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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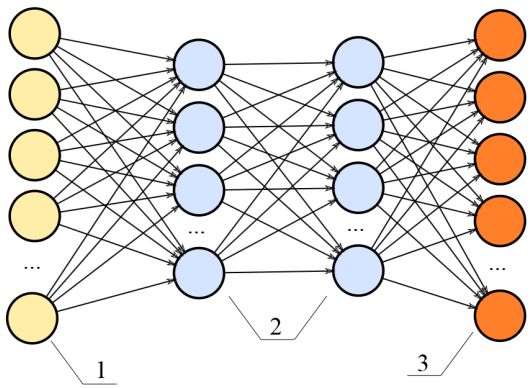
Definition

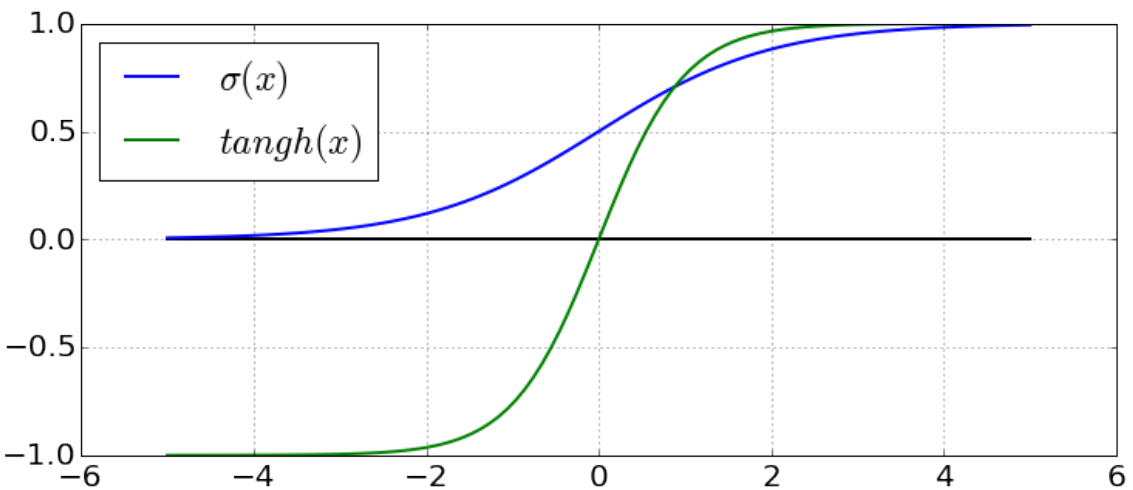
- linear / logistic regression - simplest case
- acyclic directed graph
- verticals called neurons
- edges correspond to certain weighs



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

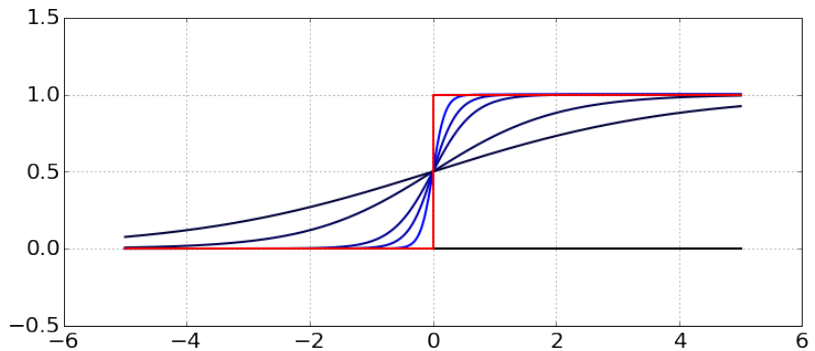
Definition

- 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: $\text{tangh}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

