Introduction to Artificial Neural Networks

Pattern recognition

March 17, 2021

Outline

- Biological neural networks
  - Motivation
  - Biological neurons
- Artificial neural networks
  - Symbolism vs. Connectionism
  - Historical background & bio-inspiration
  - First artificial neurons
  - XOR problem
  - MLP
  - Back-propagation
  - Types of ANN and learning

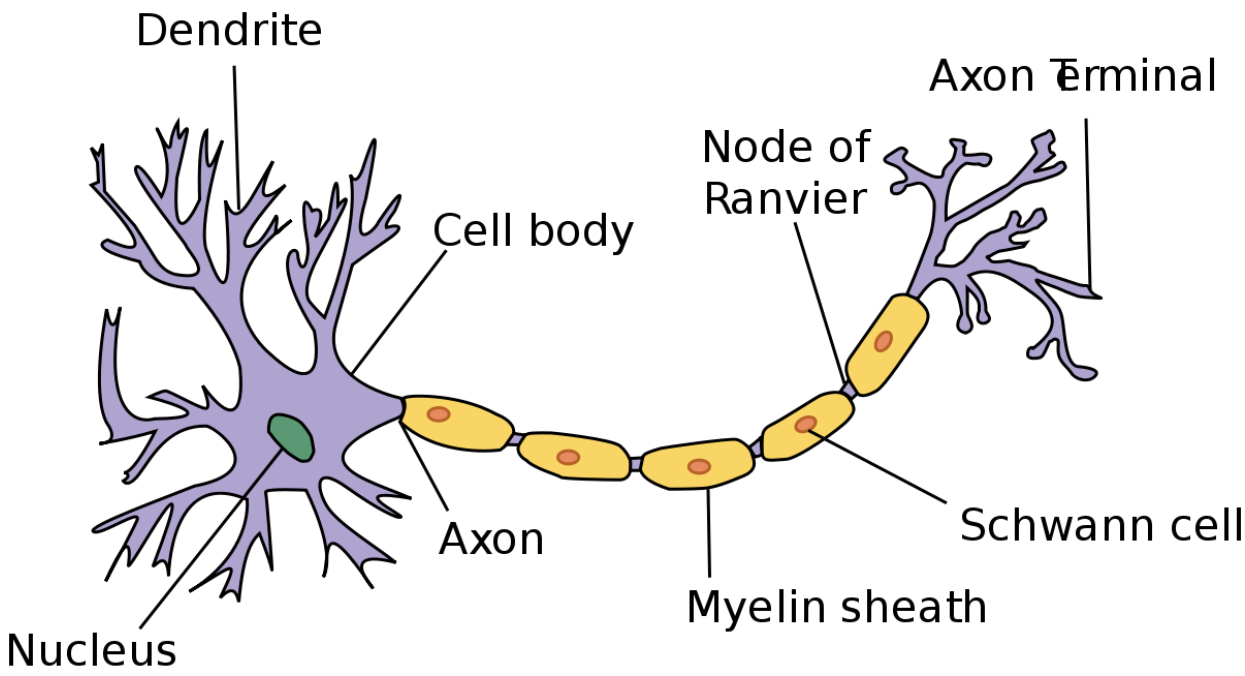
Biological Neural Networks

Why bio-inspiration

- Success in many other fields
  - basically, "nature" had time to develop some pretty good systems ($\sim$evolution)
- Human brain:
  - neurons are slow compared to logic gates/transistors (order of milliseconds)
  - yet the brain is faster and more accurate on some tasks $\rightarrow$ massive parallelism
    - $\sim 10^{11}$ neurons
    - $\sim 10^{15}$ synapses (approx. 10 000 synapses per neuron)
  - robustness & good generalization
  - (biological) neural networks with similar structure can adapt to perform different tasks on different modalities

