Multilayer perceptron

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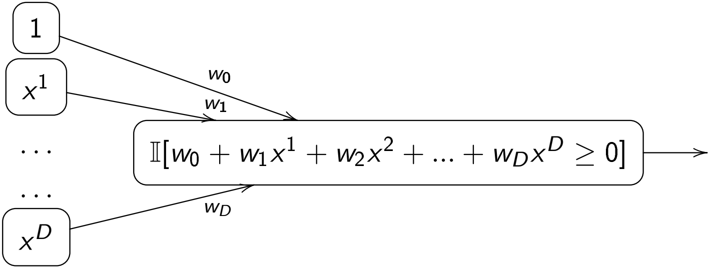
Table of Contents

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.

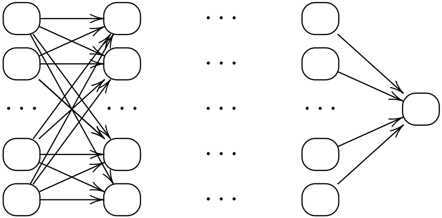
Simple model of a neuron



- 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
- w_0 stands for bias

Multilayer perceptron architecture[1]

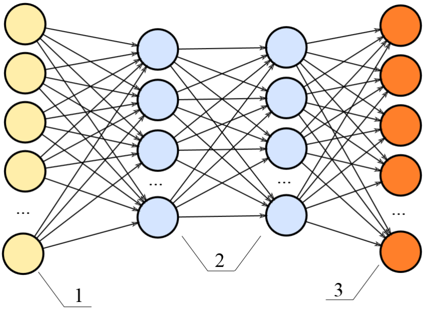
- Hierarchically nested set of neurons.
- Each node has its own weights.



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

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

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

Output generation

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

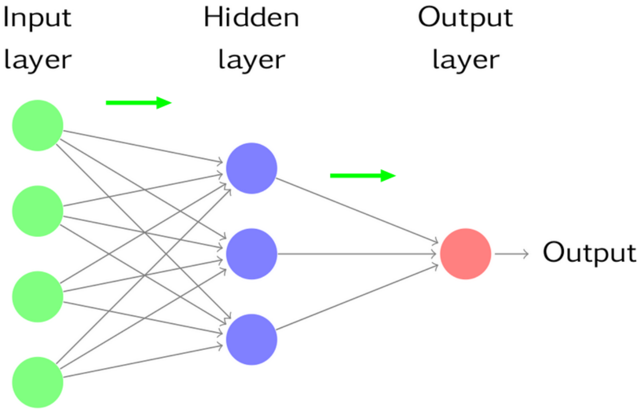


Table of Contents

Number of layers selection

- Consider indicator activations.
- **# layers selection for 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
- So 3 layered NN can approximate all regular[2] sets!

[2] With well-defined volume - Borel measurable.

Number of layers selection

- Consider indicator & identity (linear) activations.
- **# layers selection for 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)
- So 3 layered NN can approximate all regular[3] dependencies!

[3] Function should be Borel measurable.

Number of layers selection

Sufficient amount of layers

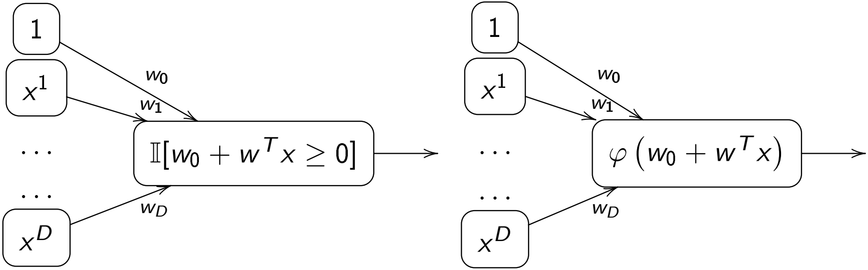
Any continuous function on a compact space can be uniformly approximated by 2-layer neural network with linear output and any (without polynomial) activation functions.

- In practice #layers=2 is enough, but may require too many neurons.
- So often it is more convenient to use more layers with less total amount of neurons
  - less parameters=>less overfitting.

