Neural networks

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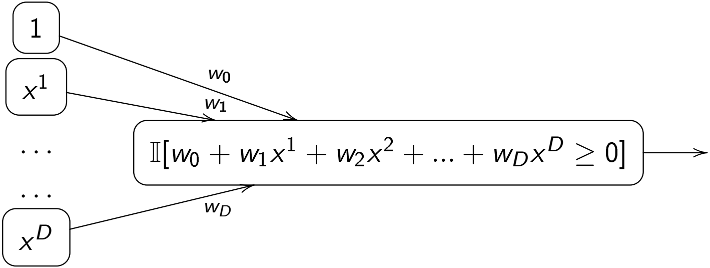
Table of Contents

History

- Neural networks originally appeared as an attempt to model human brain


- Human brain consists of multiple interconnected neuron cells
    - cerebral cortex (the largest part) is estimated to contain 15–33 billion neurons
    - communication is performed by sending electrical and electro-chemical signals
    - signals are transmitted through axons - long thin parts of neurons.

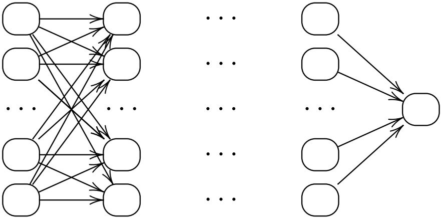
Simple model of a neuron



- Neuron get's activated in the half-space, defined by $w_0 + w_1 x^1 + w_2 x^2 + ... + w_D x^D \geq 0$.
- Each node is called a neuron
- Each edge is associated a weight
- Constant feature 1 stands for bias

Multilayer perceptron architecture[1]

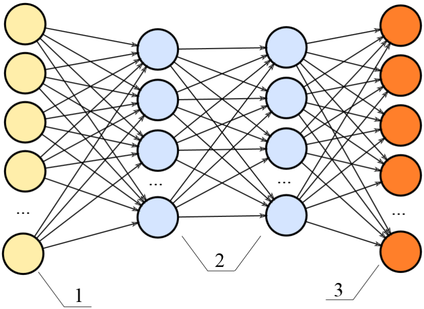
- Hierarchically nested set of neurons.
- Each node has its own weights.



This is structure of multilayer perceptron - acyclic directed graph.

[1] Propose neural networks estimating OR,AND,XOR functions on boolean inputs.

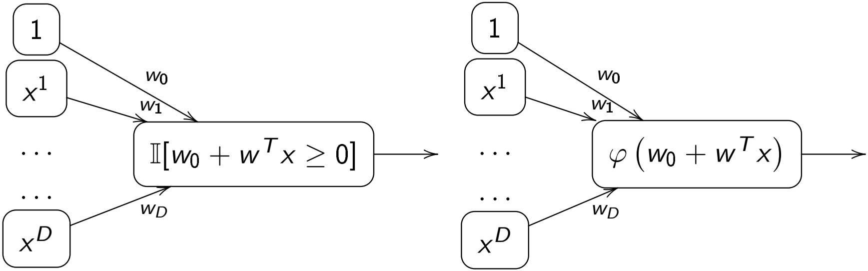
Layers



- Structure of neural network:
  - 1-input layer
  - 2-hidden layers
  - 3-output layer

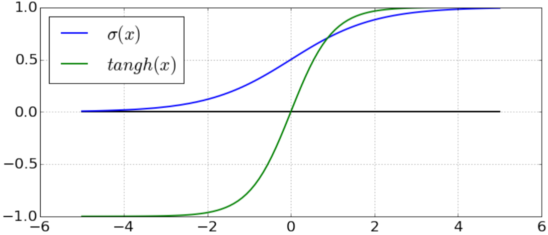
Continious activations

- Pitfall of $\mathbb{I}[]$: it causes stepwise constant outputs, weight optimization methods become inapplicable.
- We can replace $\mathbb{I}[w^T x + w_0 \ge 0]$ with smooth activation $\varphi(w^T x + w_0)$



Typical activation functions

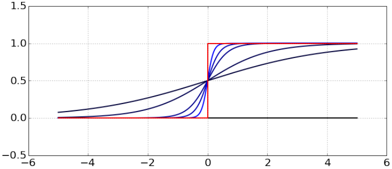
- sigmoidal: $\sigma(x) = \frac{1}{1+e^{-x}}$
  - 1-layer neural network with sigmoidal activation is equivalent to logistic regression
- hyperbolic tangent: $\text{tangh}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$



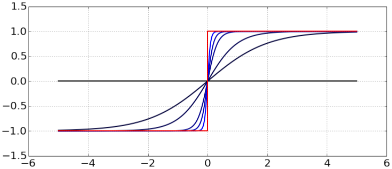
- ReLu: $\varphi(x) = [x]_+$.

