Lecture 5. Neural networks intro, backpropagation method

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Kazakh-British Technical University

October 8, 2022

Five-minute questions

- What is the name of the course?
- What is the teacher's name?
- What color is the textbook?

To make long story short

2003, silver medal

To make long story short

2009, master of math

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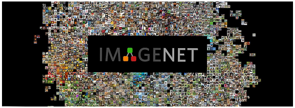
Tasks solved by neural networks

Images: 25% $\rightarrow$ 3.5%
VS 5% errors by human



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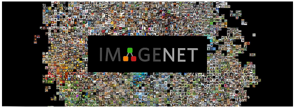

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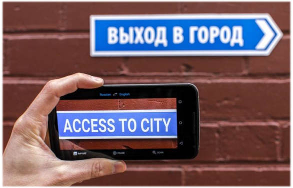

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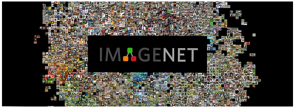

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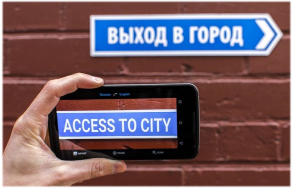
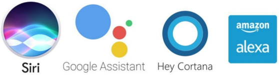


Voice



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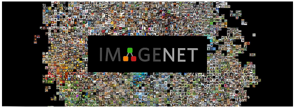

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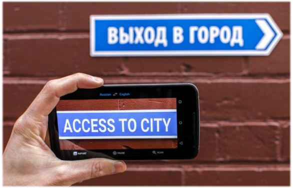

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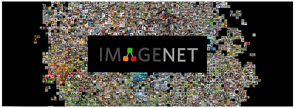

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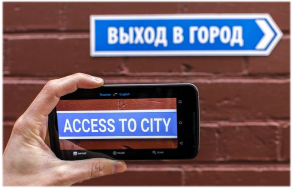

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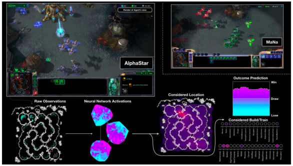

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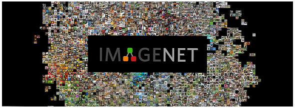

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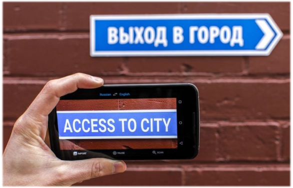

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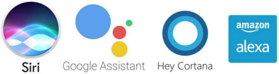
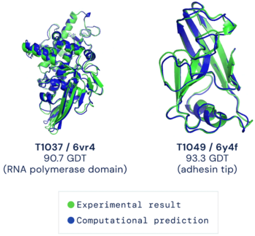


Protein structure, 2022



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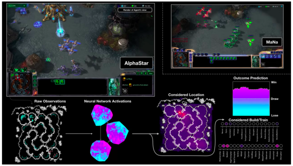
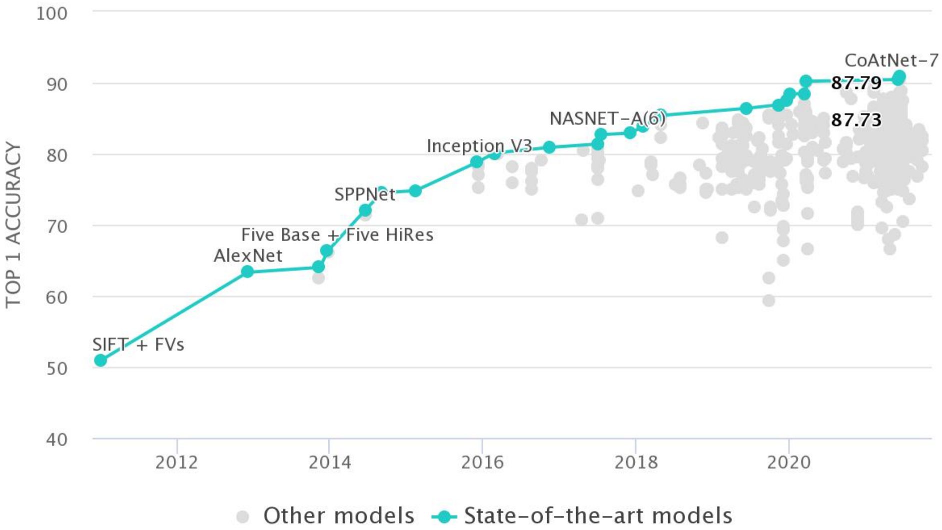




