Neural networks

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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.

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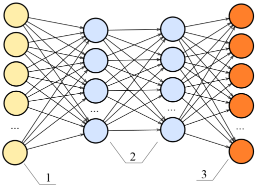
Definition

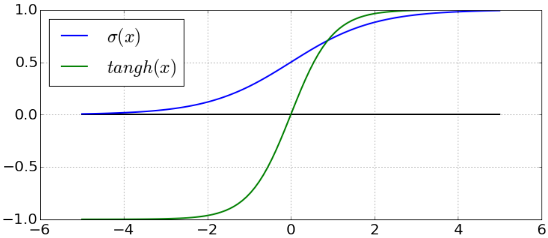
- linear / logistic regression - simplest case
- acyclic directed graph
- verticals called neurons
- edges correspond to certain weighs



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

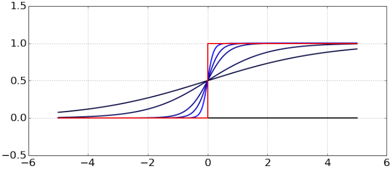
Definition

- Each neuron j is associated a non-linear transformation φ.
- For multilayer perceptron class neural networks φ belongs to a class of activation functions.
- Most common activation functions:
  - sigmoidal: $\sigma(x) = \frac{1}{1+e^{-x}}$
    - 1-layer neural network with sigmoidal activation is equivalent to logistic regression
  - hyperbolic tangent: $\text{tangh}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

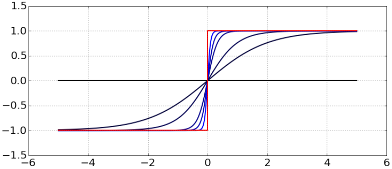


Activation functions

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 i.
- Denote: I_i - input to neuron i, O_i - output of neuron i
- Output of neuron i: $O_i = A(I_i)$, where A is activation function.
- Input to neuron i: $I_i = \sum_{k \in inc(i)} w_{ki} O_k + w_{k0}$,
    - w_{k0} is the bias term
    - $inc(i)$ is a set of neurons with outgoing edges to neuron i.
    - further we will assume that at each layer there is a vertex with constant output $O_{const} \equiv 1$, so we can simplify notation

$$I_i = \sum_{k \in inc(i)} w_{ki} O_k$$

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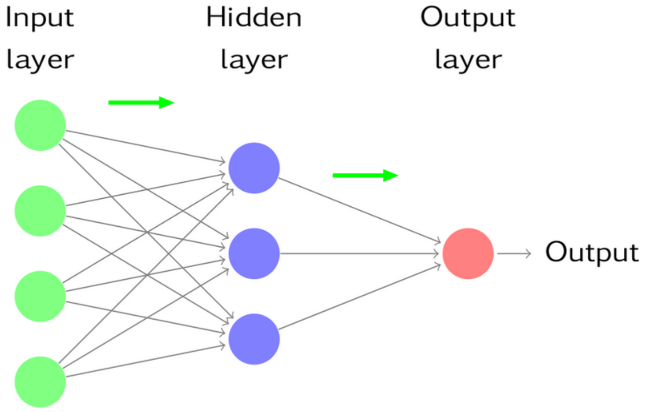
Output generation

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

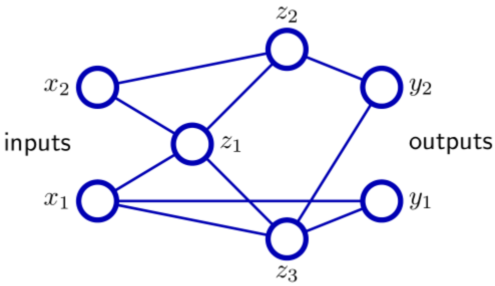


Output generation

- Output layer transformations
  - regression: $\varphi(I) = I$
  - classification:
    - 2 classes: sigmoid, indicating target class probability
      $$\varphi(I) = \frac{1}{1 + e^{-I}}$$
    - multiple classes: softmax, indicating probabilities of each class:
      $$\varphi(I_i) = \frac{e^{O_i}}{\sum_{k \in OL} e^{O_k}}, \, i \in OL$$
      where OL denotes neuron indices at 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.

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 polyhedron
    - 3-layer network can uniformly approximate arbitrary continuous function (as sum of indicators of various 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 fewer amount of neurons
  - model becomes more interpretable and tunable

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

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

Network optimization: classification

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

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

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

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

Network optimization: classification

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

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

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

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

- 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:

while (stop criteria not met):

$$w^{k+1} = w^k - \eta \nabla E(w^k)$$

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

Neural network optimization

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

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

or better

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

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

- Instability with respect to:
    - different starting parameter values
    - different subsamples
    - different feature selections
- Solutions
    - select best optimum from local optima
    - average predictions for different local optima

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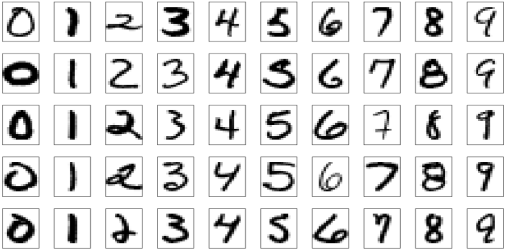
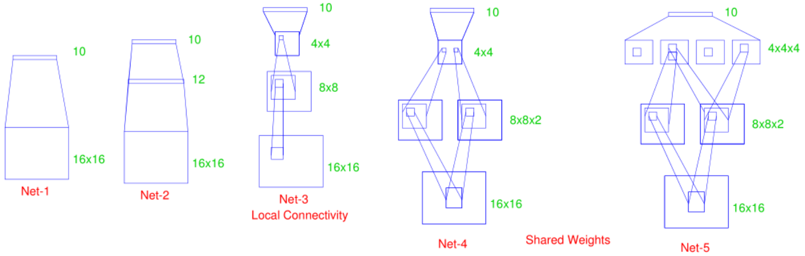
Case study (due to Hastie et al. The Elements of Statistical Learning)

ZIP code recognition task

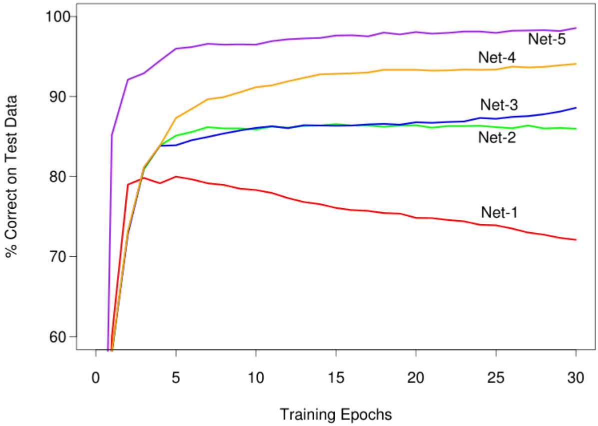


Neural network structures

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


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

Addition

- Deep learning
- Neural networks may model not only real value outputs, but densities
  - each output - frequency of histogram bin
  - each output - parameter of a distribution

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