Activation functions

Activation functions are smooth approximations of step functions:



$\sigma(ax)$ limits to 0/1-step function as $a \to \infty$



tangh(ax) limits to -1/1-step function as $a \to \infty$

Definition details

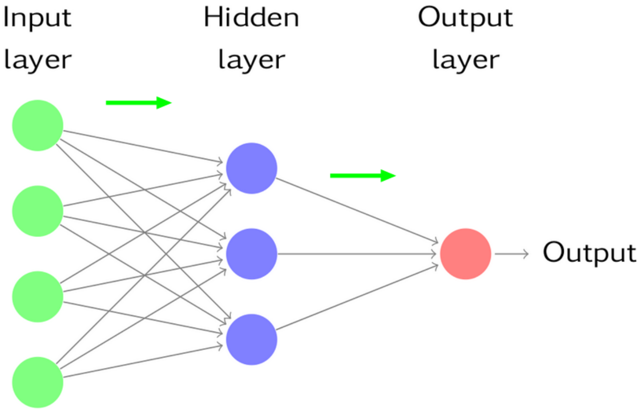
- Label each neuron with integer j.
- Denote: I_j - input to neuron j, O_j - output of neuron j
- Output of neuron j: $O_j = \varphi(I_j)$.
- Input to neuron j: $I_j = \sum_{k \in inc(j)} w_{kj} O_k + w_{0j}$,
    - w_{0j} is the bias term
    - $inc(j)$ is a set of neurons with outging edges incoming to neuron j.
    - further we will assume that at each layer there is a vertex with constant output $O_{const} \equiv 1$, so we can simplify notation

$$I_j = \sum_{k \in inc(j)} w_{kj} O_k$$

Table of Contents

Output generation

- Forward propagation is a process of successive calculations of neuron outputs for given features.



Activations at output layer

- Regression: $\varphi(I) = I$
- Classification:
  - binary: $y \in \{+1, -1\}$

$$\varphi(I) = p(y = +1|x) = \frac{1}{1 + e^{-I}}$$

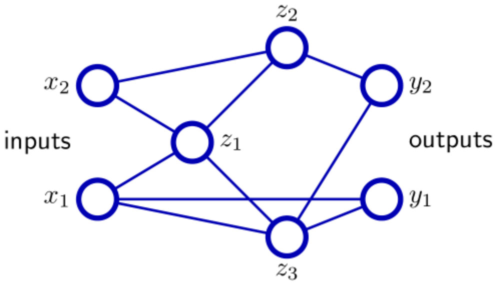
  - multiclass: $y \in 1, 2, ...C$

$$\varphi(O_1, ...O_C) = p(y = j|x) = \frac{e^{O_j}}{\sum_{k=1}^{C} e^{O_k}}, j = 1, 2, ...C$$

where $O_1, ...O_C$ are outputs of output layer.

Generalizations

- each neuron j may have custom non-linear transformation φ_j
- weights may be constrained:
  - non-negative
  - equal weights
  - etc.
- layer skips are possible



- Not considered here: RBF-networks, recurrent networks.

Number of layers selection

- Number of layers usually denotes all layers except input layer (hidden layers+output layer)
- We will consider only continuous activation functions.
- Classification:
  - single layer network selects arbitrary half-spaces
  - 2-layer network selects arbitrary convex polyhedron (by intersection of 1-layer outputs)
    - therefore it can approximate arbitrary convex sets
  - 3-layer network selects (by union of 2-layer outputs) arbitrary finite sets of polyhedra
    - therefore it can approximate almost all sets with well defined volume (Borel measurable)

Number of layers selection

- Regression
  - single layer can approximate arbitrary linear function
    - 2-layer network can model indicator function of arbitrary convex polyhedron
    - 3-layer network can uniformly approximate arbitrary continuous function (as sum weighted sum of indicators convex polyhedra)

Sufficient amount of layers

Any continuous function on a compact space can be uniformly approximated by 2-layer neural network with linear output and wide range of activation functions (excluding polynomial).