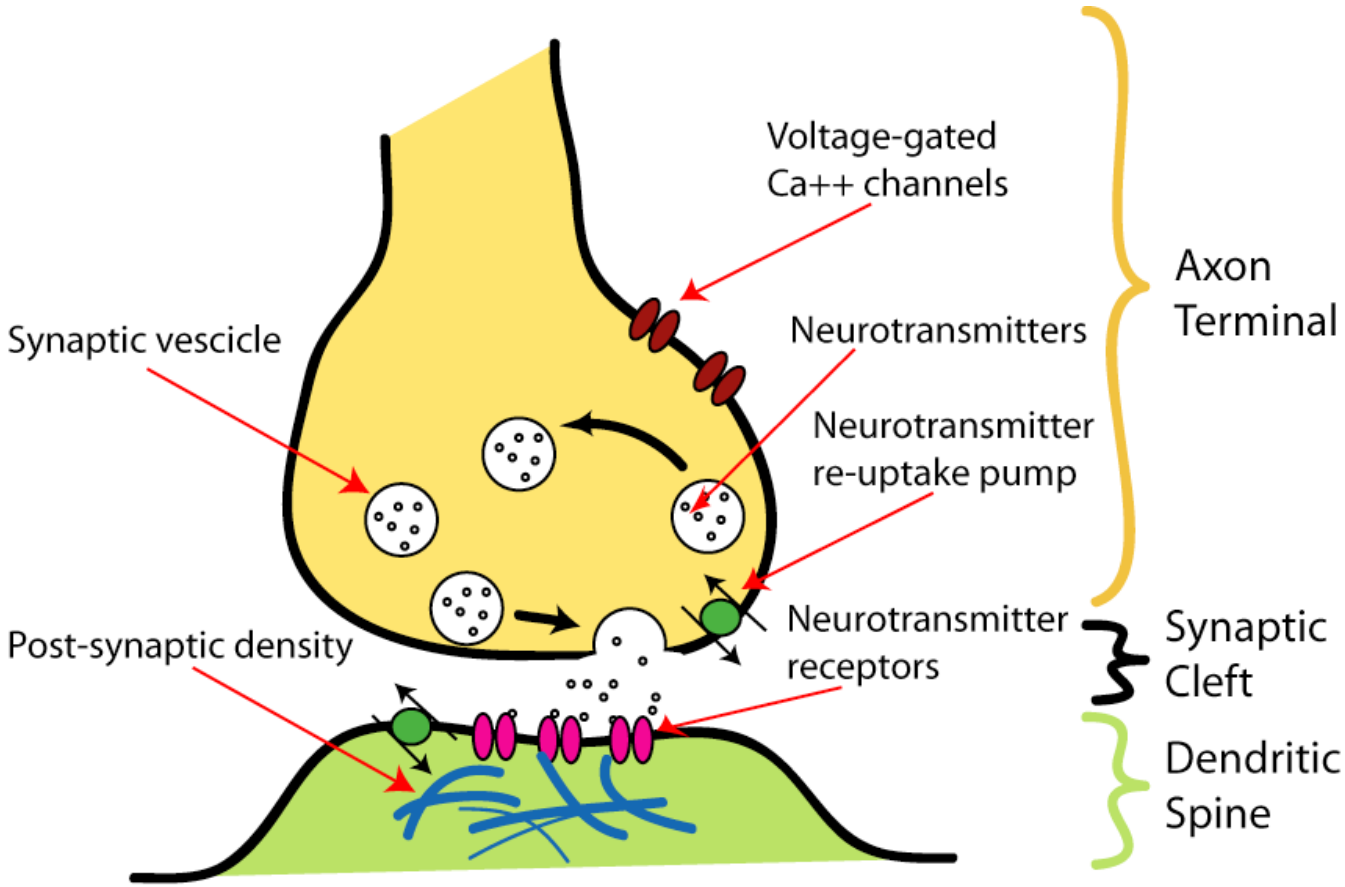
Biological neuron

- *Dendrites* collect information (electro-chemical signals)
- *Soma* ("body") integrates information
- If threshold is reached $\rightarrow$ the neuron fires
  - Information is transmitted mostly via frequency modulation
- Firing transmitted via *axon*



Biological neuron – synapse

- Mediates the interaction between neurons
- The signal is converted from electrical activity to chemical (release of neurotransmitter) and back to electrical (activation of neurotransmitter receptors)
- Can have excitatory or inhibitory effect



Artificial Neural Networks

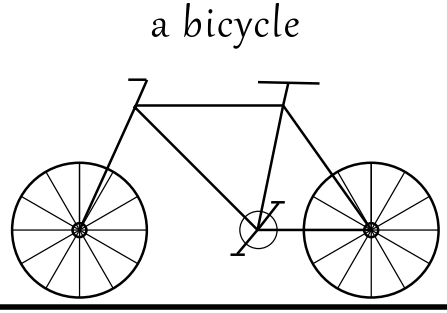
Connectionism

- Information processing theory
- **Symbolism**:
  - Entities in the world are represented using symbols (i.e., sort of "unitary" representations of things)
  - Information processing done by manipulating the symbols as a whole
    - E.g., propositional logic
  - View of human brain:
    - Humans are symbolic species – the symbolic part distinguishes us from the rest of the animals
    - Brain runs "a program" – the substrate is irrelevant
  - AI started as a symbolic field (many actual AI systems deployed in the field are symbolic even today)
    - advantage: more tangible and interpretable algorithms/computations
- **Connectionism:**
  - Inspired by (human) brain – huge network of simple processing units
  - Information processing done via interaction between the units
  - View of human brain:
    - The form of human brain is important
    - Function of the brain cannot be understood without the connectionist view
  - Thanks to the most well known connectionist model – artificial neural network – connectionism is rapidly taking over the field of AI (e.g. search engines, various recognition systems)

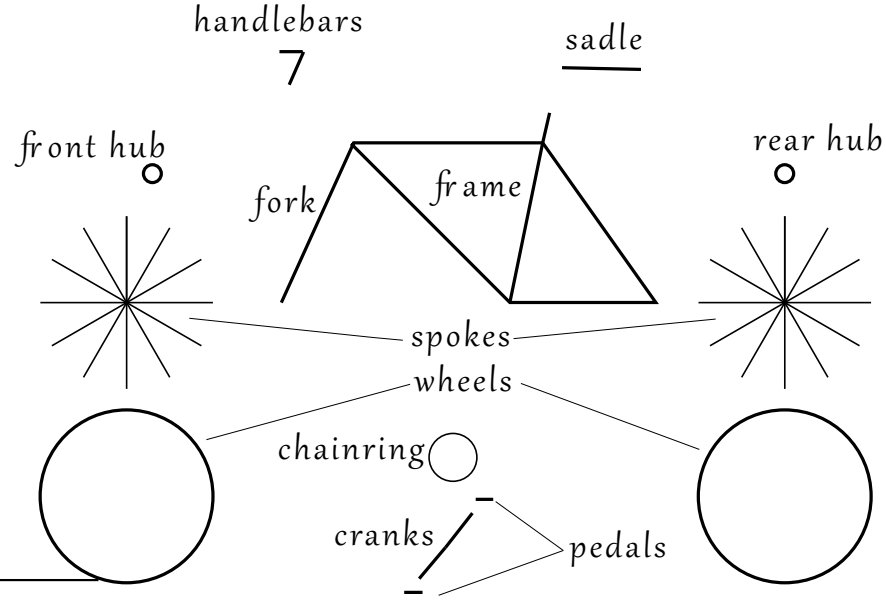
Connectionism vs. Symbolism

- *An oversimplified analogy*

What a symbolist sees:



What a connectionist sees: [1],[2]



[1] Parts of symbols or subsymbols in ANNs are learned and are almost never "nice" parts of objects as it would be if ANN parameters were designed by hand.

[2] There are, however, older connectionist models based around "nice" object parts.

History – first neural model

- Warren McCulloh and Walter Pitts (1943) – Threshold Logic Unit
- Binary firing function
- Excitation $\boldsymbol{x}^{exc}$ and inhibition $\boldsymbol{x}^{inh}$ inputs, firing threshold θ

$$\xi = \sum_{i=1}^{n} x_i^{exc} - \sum_{j=1}^{m} x_i^{inh} \tag{1}$$

$$y = \begin{cases} 1 & \xi \geq \theta \\ 0 & \xi < \theta \end{cases} \tag{2}$$

History – first neural model

- equation (1) can be rewritten with weights:

$$\xi = \sum_{i=1}^{n} x_i * w_i, w_i \in \{-1, 1\} \tag{3}$$

- equation (2) can then be changed to:

$$y = \begin{cases} 1 & \xi - \theta \geq 0 \\ 0 & \xi - \theta < 0 \end{cases} \tag{4}$$

- Putting it together and rearranging a bit – we get a spoiler of the future ANN model:

$$y = step\left(\sum_{i=1}^{n} x_i * w_i - \theta\right) \tag{5}$$

- There is still no learning
- Only simple binary functions

Hebbian learning rule

- The famous phrase:

"Neurons that fire together wire together"

