Neural networks

Victor Kitov

v.v.kitov@yandex.ru

Yandex School of Data Analysis

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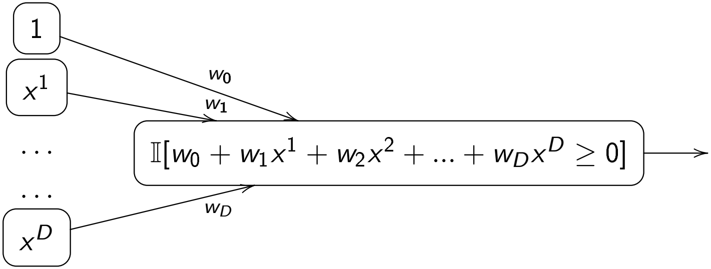
History

- 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

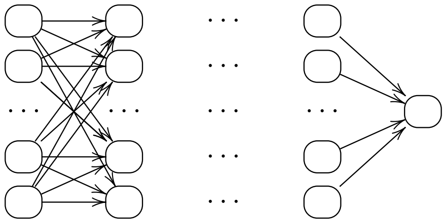

1
x^1
x^D
w_0
w_1
w_D
$\mathbb{I}[w_0 + w_1 x^1 + w_2 x^2 + ... + w_D x^D \geq 0]$

- 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]

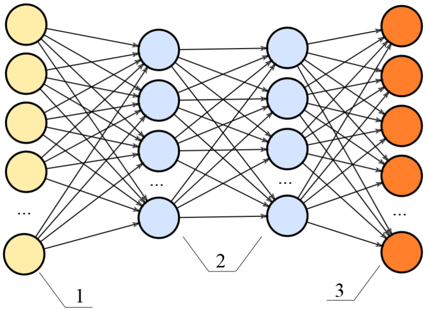
Multilayer perceptron:

- Each node has its own weights.
- Nodes&edges form directed acyclic graph.
- Multiple layers of neurons.
- Neurons of two consecutive layers are fully connected.



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

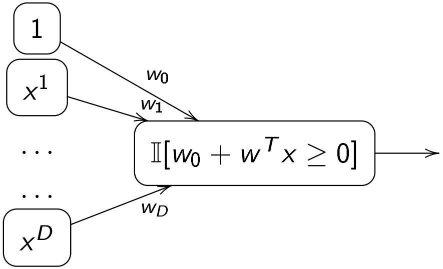
Layers

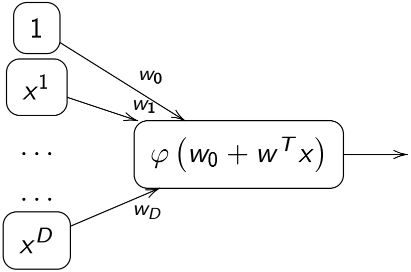


- Structure of neural network:
    - 1-input layer
    - 2-hidden layers
    - 3-output layer

Continious activations

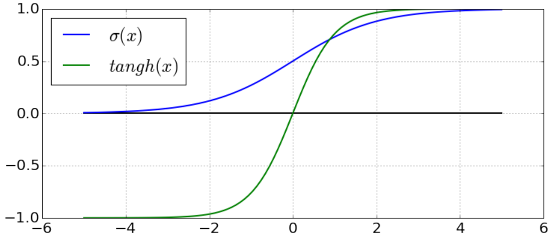
- Pitfall of $\mathbb{I}[]$: it causes stepwise constant outputs, weight optimization methods become inapliccable.
- We can replace $\mathbb{I}[w^T x + w_0 \geq 0]$ with smooth activation $\varphi(w^T x + w_0)$