Table of Contents

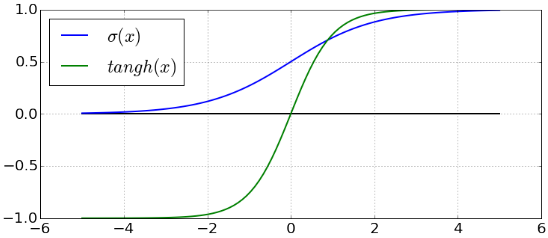
Continuous activations

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



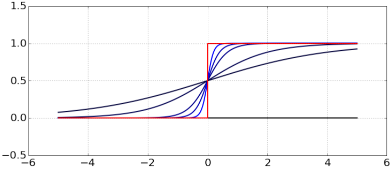
Typical activation functions

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

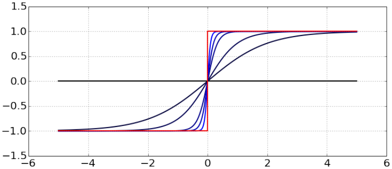


Activation functions

Activation functions are smooth approximations of step functions:



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

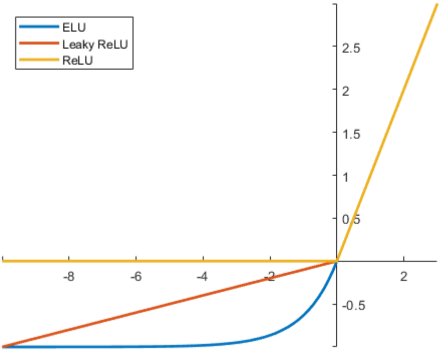


tangh(ax) limits to -1/1-step function as $a \to \infty$

Activation functions

- Rectified linear unit (ReLU): $\varphi(x) = x\mathbb{I}[x \geq 0]$
- SoftPlus: $\varphi(x) = \ln(1 + e^x)$
- Leaky ReLU: $\varphi(x) = \begin{cases} x, & x \geq 0 \\ 0.01x, & x < 0 \end{cases}$
- Parametric ReLU (PReLU): $\varphi(x|\alpha) = \begin{cases} x, & x \geq 0 \\ \alpha x, & x < 0 \end{cases}$
- Exponential LU (ELU): $\varphi(x) = \begin{cases} x, & x \geq 0 \\ \alpha(e^x - 1), & x < 0 \end{cases}$

ReLU visualization



Activation functions

MaxOut: $\varphi(x) = \max\{w_1^T x + b_1, w_2^T x + b_2\}$
Gaussian: $\varphi(x|\mu, \sigma^2) = exp\left(-\frac{\|x-\mu\|^2}{2\sigma^2}\right)$

Recommendations:

- do not use sigmoid (saturates, non-centered output)
- start from ReLU
- if many "dead" neurons - use leaky ReLU, PReLU, ELU, etc.

Activations at output layer

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

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

  - 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.

Table of Contents

4 Optimization
- Loss functions
- Optimization

Regression

- Scalar regression $y \in \mathbb{R}$:

$$MSE(x, y) = (\widehat{y}(\mathbf{x}) - y)^2$$

- Vector regression $\mathbf{y} \in \mathbb{R}^K$:

$$MSE(x, y) = \|\widehat{\mathbf{y}}(\mathbf{x}) - \mathbf{y}\|_2^2$$

- Total loss: summed loss over objects of the training set.

Classification (class probabities output)

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

$$NLL(x, y) = -\ln p(y = 1|x)^{y}[1 - p(y = 1|x)]^{1-y}$$

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

$$NLL(x, y) = -\ln \prod_{c=1}^{C} p(y = c|x)^{y_c}, \qquad y_c = \mathbb{I}\{y = c\}$$

- Total loss: summed loss over objects of the training set.

Classification (class scores output)

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

$$hinge(x, y) = [O_{-y}(x) + 1 - O_y(x)]_+$$

- C classes ($y \in \{1, 2, ...C\}$):

$$hinge_1(x, y) = \left[\max_{c \neq y} O_c + 1 - O_y\right]_+$$

$$hinge_2(x, y) = \sum_{c \neq y} [O_c + 1 - O_y]_+$$

- Total loss: summed loss over objects of the training set.