https://paperswithcode.com/sota/image-classification-on-imagenet

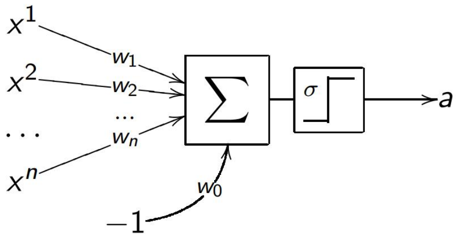
Linear model

recall

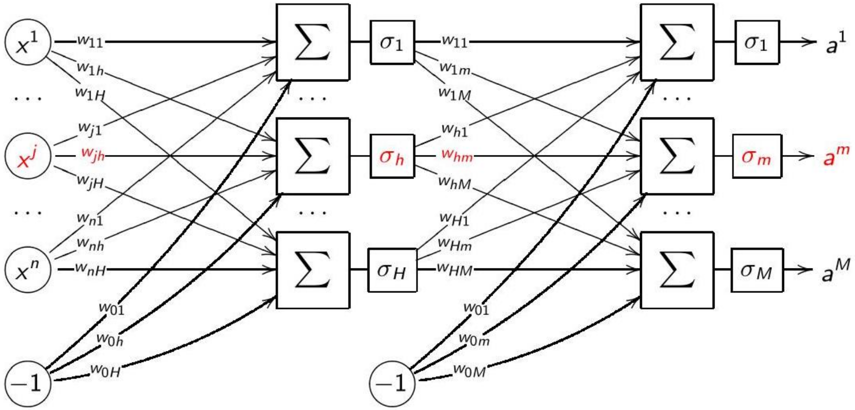
$x^1, x^2, \dots, x^n \in \mathbb{R}$ — numerical features of one object x
$w_0, w_1, \dots, w_n \in \mathbb{R}$ — weights of features

$$a(x, w) = \sigma(\langle w, x \rangle) = \sigma\left(\sum_{j=1}^{n} w_j f_j(x) - w_0\right),$$

$\sigma(z)$ — activation function, for example one of the: $\mathrm{sign}(z)$, $\frac{1}{1+e^{-z}}$, $(z)_+$



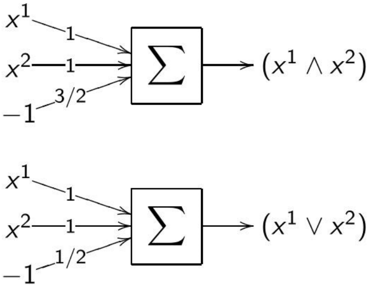
Neural network as combination of linear models

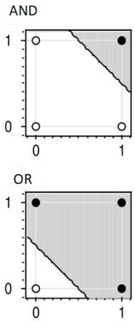


Neural implementation of logic functions

Functions AND, OR, NOT from binary variables x^1 and x^2:

$$x^1 \wedge x^2 = [x^1 + x^2 - \tfrac{3}{2} > 0]$$
$$x^1 \vee x^2 = [x^1 + x^2 - \tfrac{1}{2} > 0]$$
$$\neg x^1 = [-x^1 + \tfrac{1}{2} > 0]$$





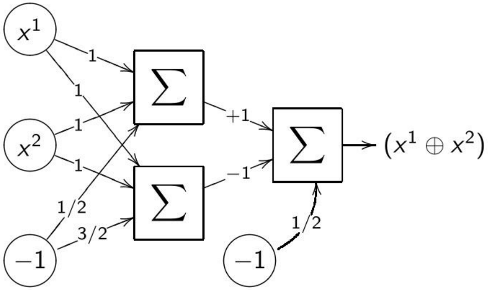
Logic function XOR

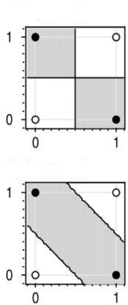
Function $x^1 \bigoplus x^2 = [x^1 \neq x^2]$

Is not implementable by one neuron

There are two ways to implement:

- By adding a non-linear feature $x^1 \bigoplus x^2 = [x^1 + x^2 - 2x^1x^2 - \frac{1}{2} > 0]$
- With a network (two-layer superposition) of AND, OR, NOT functions: $x^1 \bigoplus x^2 = [(x^1 \vee x^2) - (x^1 \wedge x^2) - \frac{1}{2} > 0]$.