- Donald Hebb (1949) – "The Hebbian learning rule"
- Weights are changed as the neuron fires
  - correct firing $\Rightarrow$ responsible connections (weights) are strengthened
  - incorrect firing $\Rightarrow$ responsible connections (weights) are weakened

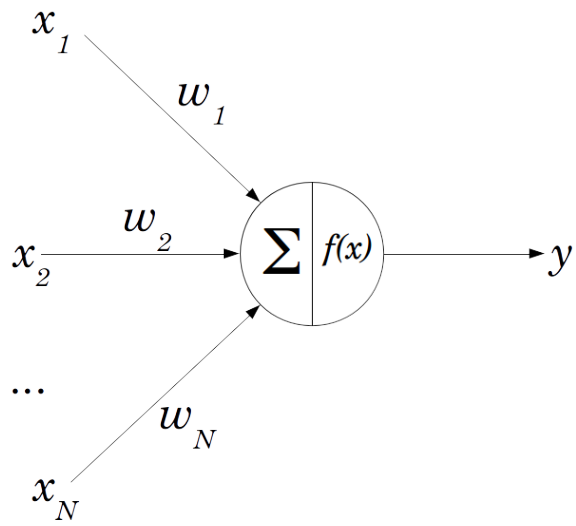
$$w_{ij}(t+1) = w_{ij}(t) + \eta o_i o_j \tag{6}$$

where w_{ij} is weight (strength of connection) between neurons "i" and "j" and o_i, o_j are outputs of these neurons; η is the learning rate (usually $\ll 1$)

- works for outputs $\in \{-1, 1\}$
- "output" was also interpreted as output from the input neurons, i.e. the inputs, thus Δw can also be interpreted as $\eta \times input \times ouput$

Perceptron

- Frank Rosenblatt (1957) neural model – perceptron
- Combination of the McCulloh & Pitts model and Hebbian learning



$$y = f\left(\sum_{i=1}^{n} x_i w_i - \theta\right) \tag{7}$$

or

$$y = f\left(\sum_{i=1}^{n+1} x_i w_i\right), x_{n+1} = -1 \tag{8}$$

- The **activation function** f has to be *bounded*, *monotonous*, *differentiable*; e.g. the sigmoid function σ (originally, step function was used)

Perceptron learning

- Activation:

$$y = f\left(\sum_{i=1}^{n+1} x_i w_i\right)$$

- Target output: $\hat{y}$
- Learning rule:

$$w_i(t+1) = w_i(t) - \alpha(y - \hat{y})x_i \tag{9}$$

If you would like to have less negativity in your life, eq. (9) can be rewritten as $w_i(t+1) = w_i(t) + \alpha(\hat{y} - y)x_i$

ADAptive LInear NEuron

- Improvement of the perceptron, mainly of the learning rule
- Step function changed to a linear function (differentiability)
- Error/cost function (SSE):

$$J(w) = \frac{1}{2}\sum_{j}\left(\hat{y}^j - y^j\right)^2 \tag{10}$$

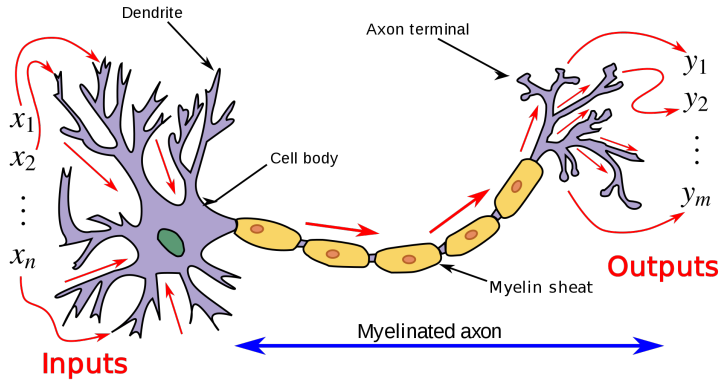
- Weight update computed from the derivative:

$$w(t+1) = w(t) + \alpha\sum_{j}\left(\hat{y}^j - y^j\right)x^j$$

- Update computed from the entire **batch** of samples (j) (previously after each sample)
- Real valued outputs and targets (previously binary outputs)

Bio-inspiration of the artificial neuron

- Image, such as this one, is often presented to show the relation between biological and artificial neuron:



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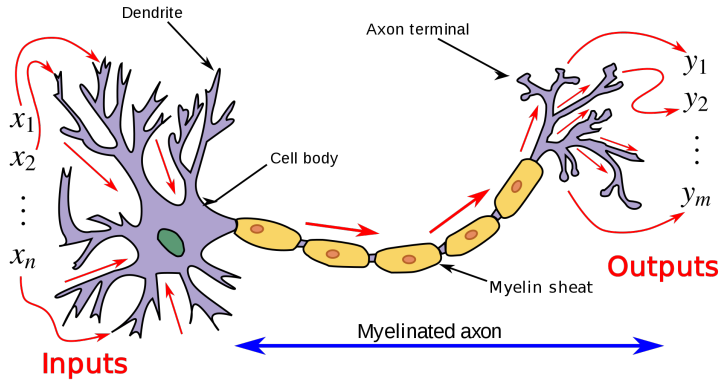

This is wrong!