Typical activation functions

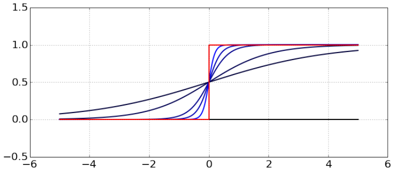
- sigmoidal: $\sigma(x) = \frac{1}{1+e^{-x}}$
  - 1-layer neural network with sigmoidal activation is equivalent to logistic regression
- hyperbolic tangent: $\text{tangh}(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$



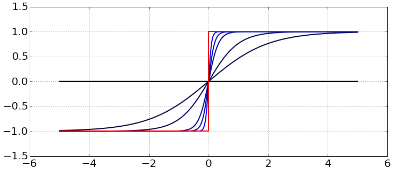
- ReLu: $\varphi(x) = [x]_{+}$.

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_{j0} 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

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

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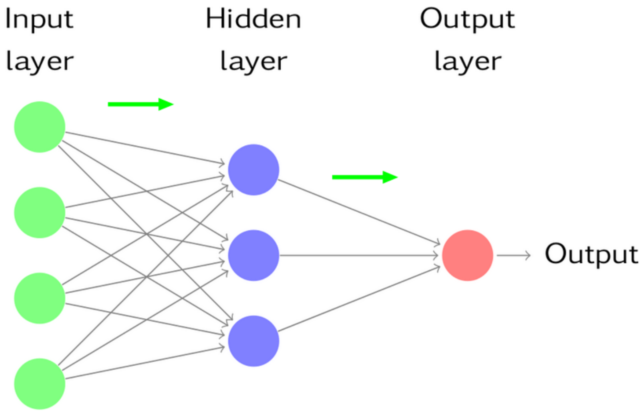
Output generation

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



Activations at output layer

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

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

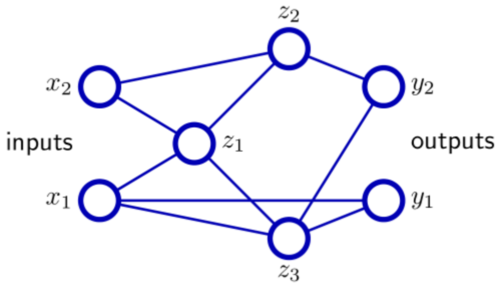
  - multiclass: $y \in \{1, 2, ...C\}$

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

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



- recurrent networks, RBF-activations.

Number of layers selection

- Number of layers usually denotes all layers except input layer (hidden layers+output layer)
- Classification with indicator activations:
    - 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 all measurable sets

Number of layers selection

- Regression with indicator activations:
    - 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.

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Network optimization: regression

- Single output:

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

Network optimization: regression

- Single output:

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

- K outputs

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

Network optimization: classification

- Two classes, $y \in \{0, 1\}$:

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

Network optimization: classification

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

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

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

Network optimization: classification

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

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

- In practice log-likelihood is maximized to avoid numerical underflow.

