# Neural networks

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# Table of Contents

# History

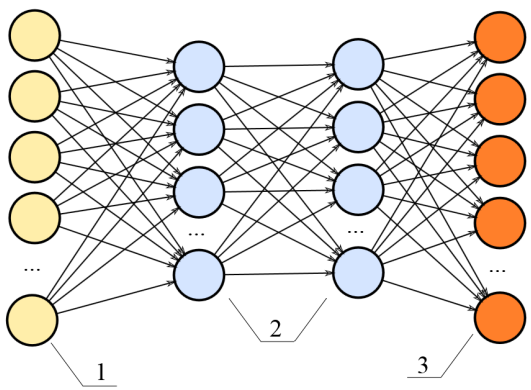
- Neural networks originally appeared as an attempt to model human brain

- 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.

# Table of Contents

# Definition

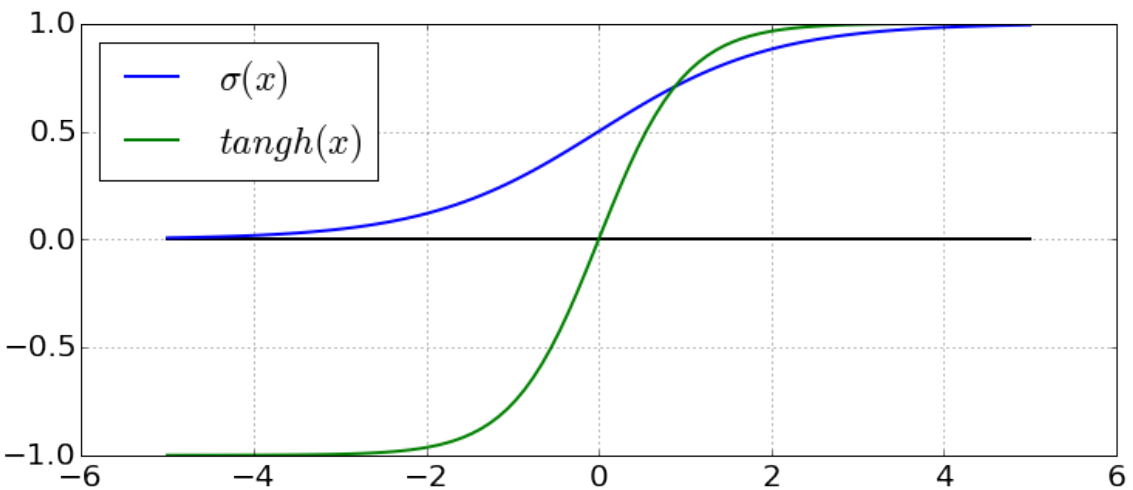
- acyclic directed graph
- verticals called neurons
- edges correspond to certain weighs




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

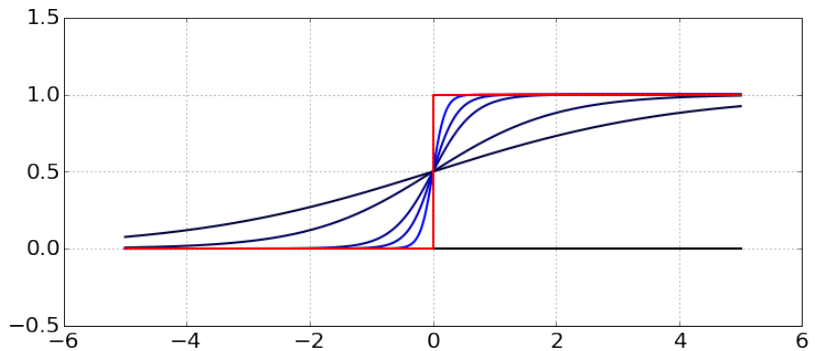
# Definition

- Each neuron $j$ is associated a non-linear transformation $\varphi$.
- For multilayer perceptron class neural networks $\varphi$ 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: $\text{tangh}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