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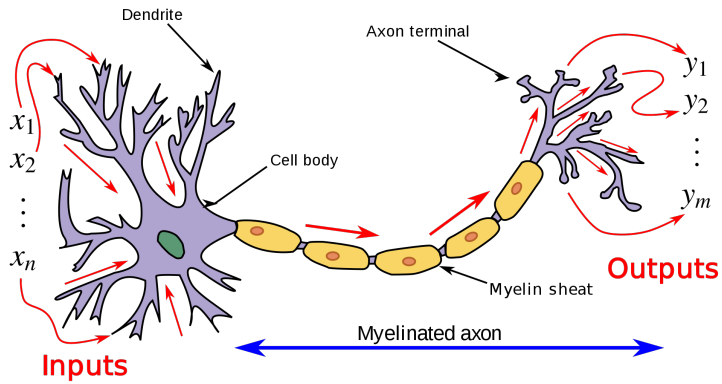
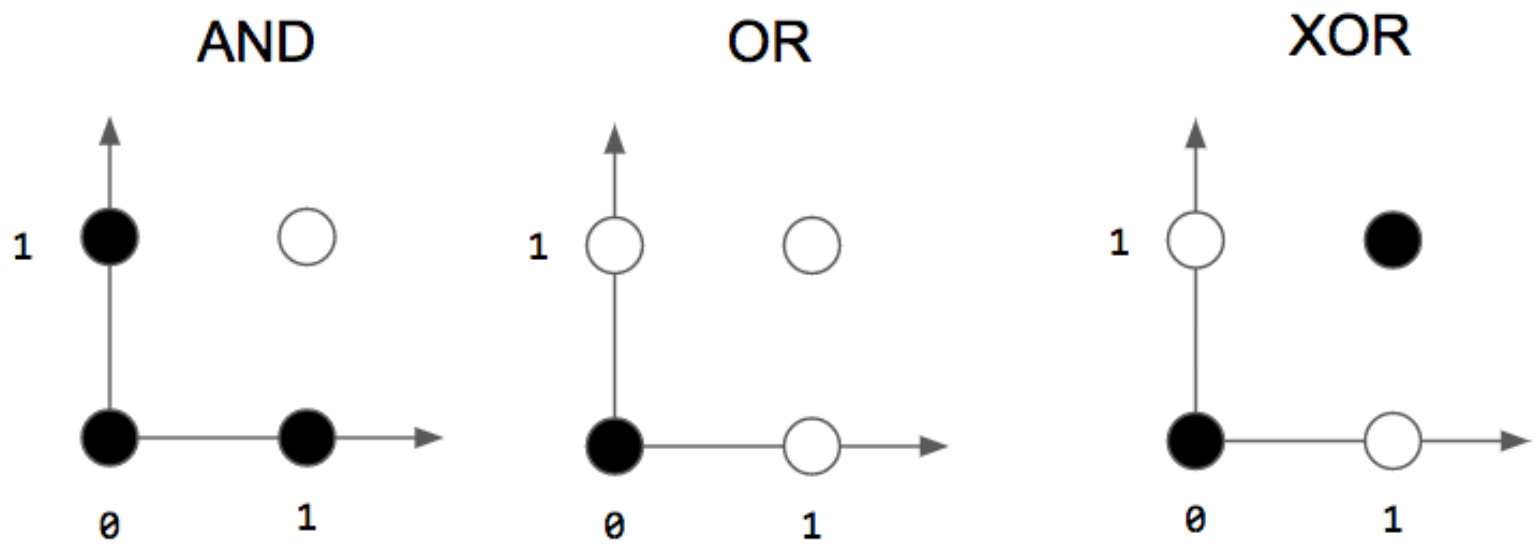


This is wrong!

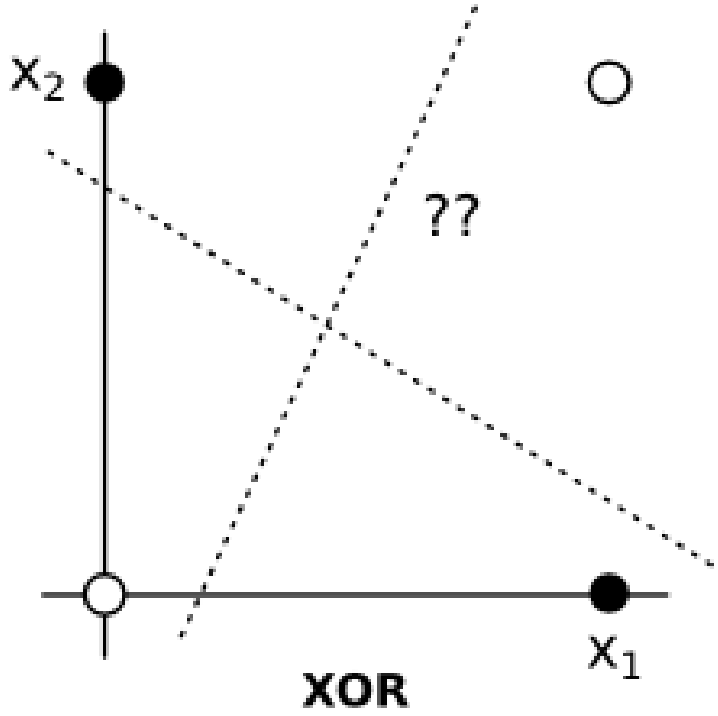
- More accurate view: a single mathematical model of neuron (a.k.a. artificial neuron) represents (i.e. model the behavior of) a group of biological neurons
- But mathematical models had diverged from the biological neurons for the sake of computational efficiency and usability
  - modeling the actual behavior of a neuron is quite complex and costly
- Remember it is bio-*inspired*, not biologically accurate
  - There is another field of research trying to develop models that would be almost as efficient as ANNs but more biologically plausible

The XOR problem

- Marvin Minsky and Seymour Papert (1969)
- It is impossible for perceptron to learn the XOR function
- A single perceptron can only classify linearly separable classes
- Logical functions:



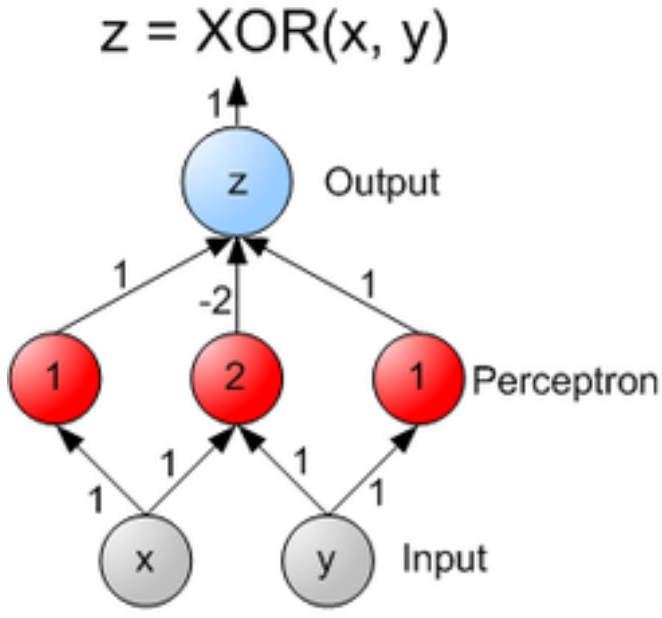
The XOR and the learning problem



- A good solution would be to stack multiple layers of perceptrons – splitting the problem into sub-problems
  - but how to adjust the weights?
- ANNs dormant for many years:
  - needed the invention of back-propagation learning algorithm
  - and more computational power

Multilayer perceptron

- Multilayer perceptron (MLP) – universal function approximator
- Rumelhart, Hinton, and Williams (1986)



