Machine Learning and Data Mining

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Machine Learning

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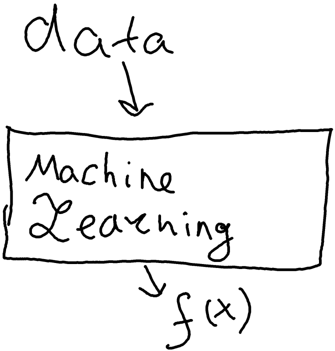


- data comes in;
- an algorithm (decision function) comes out.

Typical learning algorithm structure

- model :

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

- solver :

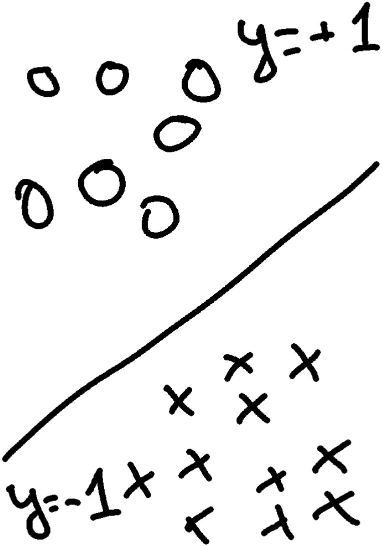
$$\text{solver} : \text{data} \to \text{model};$$

    - loss function:

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

    - optimizer: gradient descent, genetic algorithms etc.

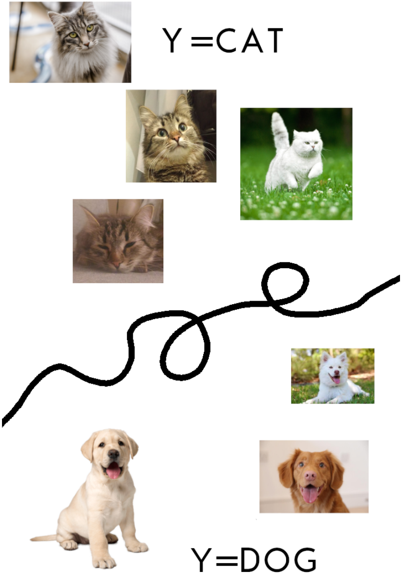
Linear models

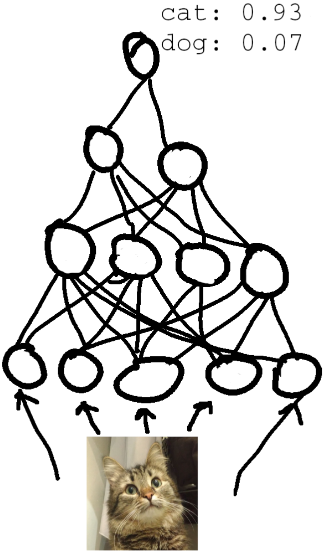


$$\begin{aligned} f(x) &= w \cdot x + b; \\ w &\in \mathrm{R}^2, b \in \mathrm{R} \end{aligned}$$

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

Non-linear models





Which ML algorithms are the best?

No Free Lunch theorem

Given:

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

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

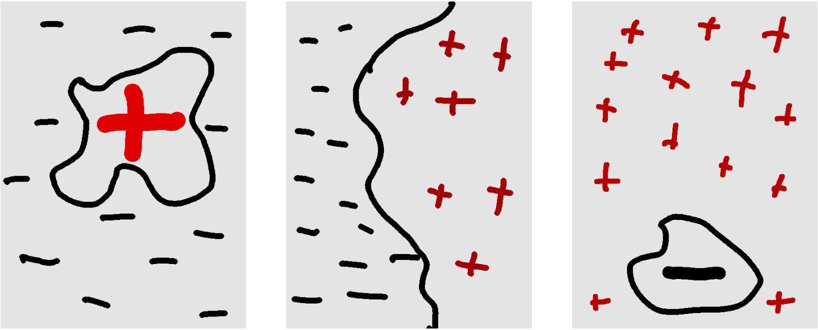
No Free Lunch theorem

Given:

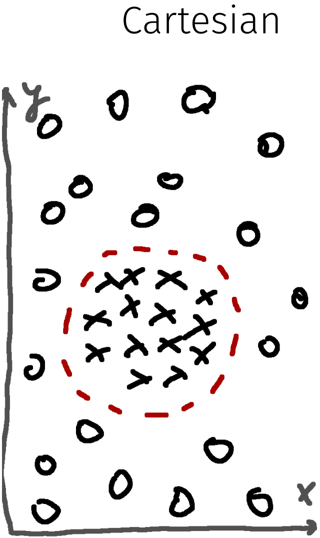
- binary classification;
- metric: off-training set accuracy;

