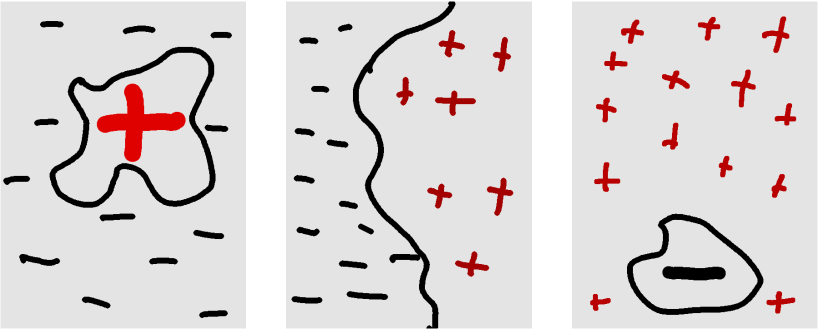
No Free Lunch theorem

Given:

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

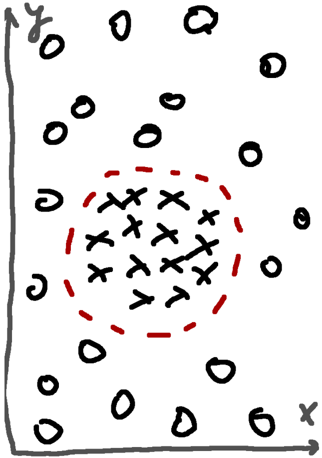
Any increase in performance on one set of problems **must** be accompanied by equivalent decrease on another.

Example

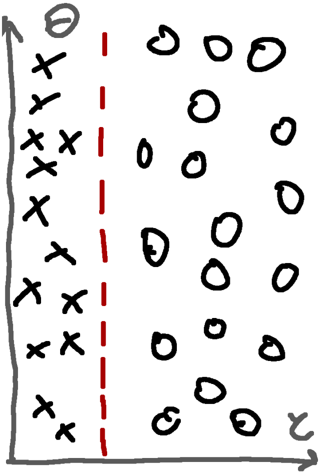


Example

Cartesian

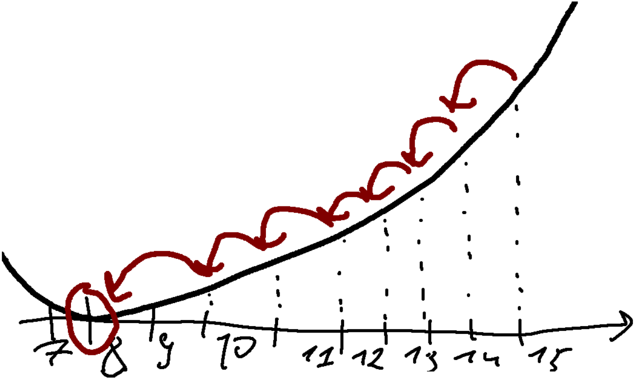


Polar



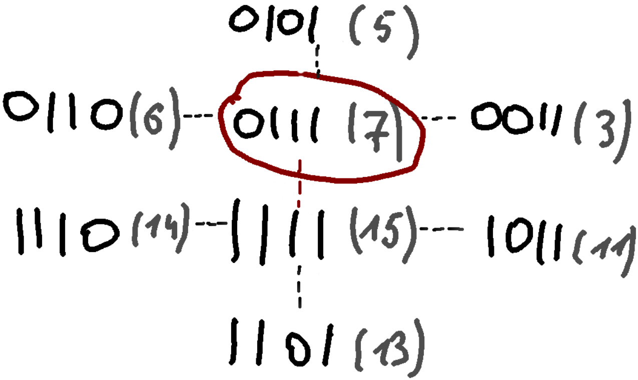
Example

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



Example

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



Neural Networks

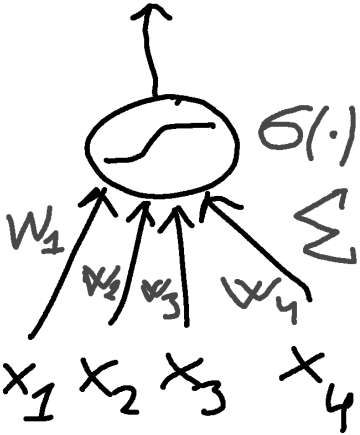
NFL vs humans

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

Family of algorithms can.

[1] assuming uniform prior over problems

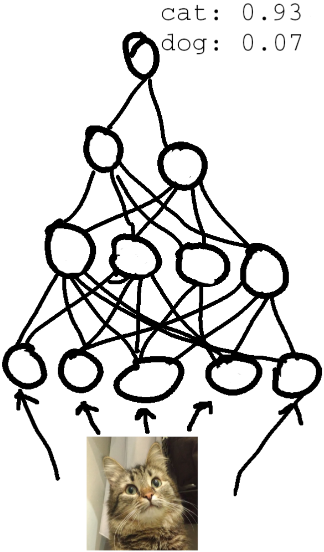
”Neuron”