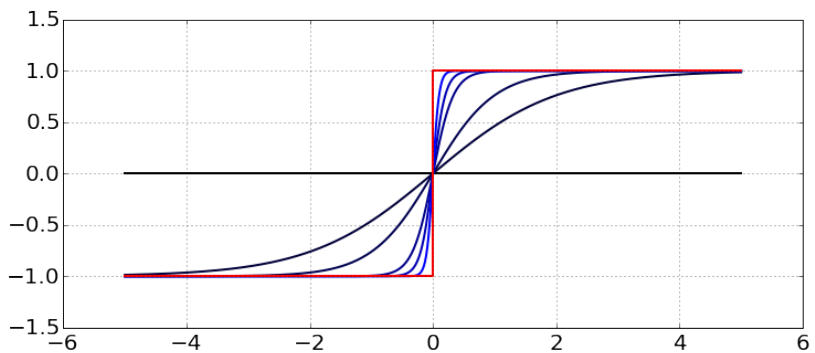


Activation functions

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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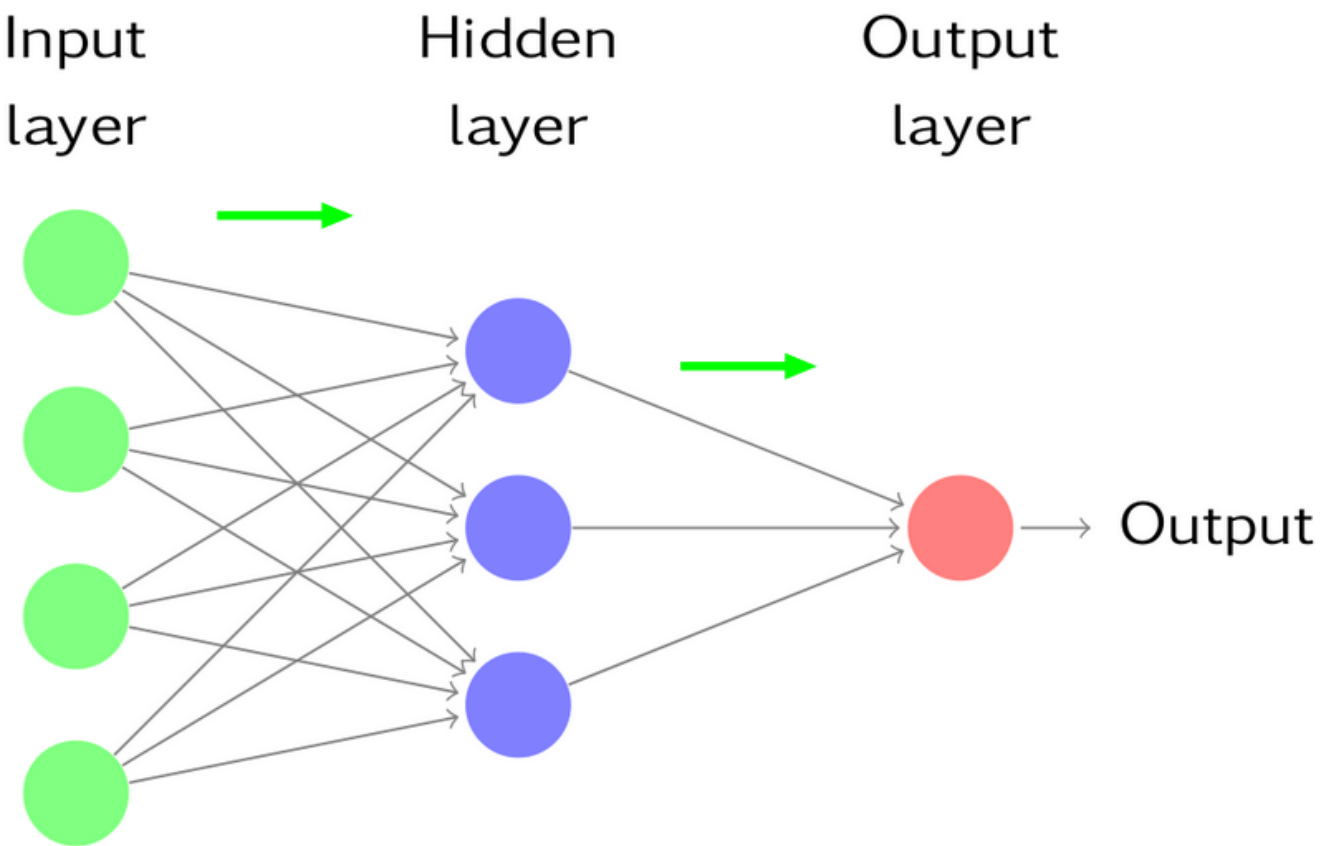
Output generation