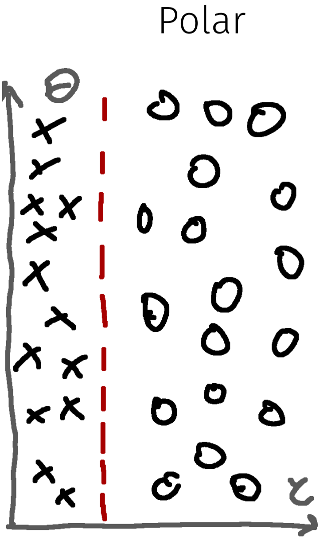
Any increase in performance on one set of problems **must** be accompanied by equivalent decrease on another.

Example



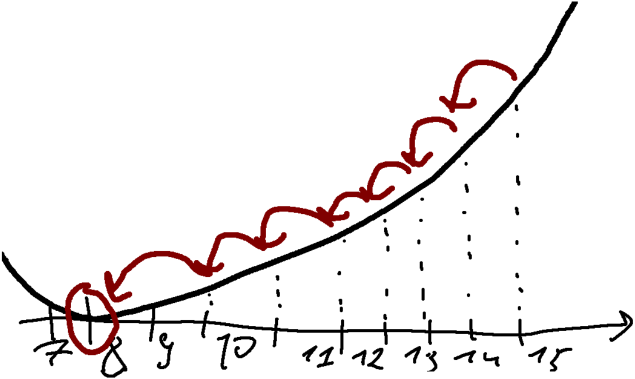
Example





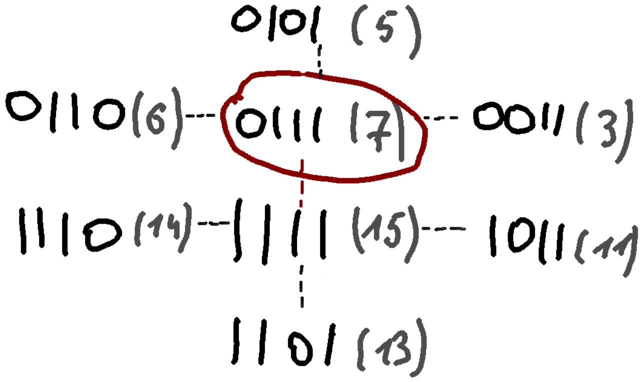
Example

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



Example

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



Neural Networks

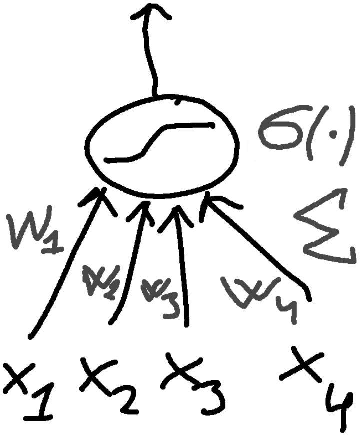
NFL vs humans

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

Family of algorithms can.

[1] assuming uniform prior over problems

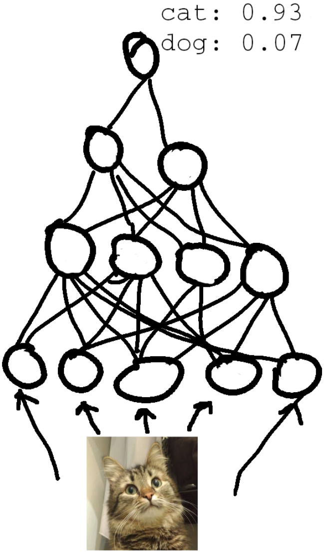
"Neuron"