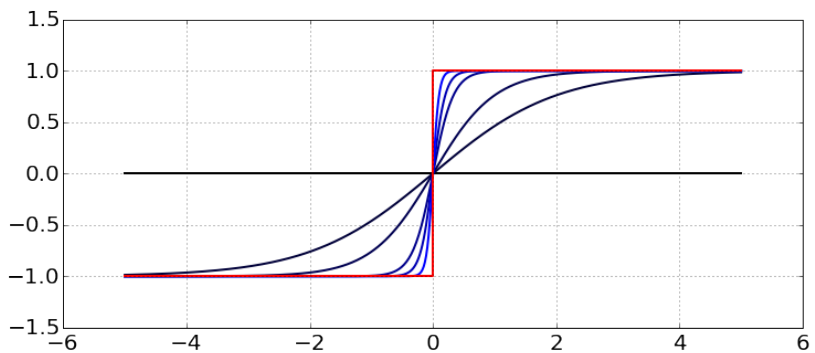


# Activation functions

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 $a \to \infty$

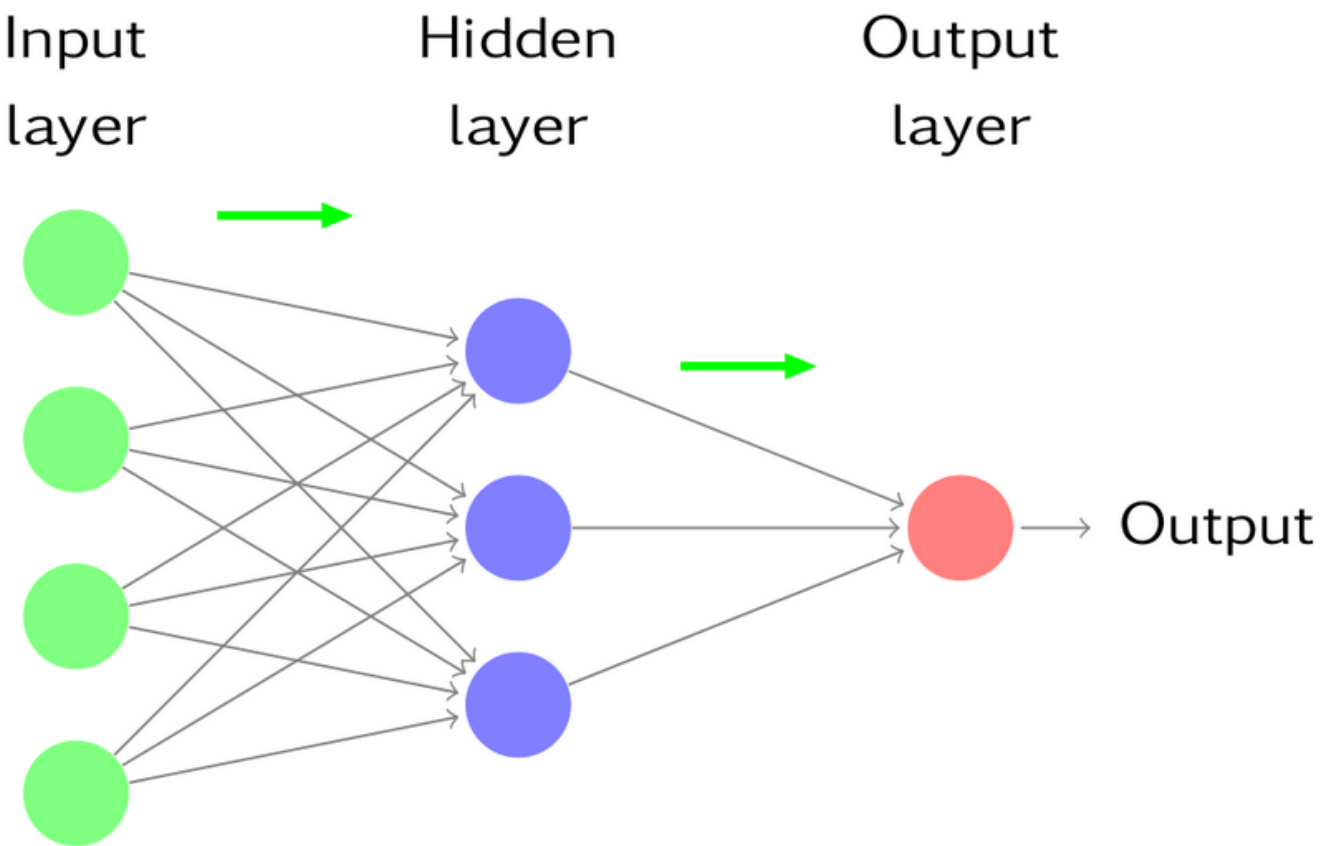
# Definition details

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

# Table of Contents

# 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

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