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

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

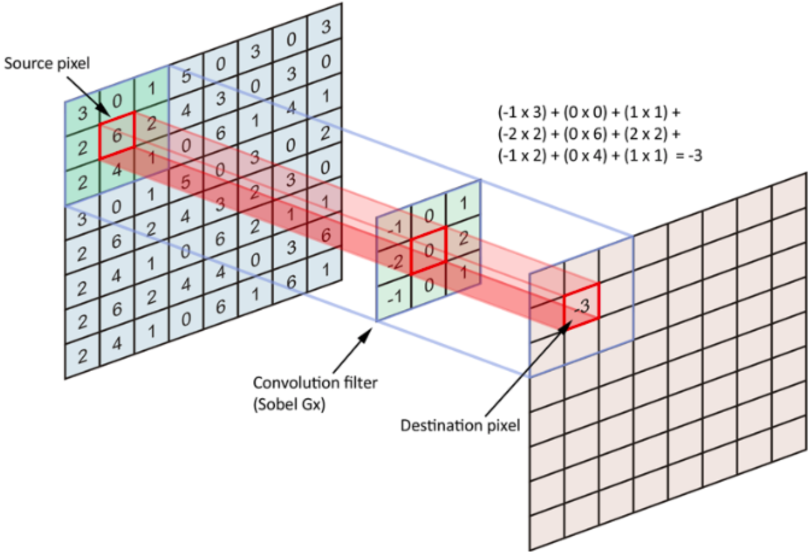
Deep learning



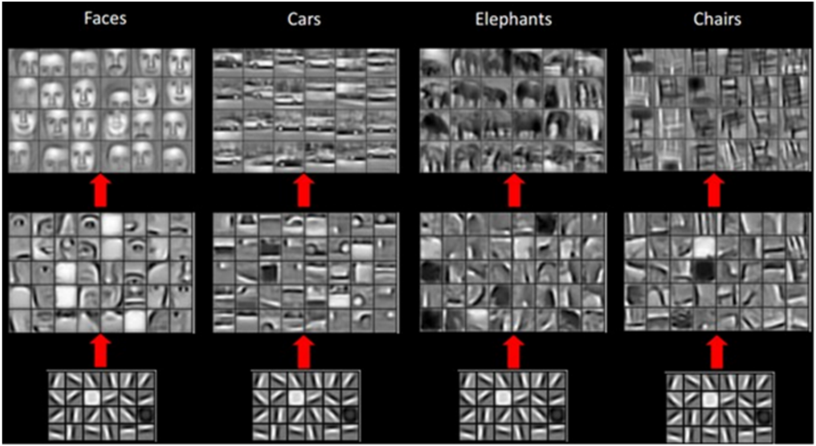
- neurons are organized into layer;
- layer are typically connected sequentially.

Convolutional Networks

Convolutional Networks

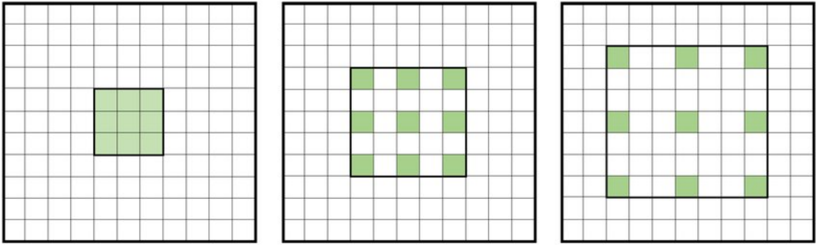


Convolutional Networks



Types of convolution

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



Kernel 3 x 3
Rate = 1

Kernel 3 x 3
Rate = 2

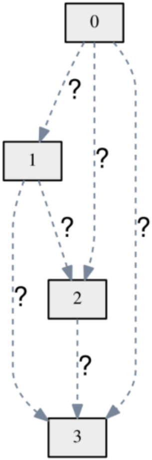
Kernel 3 x 3
Rate = 3

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

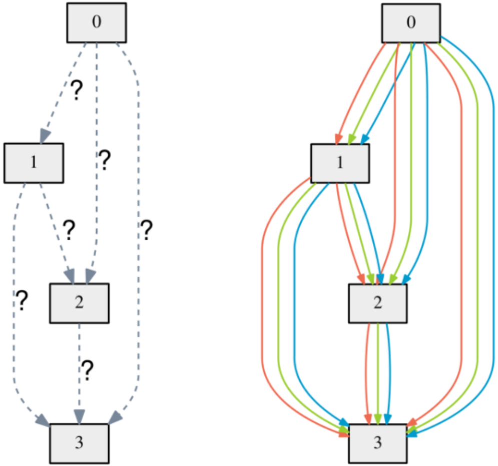


(a)

- $O_i(x)$ — 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



(a) (b)

DARTS

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

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

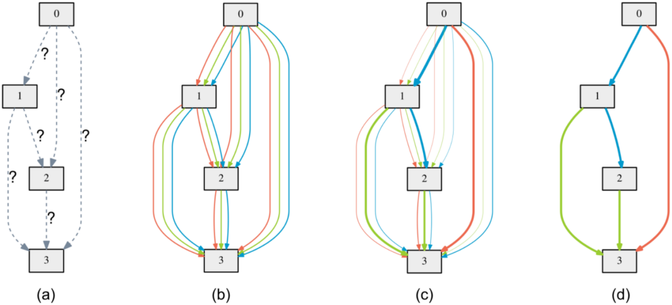


Figure 1: An overview of DARTS: (a) Operations on the edges are initially unknown. (b) Continuous relaxation of the search space by placing a mixture of candidate operations on each edge. (c) Joint optimization of the mixing probabilities and the network weights by solving a bilevel optimization problem.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

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