Neural network optimization

- Denote W - the total dimensionality of weights space, $w \in \mathbb{R}^W$.
- 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):
    $w^{k+1} := w^k - \eta \nabla E(w^k)$
    $k := k + 1$
```

- Standardization of features makes gradient descend converge faster
- Other optimization methods are more efficient (such as conjugate gradients)

Gradient calculation

- Denote $\varepsilon_i = (0, ..., 0, \overbrace{\varepsilon}^{i\text{-th position}}, 0, ...0) \in \mathbb{R}^W$
- 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

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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

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

- Stochastic simplification of model, such as dropout.

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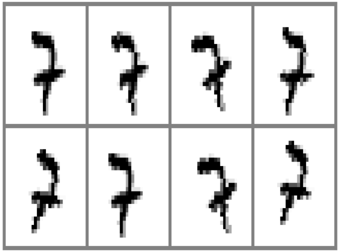
Invariance to particular transformations

- 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

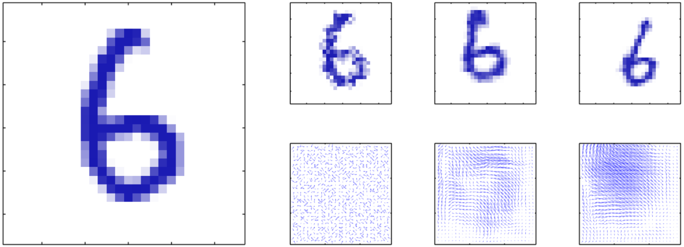


Invariance to particular transformations

- Approaches to build an invariant model to particular transformation:
  - use only features that are invariant to transformations
  - 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
  - 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



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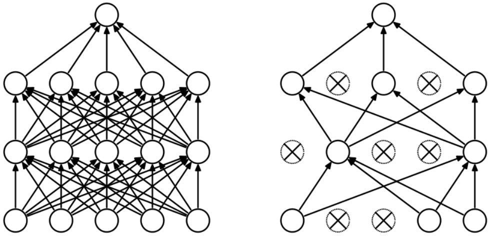
Dropout idea

Each neuron is left or removed independently from decisions about other nodes:



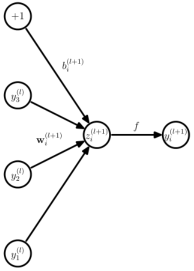
(a) Standard Neural Net (b) After applying dropout.

- Output layer nodes are never removed.
- Recommended[2] neuron removal probability $1 - p$:
    - $p = 0.5$ for inner layer nodes
    - $p = 0.8$ for input layer nodes (feature subsampling)

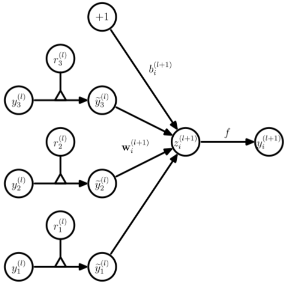
[2]Removal probabilities can be fine-tuned on cross-validation.

Dropout algorithm

- Dropout forces neurons to rely less on other neurons and to learn something valuable by themselves.
    - neurons learning becomes more robust to information learnt by other neurons.
    - resulting network becomes less overfitted.
- $r_i^{(l)}$ are i.i.d. random variables having *Bernoulli*(p) distribution.



(a) Standard network



(b) Dropout network

Definitions

Define:

- $f(x)$ - an activation function.
- y^l - vector of outputs at layer l
- z^l - vector of inputs to layer l
- L - number of layers in neural network
- $y^{(0)} = x$ - input feature vector
- $Bernoulli(p)$ returns a vector of independent Bernoulli random variables with parameter p.

Forward propagation algorithm

We need to repeat forward propagation recurrently for $l = 0, 1, ... L - 1$.

1. Usual feed-forward neural network:

$$z_i^{(l+1)} = \left(w_i^{(l+1)}\right)^T y^l + b_i^{(l+1)}$$
$$y_i^{(l+1)} = f(z_i^{(l+1)})$$

2. Feed-forward network with dropout:

$$\mathbf{r_j^{(l)}} \sim \mathbf{Bernoulli(p)}$$
$$\mathbf{\tilde{y}^l} = \mathbf{r^{(l)}} * \mathbf{y^{(l)}}$$
$$z_i^{(l+1)} = \left(w_i^{(l+1)}\right)^T \tilde{y}^l + b_i^{(l+1)}$$
$$y_i^{(l+1)} = f(z_i^{(l+1)})$$

Application of dropout

- **Learning**
    - while weights not converge:
        1. sample random subnetwork (“thinned network”) with dropout
        2. apply one step of stochastic gradient descent to thinned network

  Comment: due to weights sharing across all thinned networks the number of parameters is the same as in original network.
- **Prediction**
    - use full networks with all nodes, but multiply each weight by p
    - such scaling approximates average output of randomly sampled thinned network[3].

[3]Approximation is precise for networks without non-linearities. With non-linearities - not. We may also use Monte-Carlo sampling in the latter case.

Conclusion on neural networks

- 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