- In practice often it is more convenient to use more layers with less total amount of neurons
  - model becomes more interpretable and easy to fit.

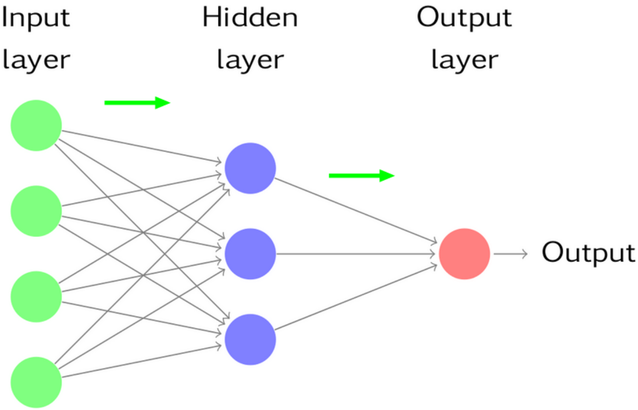
Neural network architecture selection

- Network architecture selection:
    - increasing complexity (control by validation error)
    - decresing complexity ("optimal brain damage")
        - may be used for feature selection

Table of Contents

Weight space symmetries

- Consider a neural network with 1 hidden layer
  - with $tangh(x)$ activation functions
  - consisting of M neurons



Weight space symmetries

- The following transformations in weight space lead to neural networks with equivalent outputs:
    - for any neuron in hidden layer: simultaneous change of sign of input and output weights
        - 2^M possible equivalent transformations of such kind
    - for any pair of neurons in the hidden layer: interchange of input weights between the neurons and simultaneous interchange of output weights
        - this is equivalent to reordering of neurons in the hidden layer, so there are $M!$ such orderings
    - $2^M M!$ equivalent transformations exist in total.
    - For neural network with K hidden layers, consisting of M_k, $k = 1, 2, ...K$ neurons each, we obtain $\prod_{k=1}^{K} 2^{M_k} M_k!$ equivalent neural networks.
    - In general case these are the only symmetries existing in the weights space.

Table of Contents

Network optimization: regression

- Single output:

$$\frac{1}{N}\sum_{n=1}^{N}(\widehat{y}_n(x_n)-y_n)^2 \to \min_{w}$$

Network optimization: regression

- Single output:

$$\frac{1}{N}\sum_{n=1}^{N}(\widehat{y}_n(x_n)-y_n)^2 \to \min_w$$

- K outputs

$$\frac{1}{NK}\sum_{n=1}^{N}\sum_{k=1}^{K}(\widehat{y}_{nk}(x_n)-y_{nk})^2 \to \min_w$$

Network optimization: classification

- Two classes ($y \in \{0, 1\}$, $p = P(y = 1)$):

$$\prod_{n=1}^{N} p(y_n = 1|x_n)^{y_n}[1 - p(y_n = 1|x_n)]^{1-y_n} \to \max_w$$

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- C classes ($y_{nc} = \mathbb{I}\{y_n = c\}$):

$$\prod_{n=1}^{N} \prod_{c=1}^{C} p(y_n = c|x_n)^{y_{nc}} \to \max_w$$

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$$\prod_{n=1}^{N} \prod_{c=1}^{C} p(y_n = c|x_n)^{y_{nc}} \to \max_w$$

- In practice log-likelihood is maximized.

Neural network optimization

- Let W denote the total dimensionality of weights space
- Let $E(\widehat{y}, y)$ denote the loss function of output
- We may optimize neural network using gradient descent:

```
k = 0
initialize randomly w^0 # small values for sigmoid and tangh

while (stop criteria not met):
     w^{k+1} := w^k − η∇E(w^k)
    k := k + 1
```

- Standardization of features makes gradient descend converge faster
- Other optimization methods are more efficient (such as conjugate gradients)
- Denote W - total number of edges (and weights) in the neural net.