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- With the help of linear operations and one non-linear activation function σ any continuous function can be approximated with any desired accuracy
- For some special classes of deep neural networks, they have been proven to have exponentially greater expressive power than shallow networks.

  V. Khrulkov, A. Novikov, I. Oseledets. Expressive power of recurrent neural networks, Feb 2018, ICLR

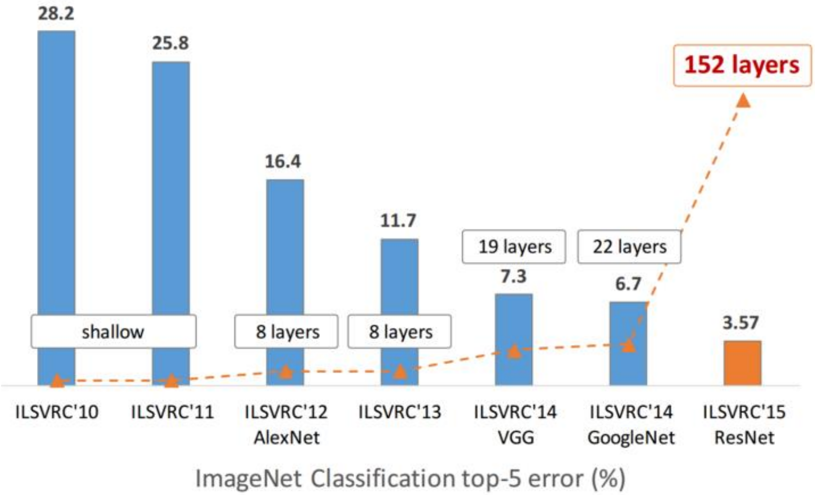
ImageNet

Annotated Image Dataset Project

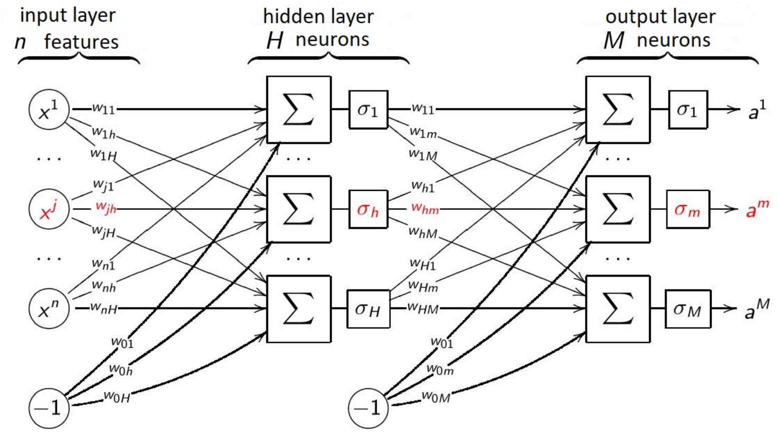
- 14M+ images
- 20K+ classes

The development of convolutional networks

Or a brief history of ImageNet



Two-layer neural network with M-dimensional output



Model parameter vector $w \equiv (w_{jh}, w_{hm}) \in \mathbb{R}^{Hn+H+MH+M}$

Question 1

Where do these amounts of parameters come from?