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

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

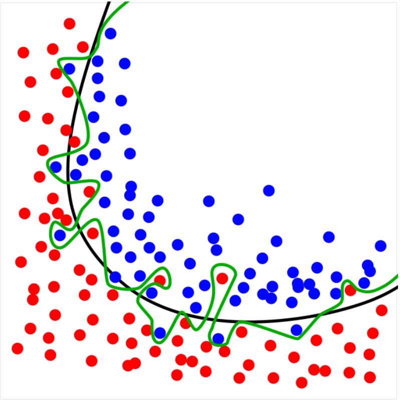
Deep learning



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

Overfitting

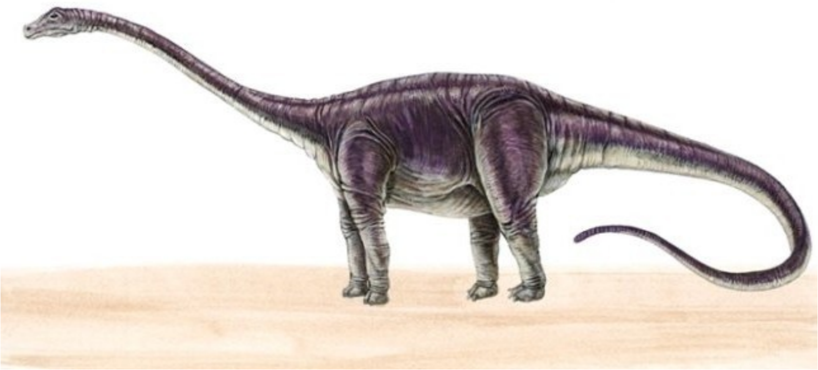
Overfitting



- dense Neural Networks tend to have a huge number of parameters;
- they can memorize examples!

Put yourself into network shoes.

It is a Diplodocus:



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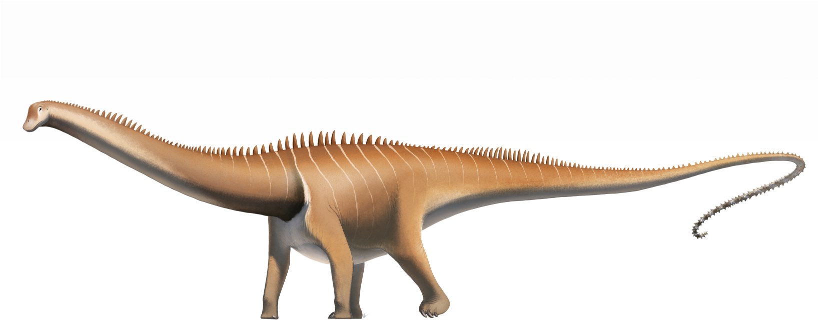
It is a Diplodocus:



Put yourself into network shoes.

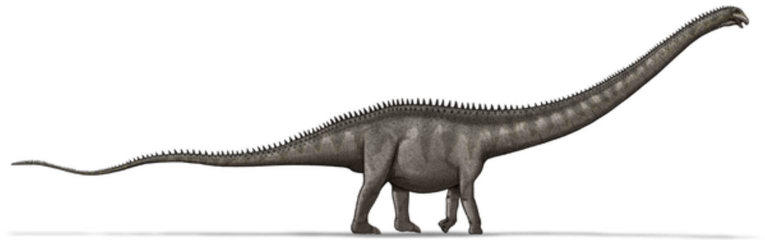
It is not a Diplodocus:

Put yourself into network shoes.

It is not a Diplodocus:

Put yourself into network shoes.

Is it a Diplodocus?



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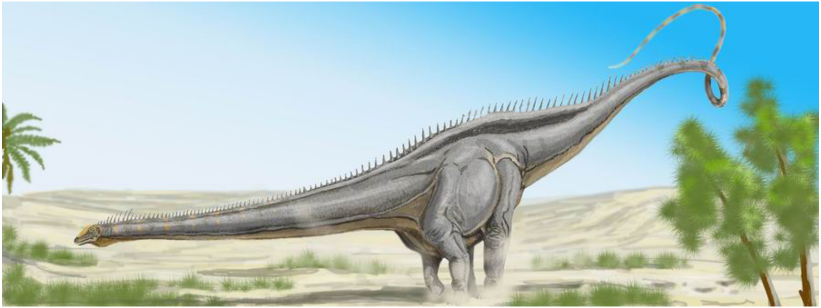
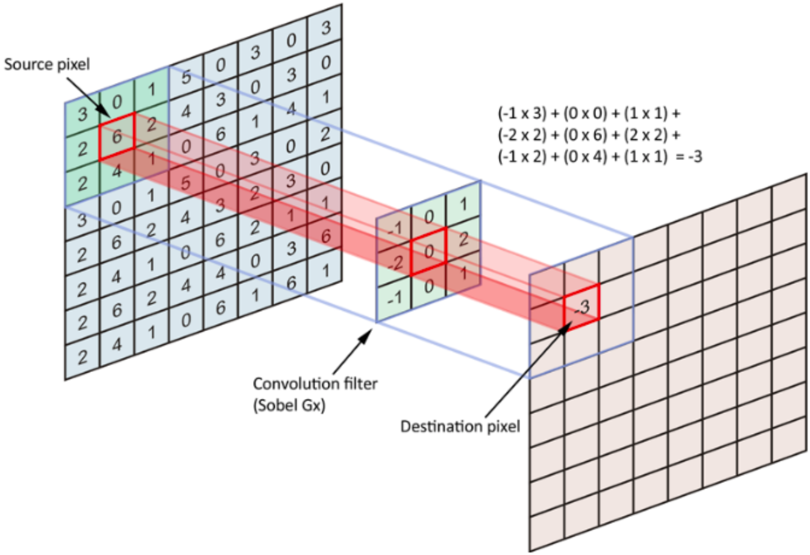
Put yourself into network shoes.