Gradient calculation

- Direct $\nabla E(w)$ calculation, using

$$\frac{\partial E}{\partial w_i} = \frac{E(w+\varepsilon_i) - E(w)}{\varepsilon} + O(\varepsilon)$$

or better

$$\frac{\partial E}{\partial w_i} = \frac{E(w+\varepsilon_i) - E(w-\varepsilon_i)}{2\varepsilon} + O(\varepsilon^2)$$

has complexity $O(W^2)$ [W forward propagations to evaluate W derivatives]

Backpropagation algorithm needs only $O(W)$ to evaluate all derivatives.

Multiple local optima problem

- Optimization problem for neural nets is **non-convex**.
- Different optima will correspond to:
    - different starting parameter values
    - different training samples
- So we may solve task many times for different conditions and then
    - select best model
    - alternatively: average different obtained models to get ensemble

Table of Contents

Definitions

- Denote w_{ij} be the weight of edge, connecting i-th and j-th neuron.
- Define $\delta_j = \frac{\partial E}{\partial I_j} = \frac{\partial E}{\partial O_j}\frac{\partial O_j}{\partial I_j}$
- Since E depends on w_{ij} through the following functional relationship $E(w_{ij}) \equiv E(O_j(I_j(w_{ij})))$, using the chain rule we obtain:
$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial I_j}\frac{\partial I_j}{\partial w_{ij}} = \delta_j O_i$$
because $\frac{\partial I_j}{\partial w_{ij}} = \frac{\partial}{\partial w_{ij}}\left(\sum_{k\in inc(j)} w_{kj} O_k\right) = O_i$, where $inc(j)$ is a set of all neurons with outgoing edges to neuron j.
- $\frac{\partial E}{\partial I_j} = \frac{\partial E}{\partial O_j}\frac{\partial O_j}{\partial I_j} = \frac{\partial E}{\partial O_j}\varphi'(I_j)$, where φ is the activation function.

Output layer

- If neuron j belongs to the output node, then error $\frac{\partial E}{\partial O_j}$ is calculated directly.
- For output layer deltas are calculated directly:

$$\delta_j = \frac{\partial E}{\partial O_j}\frac{\partial O_j}{\partial I_j} = \frac{\partial E}{\partial O_j}\varphi'(I_j) \tag{1}$$

- example for training set = {single point x and true vector of outputs $(y_1, ...y_{|OL|})$}:
  - for $E = \frac{1}{2}\sum_{j\in OL}(O_j - y_j)^2$:

$$\frac{\partial E}{\partial O_j} = O_j - y_j$$

  - for $\varphi(I) = sigm(I)$:

$$\varphi'(I_j) = \sigma(I_j)\,(1 - \sigma(I_j)) = O_j(1 - O_j)$$

  - finally

$$\delta_j = (O_j - y_j)\,O_j(1 - O_j)$$

Inner layer

- If neuron j belongs some hidden layer, denote $out(j)=\{k_1,k_2,...k_m\}$ the set of all neurons, receiving output from neuron j.
- The effect of O_j on E is fully absorbed by $I_{k_1},I_{k_2},...I_{k_m}$, so

$$\frac{\partial E(O_j)}{\partial O_j}=\frac{\partial E(I_{k_1},I_{k_2},...I_{k_m})}{\partial O_j}=\sum_{k\in out(j)}\left(\frac{\partial E}{\partial I_k}\frac{\partial I_k}{\partial O_j}\right)=\sum_{k\in out(j)}(\delta_k w_{jk})$$

- So for layers other than output layer we have:

$$\delta_j=\frac{\partial E}{\partial I_j}=\frac{\partial E}{\partial O_j}\frac{\partial O_j}{\partial I_j}=\sum_{k\in out(j)}(\delta_k w_{jk})\,\varphi'(I_j) \qquad (2)$$

- Weight derivatives are calculated using errors and outputs:

$$\frac{\partial E}{\partial w_{ij}}=\frac{\partial E}{\partial I_j}\frac{\partial I_j}{\partial w_{ij}}=\delta_j O_i \qquad (3)$$

Backpropagation

- Backpropagation algorithm:
  1. Forward propagate x_n to the neural network, store all inputs I_i and outputs O_i for each neuron.
  2. Calculate δ_i for all $i \in$output layer using (1).
  3. Backpropagate δ_i from final layer backwards layer by layer using (2).
  4. Using calculated deltas and outputs calculate $\frac{\partial E}{\partial w_{ij}}$ with (3).
- Algorithm complexity: $O(W)$, where W is total number of edges.
- Updates:
  - batch
  - stochastic
    - using minibatches of objects