- 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

$$\varphi(I) = \frac{1}{1+e^{-I}}$$

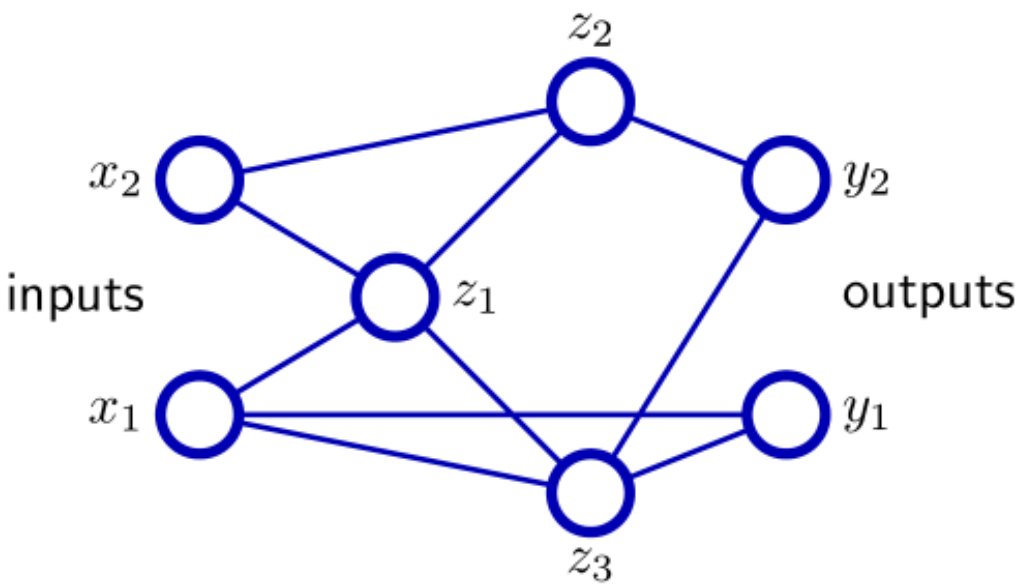
    - multiple classes: softmax, indicating probabilities of each class:

$$\varphi(I_i) = \frac{e^{O_i}}{\sum_{k \in OL} e^{O_k}}, \; i \in OL$$

      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



- 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 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