Back-propagation – gradient descent

- Gradient descent
  - Adjust weights in the direction of steepest gradient of the error/cost function
  - Ideally, error computed from every sample
  - In reality: computationally infeasible (e.g. memory problems)
  - $\rightarrow$ stochastic gradient descent (mini-batches)
- Compute gradient for the error/cost function:

$$J = \sum_{i=1}^{n} \frac{1}{2} (y_i - \hat{y}_i)^2 \tag{11}$$

- Activation function (sigmoid function):

$$y_i = \sigma \left(\sum_{j=1}^{m} x_j w_{ij} - \theta_i \right) \tag{12}$$

- Separate the sum from the function:

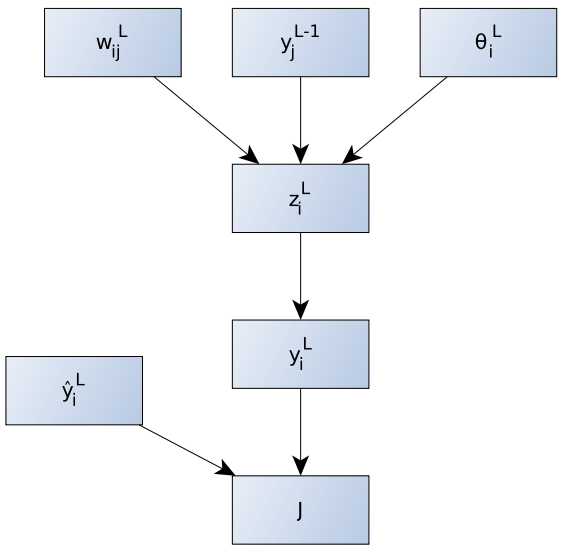
$$y_i = \sigma (z_i) \tag{13}$$

where

$$z_i = \sum_{j=1}^{n} x_j w_{ij} - \theta_i \tag{14}$$

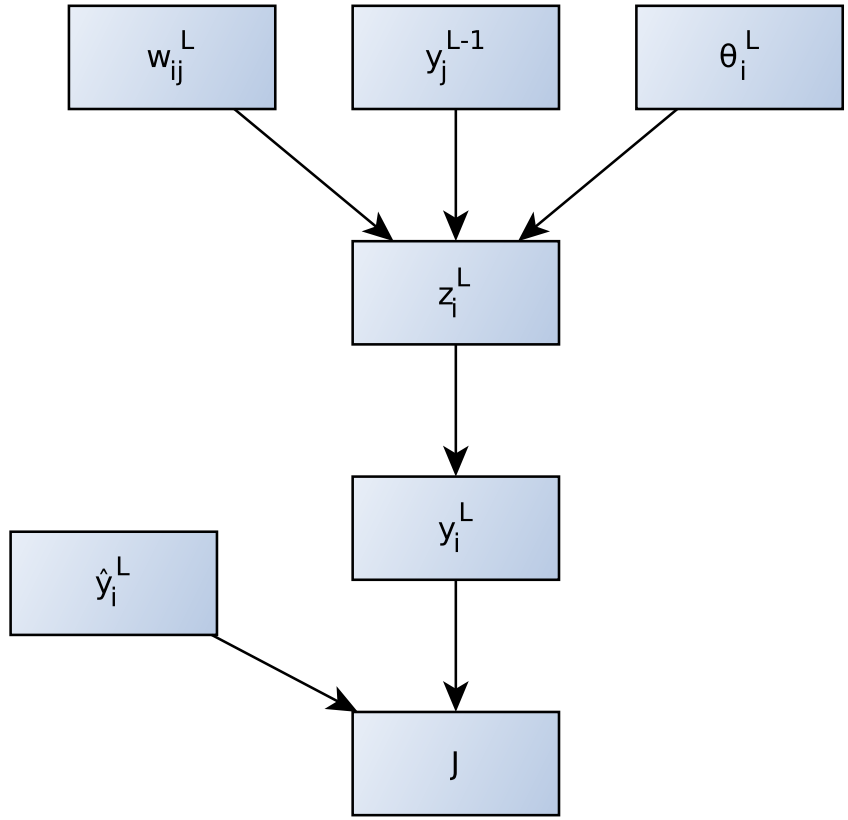
Back-propagation – gradient descent

- y_i^L output of i-th neuron in layer L
- x_j^L the j-th input for layer L; note that this is equivalent to y_j^{L-1}, i.e. the j-th output from the previous layer
- w_{ij}^L weight connecting j-th output from the previous layer with i-th neuron on layer L
- J the cost function
- $\hat{y}_i^L$ the target for the i-th neuron (the layer number could be dropped, since the targets are only available for the last layer)



- Recommended to watch:
  3Blue1Brown Series S3 - E4: Backpropagation calculus

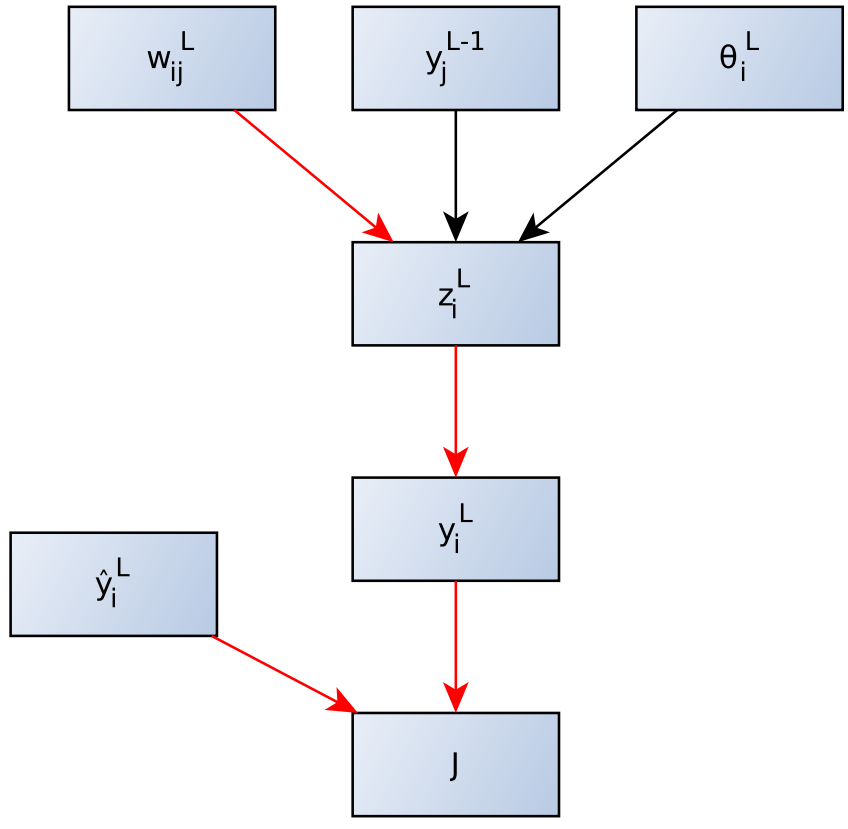
Back-propagation – gradient descent



Back-propagation – gradient descent

$$\frac{\partial J}{\partial w_{ij}^L} = \frac{\partial z_i^L}{\partial w_{ij}^L} \frac{\partial y_i^L}{\partial z_i^L} \frac{\partial J}{\partial y_i^L}$$