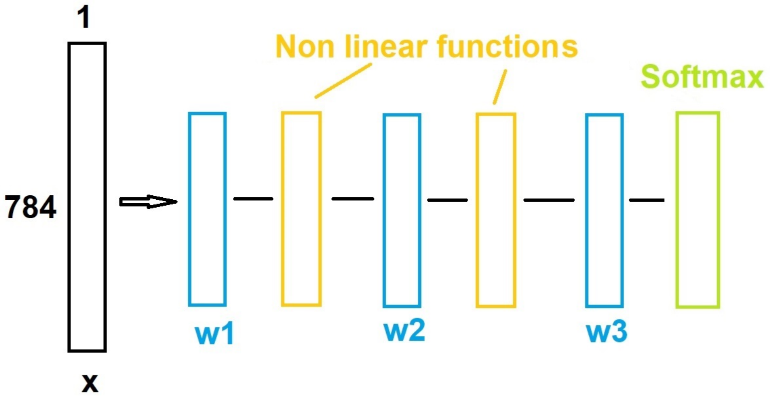
MNIST in PyTorch

Demo

Notebook at github

Source: https://nextjournal.com/gkoehler/pytorch-mnist

Neural network



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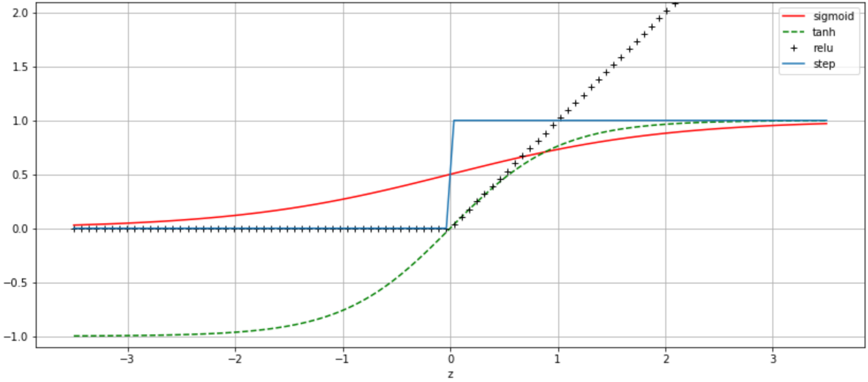
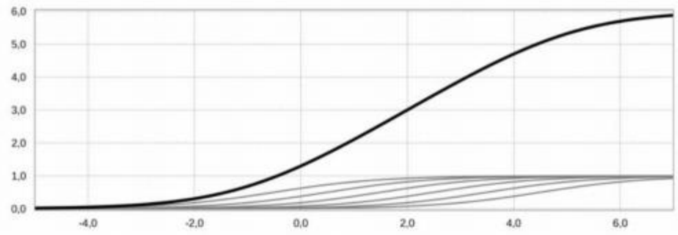
- continuous approximations of threshold function
- can lead to vanishing gradient problem and "paralysis"of the network

Let's look at the charts



$$\mathrm{ReLU}(z) = \max(0, z)$$

Motivation:
$\sigma(5) \approx 0.9933, \sigma(10) \approx 0.9999$
$f(x) = \sigma(x + \frac{1}{2}) + \sigma(x - \frac{1}{2}) + \sigma(x - \frac{3}{2}) + \sigma(x - \frac{5}{2}) + \dots$



(in Russian) Deep Learning: Dive into The World of Neural Networks, S.I. Nikolenko, A.A. Kadurin, E.O. Arkhangelskaya, Piter, 2017

ReLU — Rectified Linear Unit

$$\int \sigma(x)dx = \log(1 + e^x) + C$$

It turns out that $f(x)$ is the Riemannian sum of such an integral:

$$\int\limits_{1/2}^{\infty} \sigma(x + \frac{1}{2} - y)dy$$

$$f(x) = \sum_{i=0}^{\infty} \sigma(x + \frac{1}{2} - i) \approx \int\limits_{1/2}^{\infty} \sigma(x + \frac{1}{2} - y)dy =$$

$$= [-\log(1 + \exp(x + \frac{1}{2} - y))]_{y=1/2}^{y=\infty} = \log(1 + \exp(x)) = \text{Softplus}(x)$$

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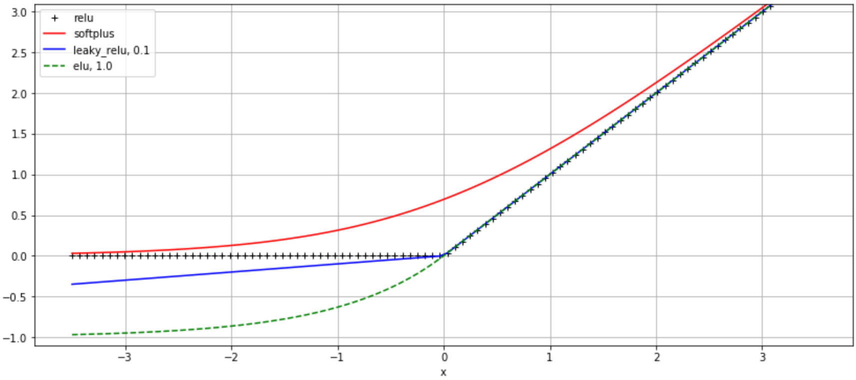
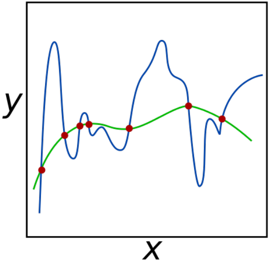