Neural network architecture selection

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

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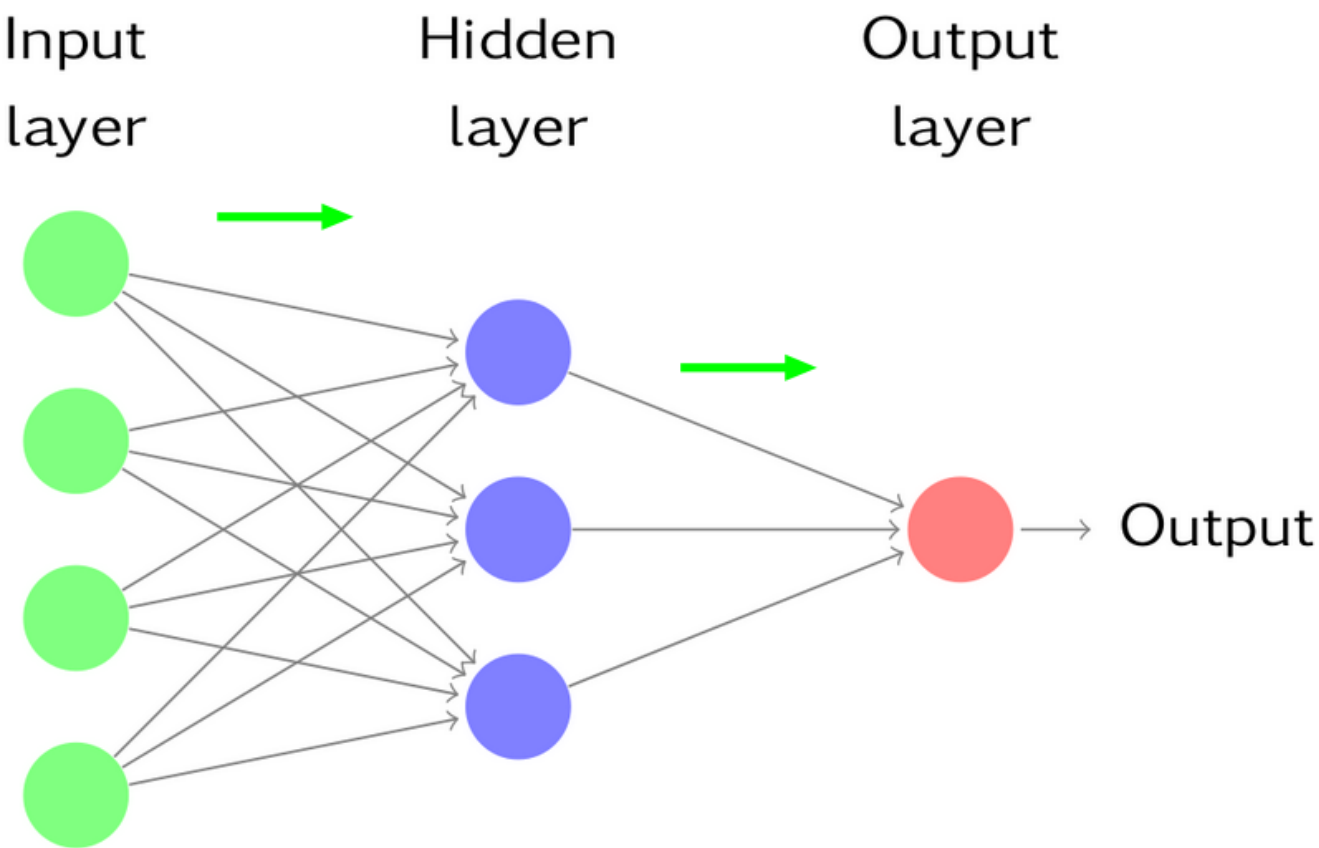
Weight space symmetries

- 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.

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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:

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- 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:

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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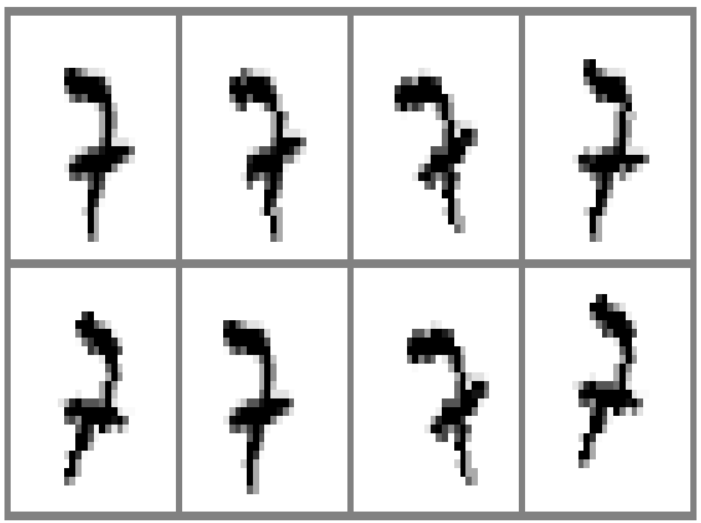
Invariances