4. Optimization
   - Loss functions
   - Optimization

Neural network optimization

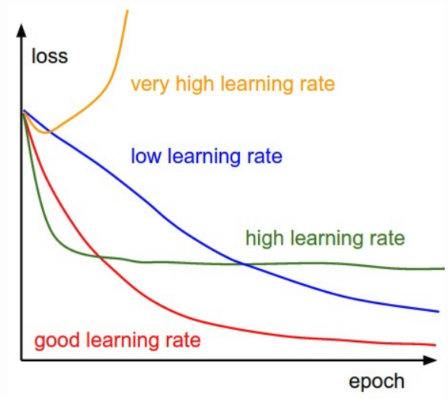
- Denote $\mathcal{L}(\widehat{y}, y)$ - the loss function, $W = \#$[weights in the network], η - step size.
- We may optimize neural network using SGD:

```
initialize randomly w # small values for sigmoid and tangh

while not (stop condition):
    sample random object (x_i, y_i)
    w := w − η∇_w L(w, x_i, y_i)
```

- Standardization of features makes GD & SGD converge faster
- Other optimization methods are more efficient (SGD+momentum, Adam)

Learning rate selection is important



Important to decrease learning rate on plateaus!

SGD with momentum

```
initialize randomly w # small values for sigmoid and tangh

while not (stop condition):
    sample random object (x_i, y_i)
    Δw := αΔw + (1 − α) ∇_w L(w, x_i, y_i) # alpha is typically 0.9.
    w := w − ηΔw
```

- Converges faster, because
  - gradient is based on several observations instead of one
  - gradient directions aggregation averages ininformative trembling:

Gradient calculation

- Direct $\nabla\mathcal{L}(w)$ calculation, using

$$\frac{\partial\mathcal{L}}{\partial w_i}=\frac{\mathcal{L}(w+\varepsilon_i)-\mathcal{L}(w)}{\varepsilon}+O(\varepsilon) \qquad (1)$$

or better

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

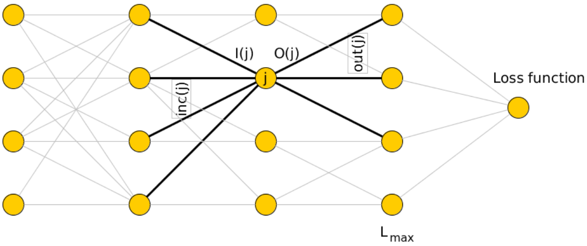
has complexity $O(W^2)$

  - need to calculate W derivatives
  - complexity for each derivative: 2W

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

Definitions

- j - neuron number, having non-linearity $\varphi_j(\cdot)$
- I_j - input to neuron j, $O_j = \varphi_j(I_j)$ - output of neuron j
- $I_j = \sum_{k \in inc(j)} w_{kj} O_k$
- $out(j)$ - set of neurons having incoming connection from neuron j.
    - bias omitted for simplicity



Definitions

- Denote w_{ij} be the weight of edge, connecting i-th and j-th neuron.
- Define $\delta_j = \frac{\partial \mathcal{L}}{\partial I_j} = \frac{\partial \mathcal{L}}{\partial O_j}\frac{\partial O_j}{\partial I_j}$
- Since $\mathcal{L}$ depends on w_{ij} through the following functional relationship $\mathcal{L}(w_{ij}) \equiv \mathcal{L}(O_j(I_j(w_{ij})))$, using the chain rule we obtain:
$$\frac{\partial \mathcal{L}}{\partial w_{ij}} = \frac{\partial \mathcal{L}}{\partial I_j}\frac{\partial I_j}{\partial w_{ij}} = \delta_j O_i$$
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.
- $\frac{\partial \mathcal{L}}{\partial I_j} = \frac{\partial \mathcal{L}}{\partial O_j}\frac{\partial O_j}{\partial I_j} = \frac{\partial \mathcal{L}}{\partial O_j}\varphi'(I_j)$, where φ is the activation function.