Regularization

$$L(W,b) = -\sum_j \ln \frac{e^{(x_j W + b)_{y_j}}}{\sum_i e^{(x_j W + b)_i}} + \lambda R(W,b)$$

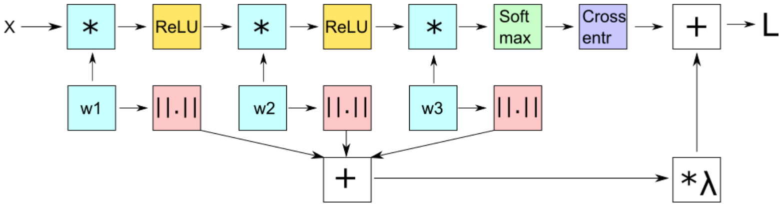
$$R(W,b) = \|W\|_2^2 + \|b\|_2^2$$

$$\|b\|_2^2 = b_0^2 + \cdots + b_k^2$$



Let's include b into W

$$L(W) = -\sum_j \ln p(c = y_j | x_j) + \lambda R(W)$$

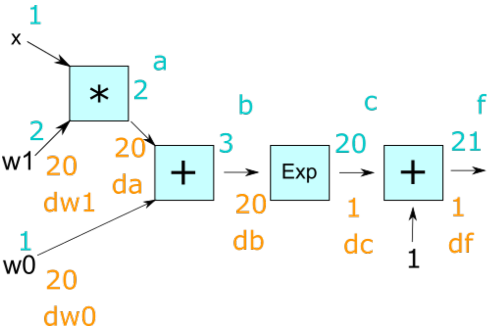


We want to find the gradients of the loss function L over all inputs of the computation graph

A simple example

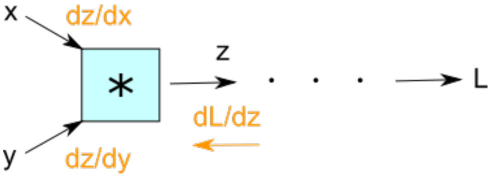
Derivative of a function composition $f(g(x)) \quad \rightarrow \frac{df}{dx} = \frac{df}{dg}\frac{dg}{dx}$

Let $f(x, w) = 1 + e^{w_1 x + w_0}$



$$\frac{\partial f}{\partial f} = 1, \ f = c + 1, \ dc = \frac{\partial f}{\partial c} = 1, \dots$$

General scheme for calculating the gradient



Backpropagation recap

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Backpropagation recap

As a result, we are able to calculate all the gradients with simple operations of the reverse pass through the graph and:

- we did not write out the entire derivative analytically
- at each step a simple function is differentiated
- we need only one pass along the calculation graph
- parallelization is possible

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- Neuron = linear classificator or regressor
- Neural network = superposition of neurons with non-linear activation functions
- Backpropagation = fast differentiation of superpositions. Allows you to train networks of almost any configuration
- Methods for improving convergence and quality:
  - training on mini-batches
  - various activation functions
  - regularization
- Was not at this lecture — will be in the next lectures of the course:
  - various optimization algorithms: adam, RMSProp
  - dropout
  - choice of initial approximation and its connection with activation functions

What else can you watch?

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- In Stanford's course: http://cs231n.github.io/optimization-2/

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- The third lecture of the course "Deep Learning on the fingers"from Semyon Kozlov (in Russian): https://www.youtube.com/watch?v=kWTC1NvL894

In the case of a two-layer neural network

Output values of the network $a^m(x_i), m = 1 \dots M$ on the object x_i:

$$a^m(x_i) = \sigma_m \left(\sum_{h=0}^{H} w_{hm} u^h(x_i) \right)$$

$$u^h(x_i) = \sigma_h \left(\sum_{j=0}^{J} w_{jh} f_j(x_i) \right)$$

Let for definiteness

$$\mathcal{L}_i(w) = \frac{1}{2} \sum_{m=1}^{M} (a^m(x_i) - y_i^m)^2$$

Intermediate task: Partial Derivatives $\frac{\partial \mathcal{L}_i(w)}{\partial a^m}$, $\frac{\partial \mathcal{L}_i(w)}{\partial u^h}$