- 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

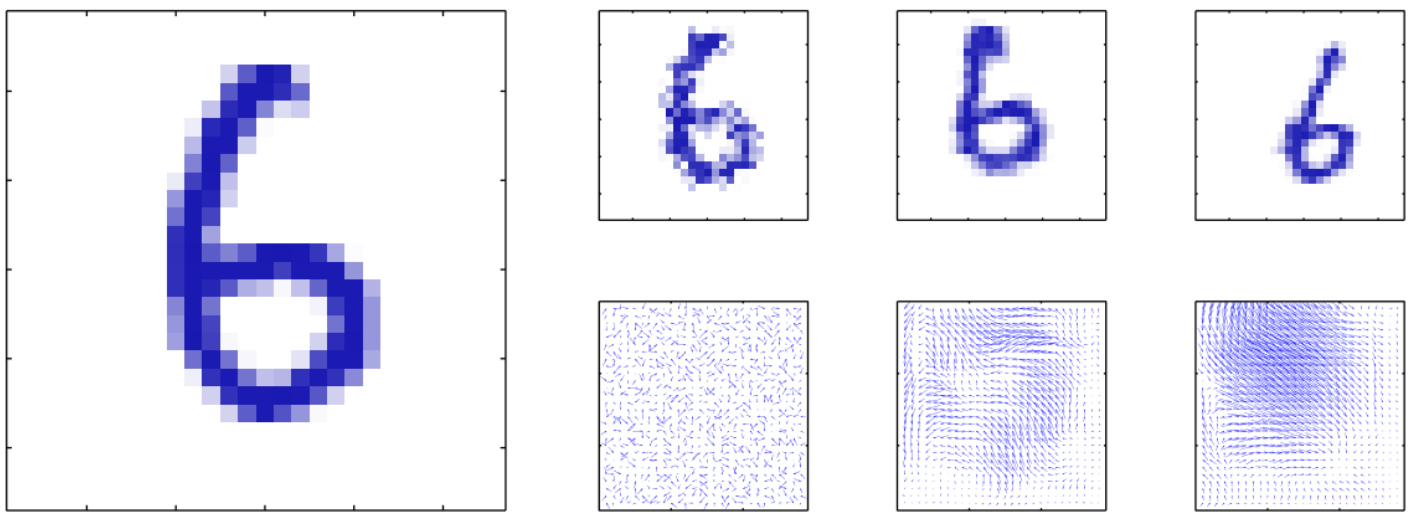


Invariances

- 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:

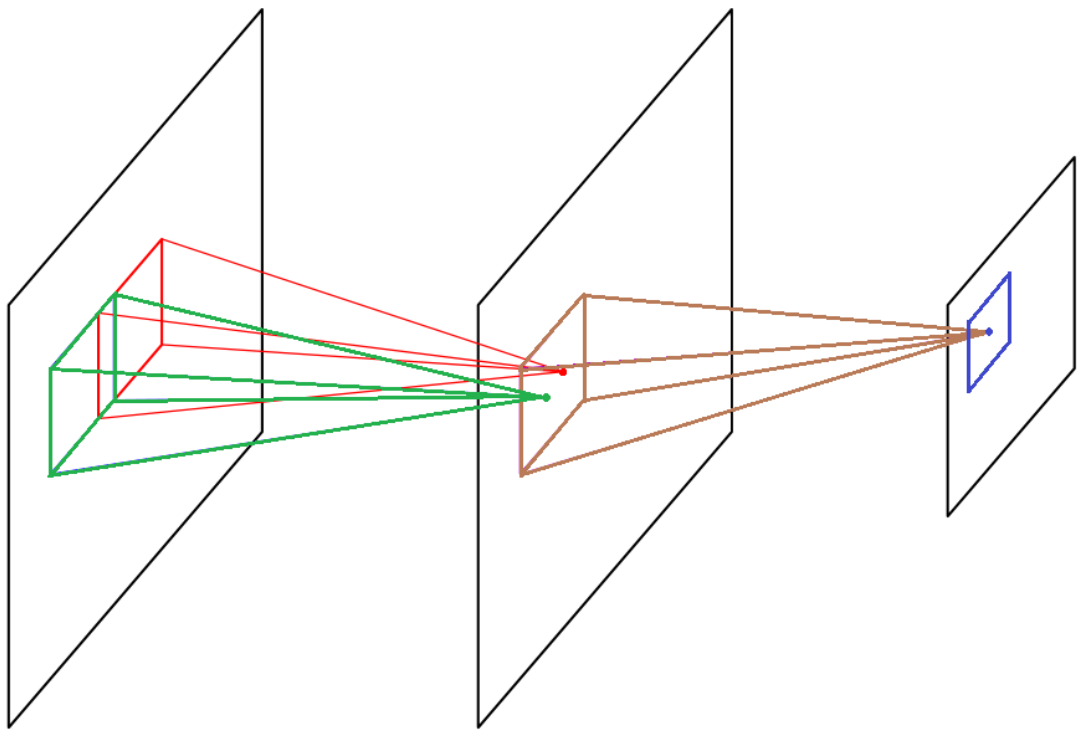
$$\left.\frac{\partial y_k}{\partial \xi}\right|_{\xi=0} = \sum_{i=1}^{D} \frac{\partial y_k}{\partial x_i}\frac{\partial x_i}{\partial \xi} = \sum_{i=1}^{D} J_{ki}\tau_i$$