$$\frac{\partial J}{\partial w_{ij}^L} = \sum_{k=1}^{n_{samples}} y_j^{L-1} \sigma' \left(z_i^L \right) \left(y_i^L - \hat{y}_i \right)$$



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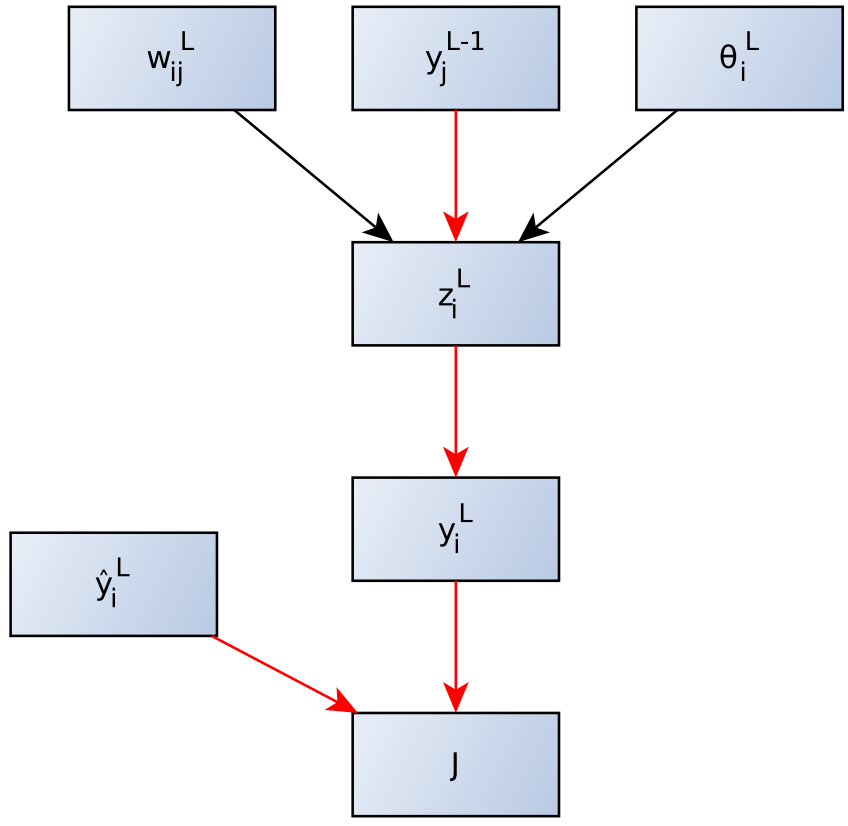
- Computation of error belonging to the previous layer:

$$\frac{\partial J}{\partial y^{L-1}} = \frac{\partial z_i^L}{\partial y^{L-1}} \frac{\partial y_i^L}{\partial z_i^L} \frac{\partial J}{\partial y^L}$$



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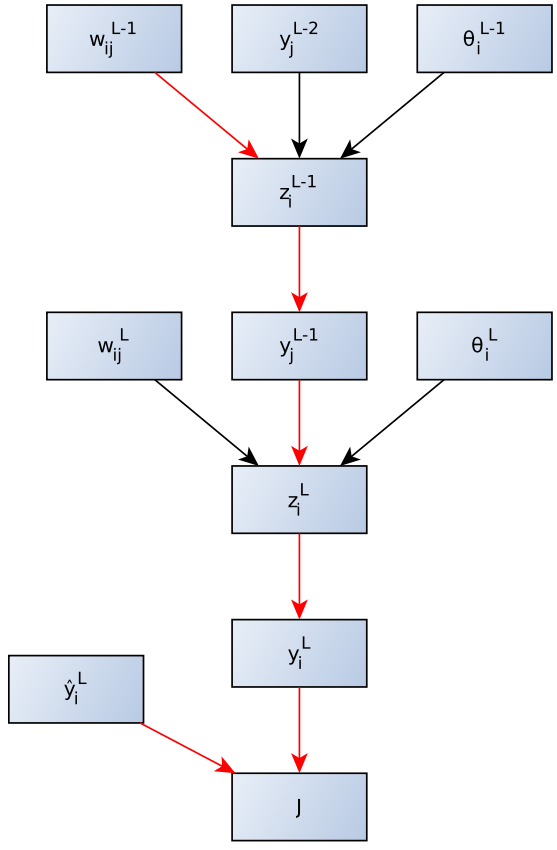

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$$\frac{\partial J}{\partial y_j^{L-1}} = \sum_{i=1}^{n} \frac{\partial z_i^L}{\partial y_j^{L-1}} \frac{\partial y_i^L}{\partial z_i^L} \frac{\partial J}{\partial y_i^L}$$

Perceptron learning – an (embarrassing) alternative

- Let's say we want to train a perceptron to compute a binary operation, for example, binary **AND**
- Possible input combinations are:

$$x_1 = [0, 0],\ x_2 = [0, 1],\ x_3 = [1, 0],\ x_4 = [1, 1]$$

- Let's put the inputs into a matrix form (the 1s in the last column are for the bias term) :

$$\mathbf{X} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

- Targets for each row: $y^T = [0, 0, 0, 1]$
- And we would like to find some weights $w^T = [w_1, w_2, w_3]$, so these equations would hold:

$$\mathbf{X}w = y$$

- How may we solve this?

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- How may we solve this?
- Yes, there are analytic solutions to this. The gradient descent approach starts to make sense when the number of weights and examples grows to large values.