Regularization

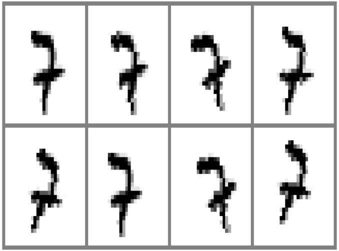
- Constrain model complexity directly
  - constrain number of neurons
  - constrain number of layers
  - impose constraints on weights
- Take a flexible model
  - use early stopping during iterative evaluation (by controlling validation error)
  - quadratic regularization

$$\tilde{E}(w) = E(w) + \lambda \sum_i w_i^2$$

Table of Contents

Invariances

- It may happen that solution should not depend on certain kinds of transformations in the input space.
- Example: character recognition task
    - translation invariance
    - scale invariance
    - invariance to small rotations
    - invariance to small uniform noise

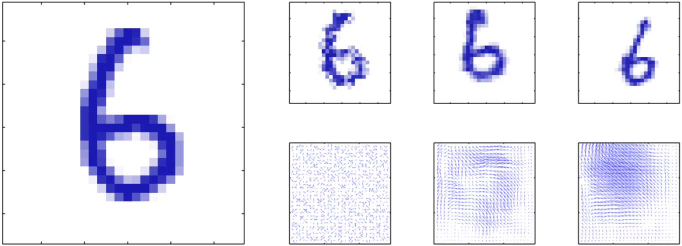


Invariances

- Approaches to build an invariant model:
  - augment training objects with their transformed copies according to given invariances
    - amount of possible transformations grows exponentially with the number of invariances
  - add regularization term to the target cost function, which penalizes changes in output after invariant transformations
    - see tangent propagation
  - extract features that are invariant to transformations
  - build the invariance properties into the structure of neural network
    - see convolutional neural networks

Augmentation of training samples

1. generate a random set of invariant transformations
2. apply these transformations to training objects
3. obtain new training objects

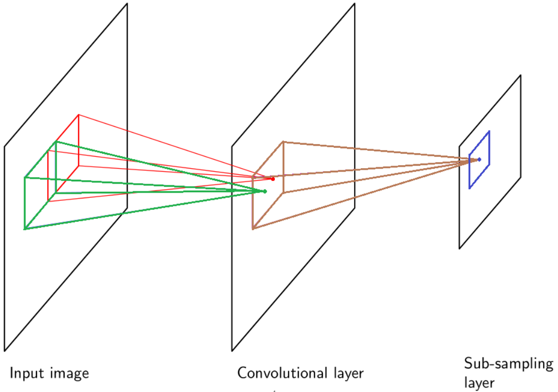


Tangent propagation

- Denote $s(x, \xi)$ be vector x after invariant transformation parametrized by ξ.
- Denote
$$\tau_n = \left.\frac{\partial s(x_n, \xi)}{\partial \xi}\right|_{\xi=0}, \quad J_{ki} = \frac{\partial y_k}{\partial x_i}$$
- We want $\left.\frac{\partial y_k}{\partial \xi}\right|_{\xi=0}$ to be as small, as possible.
- Sensitivity of y_k to small invariant transformation:
$$\left.\frac{\partial y_k}{\partial \xi}\right|_{\xi=0} = \sum_{i=1}^{D} \frac{\partial y_k}{\partial x_i}\frac{\partial x_i}{\partial \xi} = \sum_{i=1}^{D} J_{ki}\tau_i$$
- Tangent propagation - modify target cost function:
$$\tilde{E} = E + \lambda \sum_n \sum_k \left(\sum_{i=1}^{D} J_{nki}\tau_{ni} \right)^2$$

Convolutional neural networks

- Convolutional neural network:
  - Used for image analysis
  - Consists of a set of convolutional layer / sub-sampling layer pairs and aggregating layer