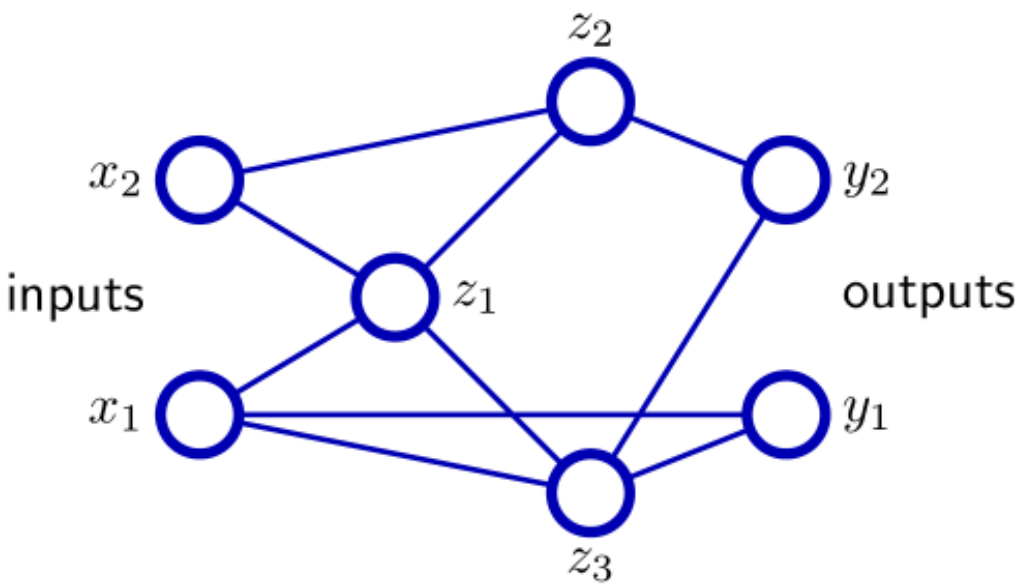
    - multiple classes: softmax, indicating probabilities of each class:

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

      where $OL$ denotes neuron indices at output layer.

# Generalizations

- each neuron $j$ may have custom non-linear transformation $\varphi_j$
- 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