Usefulness of Gradient descent

$$y = Xw, \tag{15}$$

- where X is a n by $\#dim$ matrix containing input data, y are the "labels" or output data, and w are the weights used to generate the data (unknown in real world)
- Standard representation of a system of linear equations:

$$Ax = b$$

- In our case, $b \approx y$, $A \approx X$, and $x \approx w$, therefore we can rewrite equation (15) as:

$$Xw = y$$

- and to calculate w, we want to find values satisfying:

$$w^* = \arg\min_w \|Xw - y\|^2 \tag{16}$$

Usefulness of Gradient descent

- Equation equation (16) can be solved* by:

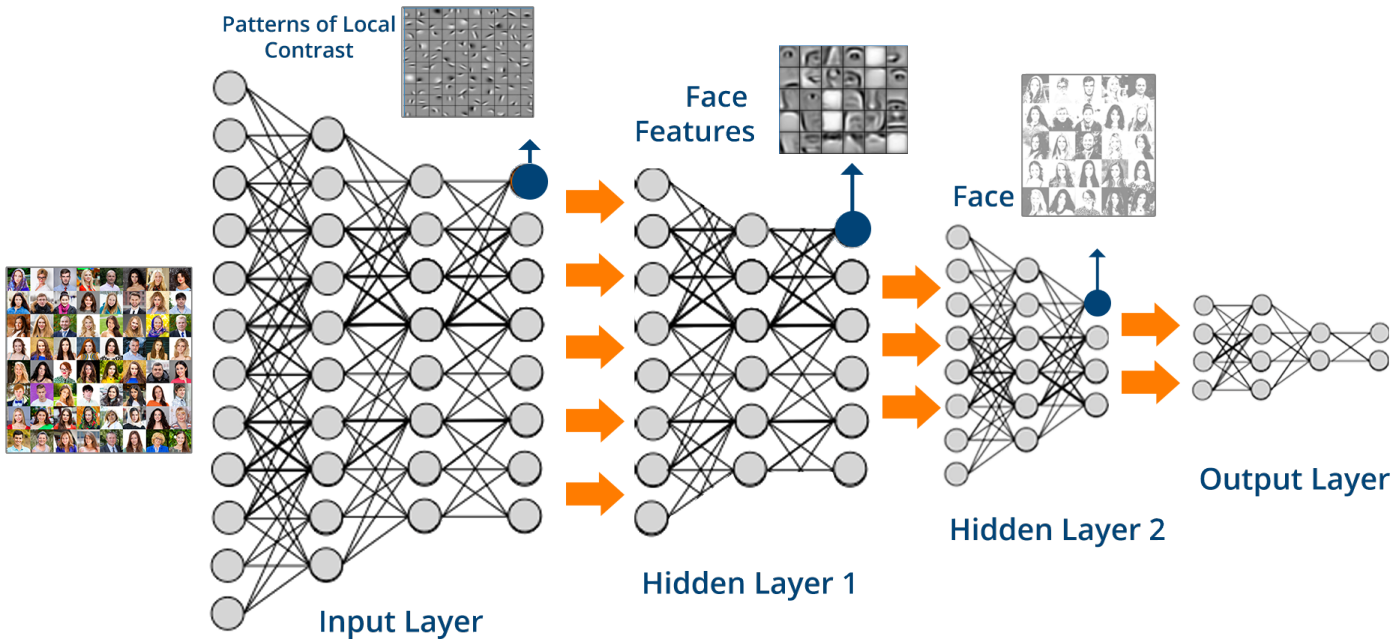
$$X^{-1}Xw = X^{-1}y$$

$$\mathcal{I}w = X^{-1}y$$

- For simple data, this method is faster and more efficient!
- So, why GD?
  - higher dimensionality
  - larger datasets
  - $\sim$ anything that cannot actually be computed via analytical solution with the available resources

Deep neural networks

- Hinton (2006)
- number of layers > 3; today $\gg 3$
- Combination of unsupervised (lower layers) and supervised (higher layers)



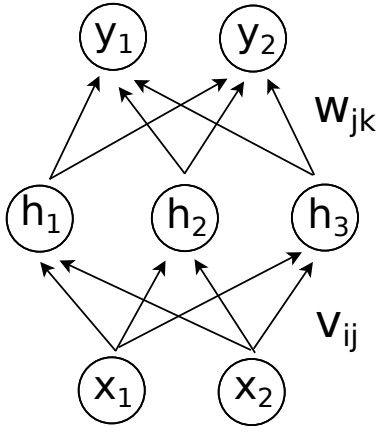
Types of learning in ANN

- **Supervised** learning: weights are adjusted according to the **desired** output (perceptron, MLP, RBF, RNN)
  $s = s(\boldsymbol{w}, \boldsymbol{x}, \hat{y})$
- **Reinforcement** learning: extension of the supervised learning; weights are adjusted according to the **reward** (MLP, RBF)
  $s = s(\boldsymbol{w}, \boldsymbol{x}, r)$
- **Unsupervised** learning: weights are adjusted according to the **statistics** of the input (Hebbian net, SOM)
  $s = s(\boldsymbol{w}, \boldsymbol{x})$

Basic structures of ANN

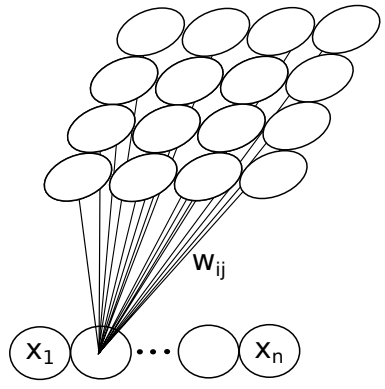
Multi-layer perceptron MLP
(Rumelhart, 1986)

- hidden layer - allows to solve linearly inseparable problems
- supervised learning - **error back-propagation (BP** or **"backprop")**
- universal function approximator
- typical task: input-output mapping, classification, regression, anomaly detection, association