Convolutional neural networks

- Convolutional layer
  - Convolutional layer consists of a number of feature maps
  - Feature map has the same dimensionality as input layer
  - Locality: each neuron in the feature map takes output from small neigborhood of input layer neurons
  - Equivalence: the same transformation is applied by each neuron in the feature map
    - obtained by constraining sets of weights to each feature map layer neuron to be equal
    - similar to convolution with moving adaptive kernel
    - effectively it is feature extraction from a region

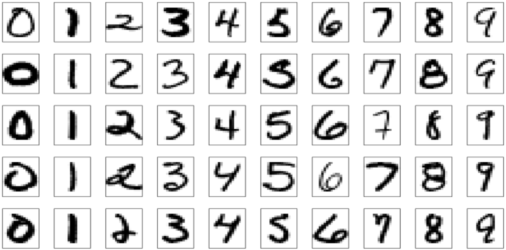
Convolutional neural networks

- Sub-sampling layer
  - Consists of a number of planes, each corresponding to respective feature map on the previous convolutional layer
  - Locality: Sub-sampling layer neurons take output from small neigborhood of respective feature map neurons
    - neigbourhoods are chosen to be contiguous and non-overlapping
  - Aggregation: input of each neuron i is: $w_{i0} + w_{i1}F$, where w_{i0}, w_{i1} are adjustable weights and F is aggregation function (sum or max of activations of respective feature map neurons)
  - Implements small translational invariance
- There may be a sequence of convolutional and sub-sampling layers
  - gradual dimensionality reduction

Table of Contents

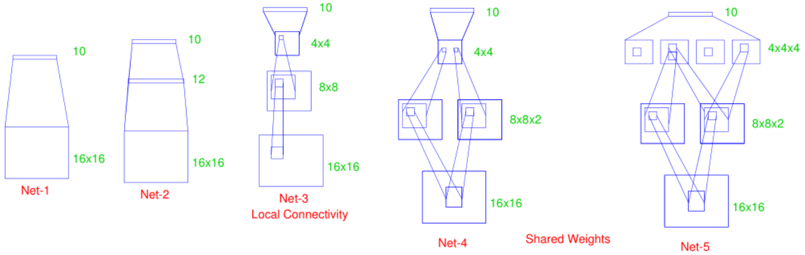
Case study (due to Hastie et al. The Elements of Statistical Learning)

ZIP code recognition task

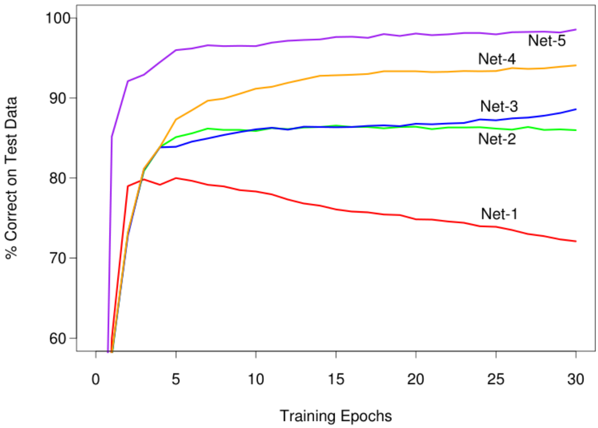


Neural network structures

Net1: no hidden layer
Net2: 1 hidden layer, 12 hidden units fully connected
Net3: 2 hidden layers, locally connected
Net4: 2 hidden layers, locally connected with weight sharing
Net5: 2 hidden layers, locally connected, 2 levels of weight sharing



Results


100
90
80
70
60
% Correct on Test Data
0
5
10
15
20
25
30
Training Epochs
Net-5
Net-4
Net-3
Net-2
Net-1

Addition

- Deep learning
- Neural networks weights may be constrained to belong to mixture density
  - $\tilde{E} \leftarrow E - \lambda P(w)$, where $P(w)$ is the mixture probability of weights
  - soft forcing of weights to group into similar clusters
- Neural networks may model not only real value outputs, but densities
  - each output - frequency of histogram bin
  - each output - either prior or mean or variance of mixture of parametrized density (normal, beta, etc.)

Conclusion

- Advantages of neural networks:
  - can model accurately complex non-linear relationships
  - easily parallelizable
- Disadvantages of neural networks:
  - hardly interpretable ("black-box" algorithm)
  - optimization requires skill
    - too many parameters
    - may converge slowly
    - may converge to inefficient local minimum far from global one