Is it Diplodocus?

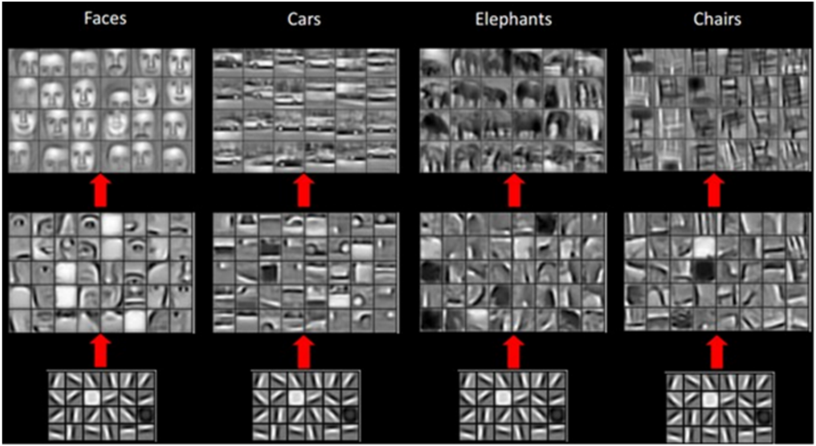


Convolutional Networks

Convolutional Networks

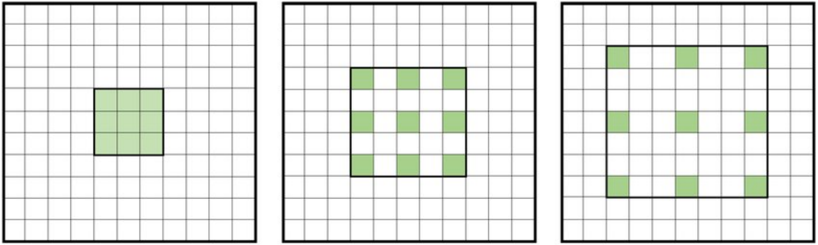


Convolutional Networks



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

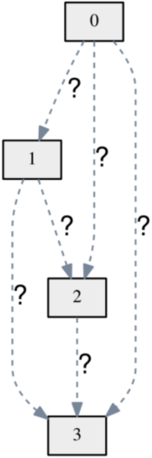
Kernel 3 x 3
Rate = 3

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

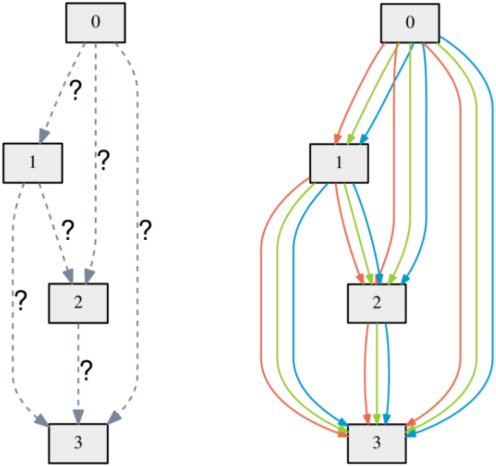


(a)

- $O_i(x)$ — 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)

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

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

DARTS

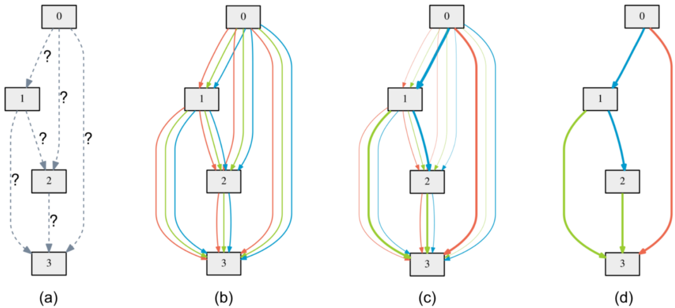


Figure 1: An overview of DARTS: (a) Operations on the edges are initially unknown. (b) Continuous relaxation of the search space by placing a mixture of candidate operations on each edge. (c) Joint optimization of the mixing probabilities and the network weights by solving a bilevel optimization problem.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

Machine Learning and Data Mining

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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.

References

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