Intermediate task: Partial Derivatives

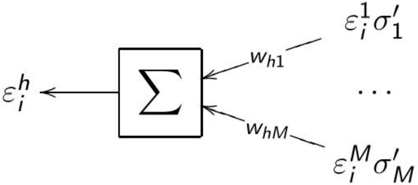
$$\frac{\partial \mathcal{L}_i(w)}{\partial a^m} = a^m(x_i) - y_i^m = \varepsilon_i^m$$

is the error at the output layer (for quadratic losses);

$$\frac{\partial \mathcal{L}_i(w)}{\partial u^h} = \sum_{m=1}^{M} (a^m(x_i) - y_i^m)\sigma'_m w_{hm} = \sum_{m=1}^{M} \varepsilon_i^m \sigma'_m w_{hm} = \varepsilon_i^h$$

— let's call it *an error on a hidden layer*.

It turns out that ε_i^h is calculated from ε_i^m if the network is run backwards:



Fast gradient calculation

Now, given the partial derivatives of $\mathcal{L}_i(w)$ with respect to a^m and u^h, it is easy to write out the gradient of $\mathcal{L}_i(w)$ with respect to the weights of w:

$$\frac{\partial \mathcal{L}_i(w)}{\partial w_{hm}} = \frac{\partial \mathcal{L}_i(w)}{\partial a^m} \frac{\partial a^m}{\partial w_{hm}} = \varepsilon_i^m \sigma_m' u^h(x_i),$$

$m = 1, \dots, M, h = 0, \dots, H$

$$\frac{\partial \mathcal{L}_i(w)}{\partial w_{jh}} = \frac{\partial \mathcal{L}_i(w)}{\partial u^h} \frac{\partial u^h}{\partial w_{jh}} = \varepsilon_i^h \sigma_h' f_j(x_i),$$

$h = 1, \dots, H, j = 0, \dots, n$

Backpropagation algorithm

1. initialize weights w_{jh}, w_{hm}
   repeat
2. select object x_i from X^ℓ (e.g. randomly)
3. forward pass
   $u_i^h = \sigma_h\left(\sum_{j=0}^J w_{jh}x_i^j\right), h = 1, \dots, H$
   $a_i^m = \sigma_m\left(\sum_{h=0}^H w_{hm}u_i^h\right), \varepsilon_i^m = a_i^m - y_i^m, m = 1, \dots, M$
   $\mathcal{L}_i = \sum_{m=1}^M (\varepsilon_i^m)^2$
4. backward
   $$\varepsilon_i^h = \sum_{m=1}^M \varepsilon_i^m \sigma'_m w_{hm}, h = 1 \dots H$$
5. gradient step
   $w_{hm} = w_{hm} - \eta\varepsilon_i^m \sigma'_m u_i^h, h = 0, \dots, H, m = 1 \dots M$
   $w_{jh} = w_{jh} - \eta\varepsilon_i^h \sigma'_h x_i^j, j = 0, \dots, n, h = 1 \dots H$
6. $Q = (1 - \lambda)Q + \lambda\mathcal{L}_i$
   until Q stabilizes

Expressive power of a neural network

$\sigma(z)$ is a sigmoid function if $\lim\limits_{z\to-\infty} \sigma(z) = 0$ and $\lim\limits_{z\to+\infty} \sigma(z) = 1$

Cybenko's theorem

(based on Kolmogorov's theorem on the representability of multidimensional functions)

If $\sigma(z)$ is a continuous sigmoid, then for any function $f(x)$ continuous on $[0,1]^n$ there are values of the parameters $w_h \in \mathbb{R}^n,\ w_0 \in \mathbb{R},\ \alpha_h \in \mathbb{R}$ that is a one-layer network

$$a(x) = \sum_{h=1}^{H} \alpha_h \sigma(\langle x, w_h \rangle - w_0)$$

approximates $f(x)$ uniformly with any accuracy ε:
$|a(x) - f(x)| < \varepsilon$, for all $x \in [0,1]^n$

G. Cybenko. Approximation by Superpositions of a Sigmoidal Function. Mathematics of Control, Signals, and Systems (MCSS) 2 (4): 303–314 (Dec 1, 1989)