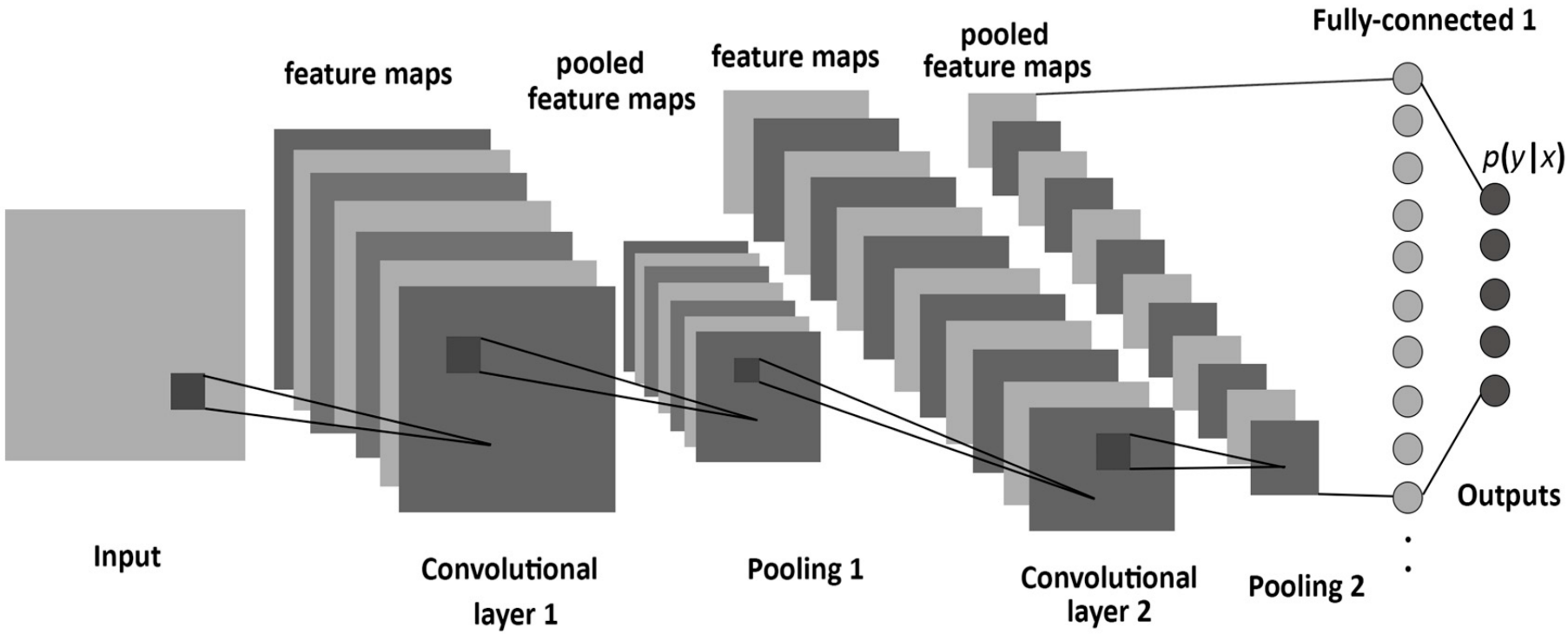
Self-organising map SOM
(Kohonen, 1997)

- unsupervised learning
- a representation of a data category is usually computed as a **local average of the data**
- similar data cluster together to same locations in the map - data topology
- typical tasks: clustering of multidimensional data, categorization



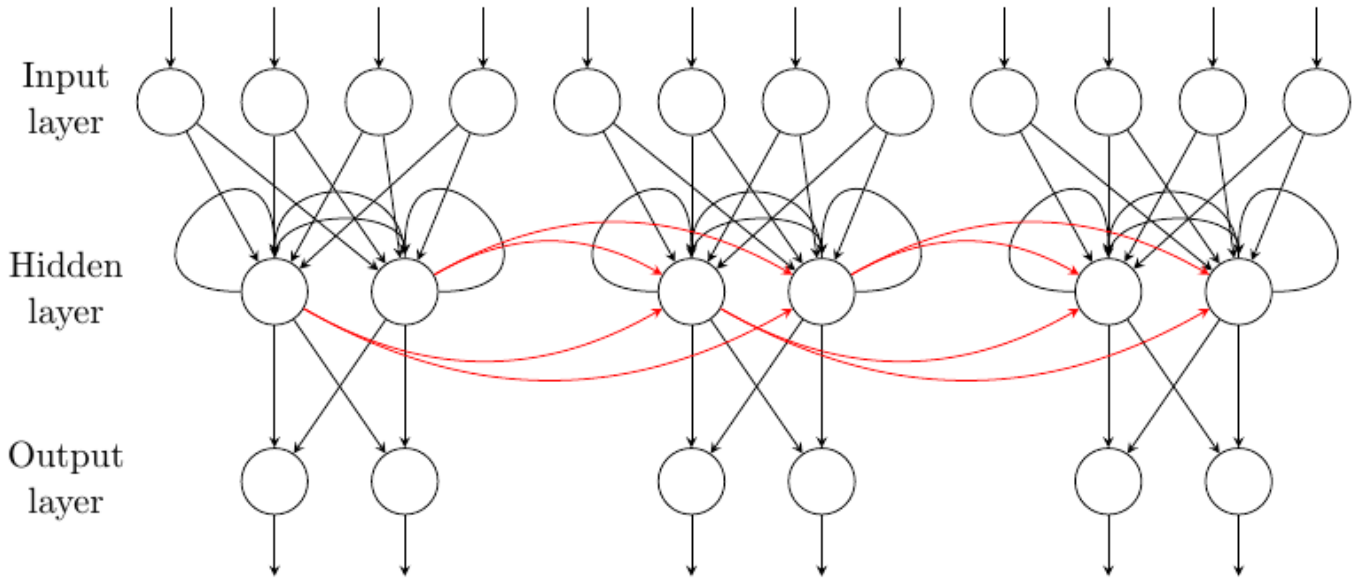
Convolutional neural networks

- Fully connected ANNs: slight shift in the input changes the output drastically
- Especially problematic in images
- Solution: move (convolve) the "receptive field" of the neuron across the image and accumulate the outputs
  $\Rightarrow$ convolutional neural networks



Recurrent neural networks

- Outputs from neurons are used as their own inputs (alongside with other inputs)
- Very powerful tool for sequential data (NL parsing, signals...)



ANN problems

- Under and over-fitting
  - Over-fitting: network represents the training data too well
    - bad performance on testing data
    - stop training when error on validation (different than testing) data increases
    - **dropout** – deactivate certain neurons during training
  - Under-fitting
    - possible causes: slow learning rate or overshooting the local minima – learning rate decay
- Vanishing gradient
  - For very deep networks, the gradient in back-prop can vanish
  - Cannot be used for training
  - Some activation functions (e.g. ReLU) diminishes this effect
- Scaling
  - Models use usually small numbers of units
  - Solutions that work well for small networks with narrow focus fail to deal with large input spaces and multiple tasks
- Data
  - Huge amount of parameters (deep networks) = requires huge amount of data

A puppy or a muffin?

Example

https://playground.tensorflow.org

Thank you for your attention