Backpropagation steps 1,2

1) If $layer(j) = L_{max}$ (lies in the output layer) $\frac{\partial \mathcal{L}}{\partial O_j}$ is calculated directly.
   - e.g. for $\mathcal{L} = \frac{1}{2}\sum_{i \in OL}(O_i - y_i)^2$: $\frac{\partial \mathcal{L}}{\partial O_j} = O_j - y_j$
2) $\frac{\partial \mathcal{L}}{\partial I_j}$ is calculated from $\frac{\partial \mathcal{L}}{\partial O_j}$:

$$\frac{\partial \mathcal{L}}{\partial I_j} = \frac{\partial \mathcal{L}(O_j)}{\partial I_j} = \frac{\partial \mathcal{L}}{\partial O_j}\frac{\partial O_j}{\partial I_j} = \frac{\partial \mathcal{L}}{\partial O_j}\varphi_j'(I_j)$$

Backpropagation steps 3,4

3) $\frac{\partial \mathcal{L}}{\partial O_j}$ is calculated from $\frac{\partial \mathcal{L}}{\partial I_j}$ of next layer:

$$\frac{\partial \mathcal{L}}{\partial O_j} = \frac{\partial \mathcal{L}\left(\{I_s\}_{s\in out(j)}\right)}{\partial O_j} = \sum_{s\in out(j)} \frac{\partial \mathcal{L}}{\partial I_s}\frac{\partial I_s}{O_j} = \sum_{s\in out(j)} \frac{\partial \mathcal{L}}{\partial I_s} w_{js}$$

4) Using $\frac{\partial \mathcal{L}}{\partial I_j}$ we can calculate $\frac{\partial \mathcal{L}}{\partial w_{ij}}$ (given that $i \in inc(j)$):

$$\frac{\partial \mathcal{L}}{\partial w_{ij}} = \frac{\partial \mathcal{L}(I_j)}{\partial w_{ij}} = \frac{\partial \mathcal{L}}{\partial w_{ij}}\frac{\partial I_j}{\partial w_{ij}} = \frac{\partial \mathcal{L}}{\partial I_j}\frac{\partial}{\partial w_{ij}}\left(\sum_{k\in inc(j)} w_{kj} O_k\right) = \frac{\partial \mathcal{L}}{\partial I_j} O_i$$

Backpropagation algorithm

FORWARD PASS: memorize I_j, O_j for all neurons.
BACKWARD PASS:
evaluate $\frac{\partial\mathcal{L}}{\partial O_j}$ for all neurons of output layer, using (1).
evaluate $\frac{\partial\mathcal{L}}{\partial I_j}$ for all neurons of output layer, using (2).
for layer L in $L_{max}-1, L_{max}-2, ...1$:
    evaluate $\frac{\partial\mathcal{L}}{\partial w_{ij}}$ for all j of layer $L+1$ and all $i \in inc(j)$, using (4).
    evaluate $\frac{\partial\mathcal{L}}{\partial O_j}$ for all neurons of layer L, using (3).
    evaluate $\frac{\partial\mathcal{L}}{\partial I_j}$ for all neurons of layer L, using (2).

Comments

- Must know $\varphi_j(\cdot)$ and $\varphi_j'(\cdot)$.
- As we may calculate $\frac{\partial \mathcal{L}}{\partial O_j}$ $\forall j$, we may estimate $\frac{\partial \mathcal{L}}{\partial x^d}$ because x^d =d-th output of input layer.
    - May be used for fine-tuning input to have desired properties
        - e.g. style transfer
        - control optimization, having minimal loss (oil production optimization)
- Backpropagation correctness is checked by comparing results with (1), (2).

Complexity

- Denote $W = \#[\text{connections in the network}]$.
- Computational complexity: $O(W)$
    - due to steps (3) and (4).
- Memory complexity: $O(W)$, need to store:
    - I_j, O_j for all neurons.
    - w_{ij} for all connected neuron pairs.

How many objects to consider?

- **Batch mode**: estimate loss on all objects
  - works only for small N
- **Minibatch mode**: estimate loss on K random objects
  - $K << N$, works on big data
  - sampling: rolling window of width K over shuffled training set
  - minibatch size $\propto$ parallelization ability of CPU or GPU (better).

Table of Contents

Multilayer perceptron as ensemble method

All network is optimized, in contrast:

- boosting keeps previous trees fixed
- stacking keeps base learners fixed.

Overfitting is more severe - need regularization.

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.

Regularization in NNs

- 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)
  - add L2/L1 regularization:

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

    - λ may be different for each layer.

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
- Everything in optimization affects final result:
  - starting conditions, optimization algorithm, learning rate size and its decrease schedule.