- 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

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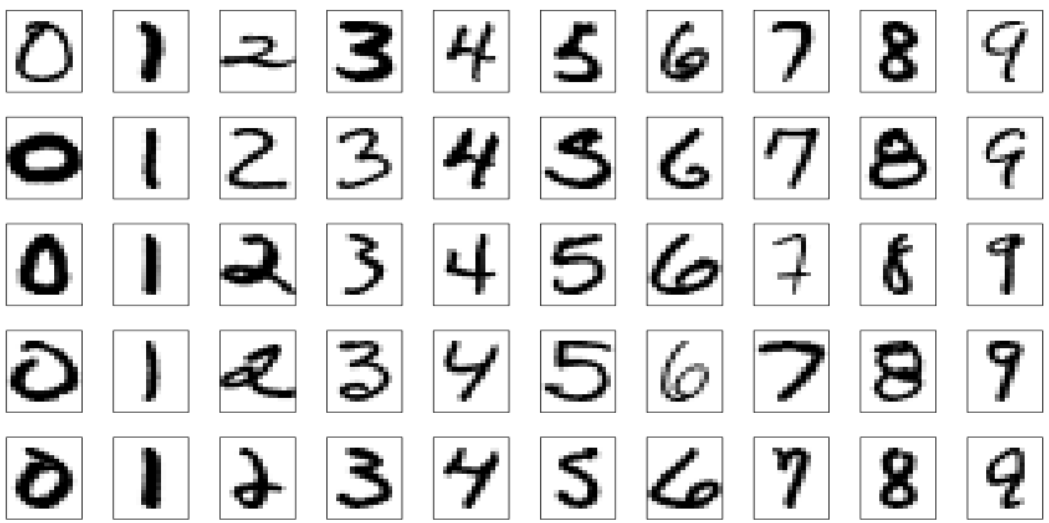
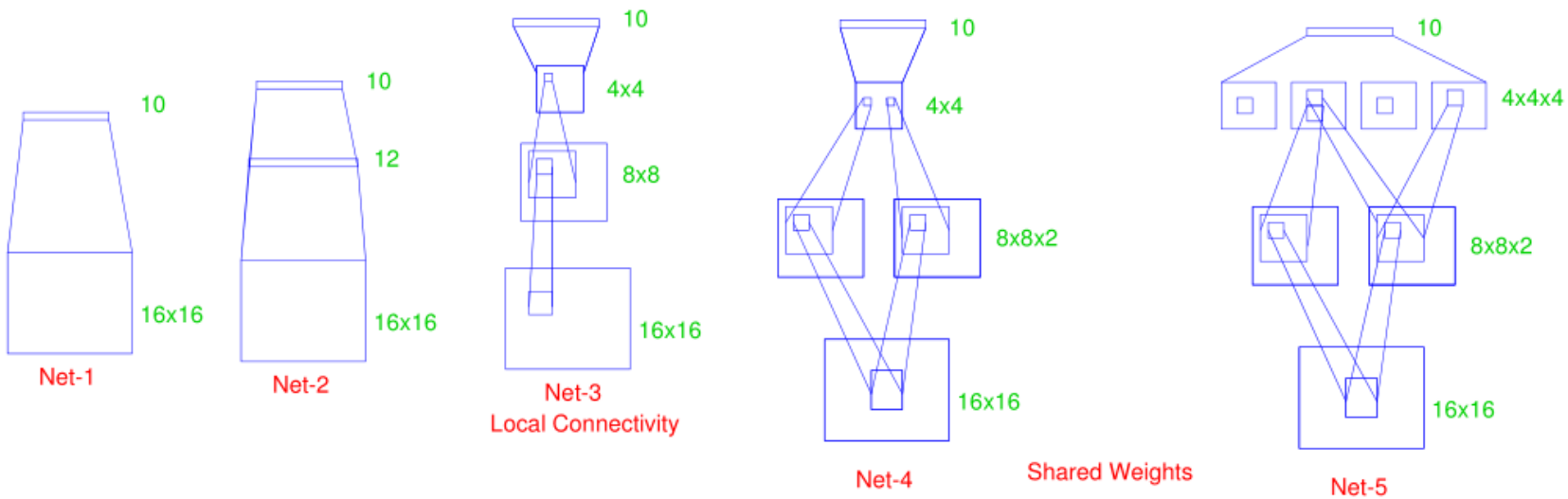
Case study (due to Hastie et al. The Elements of Statistical Learning)

ZIP code recognition task

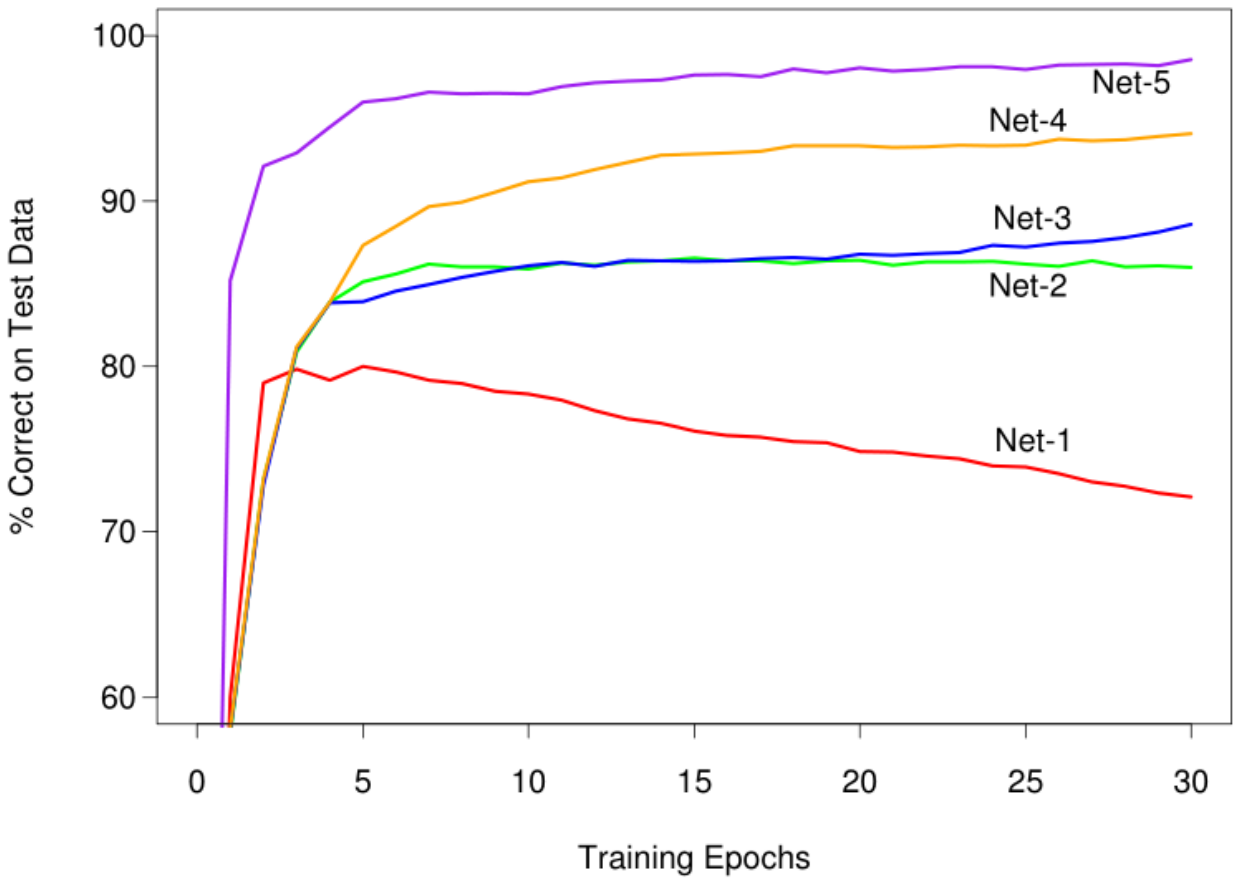


Neural network structures

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


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