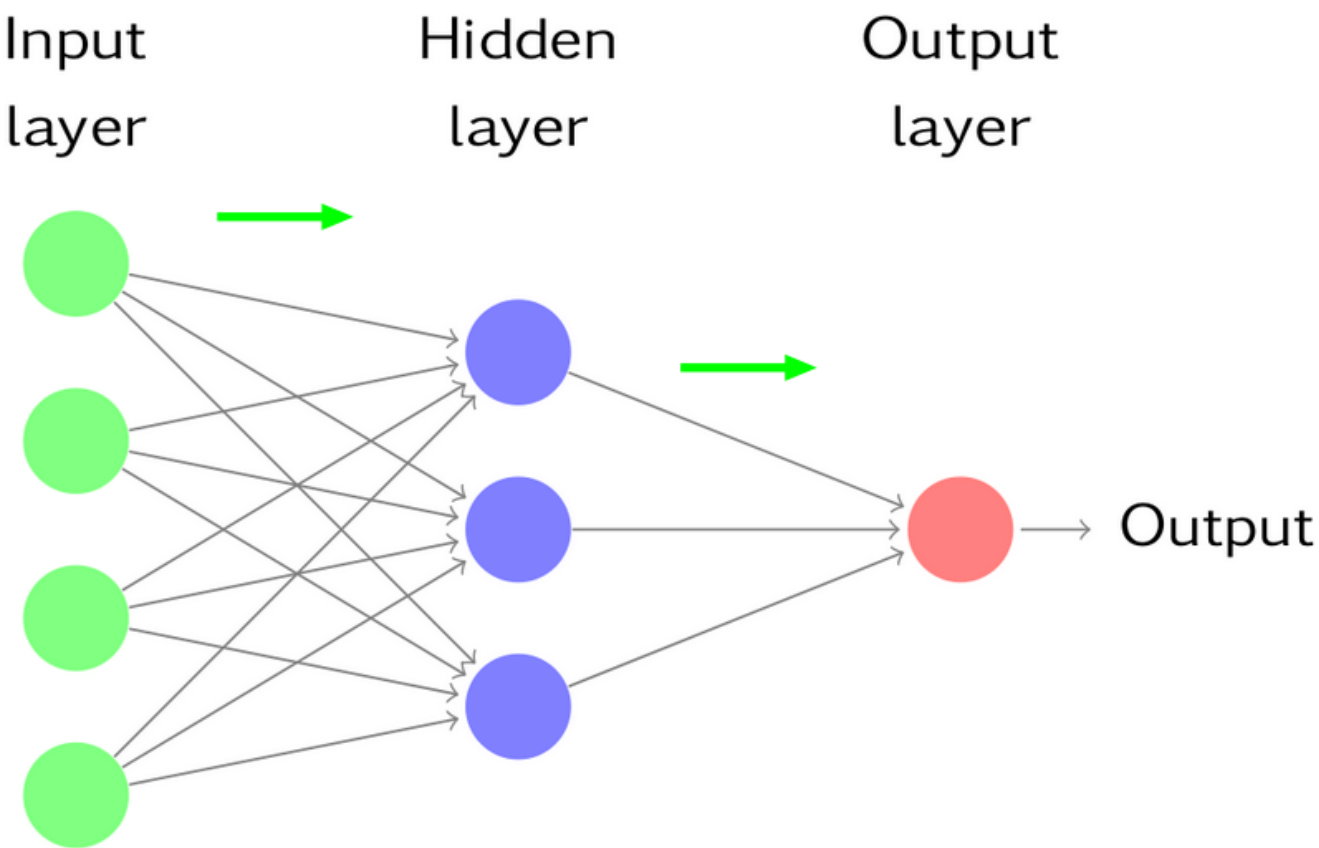
# Neural network architecture selection

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

# Table of Contents

# 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.

# Table of Contents

# Network optimization

- Regression ($y$ denotes true value and $\widehat{y}$ - its prediction)
  - single output:
    - $\frac{1}{N}\sum_{n=1}^{N}(\widehat{y}_n(x_n)-y_n)^2 \to \min_w$
  - K outputs
    - $\frac{1}{NK}\sum_{n=1}^{N}\sum_{k=1}^{K}(\widehat{y}_{nk}(x_n)-y_{nk})^2 \to \min_w$
- Classification
  - two class ($y \in \{0,1\}$ denotes true class, and $p$ is the probability of class 1):
    - $\prod_{n=1}^{N} p(x_n)^{y_n}(1-p(x_n))^{1-y_n} \to \max_w$ equivalent to $\sum_{n=1}^{N} y_n \ln p(x_n) + (1-y_n)\ln(1-p(x_n)) \to \max_w$
  - $C$ classes ($y_{nc} = \mathcal{I}\{y_n = c\}$, $p_c(x_n)$ - estimated probability of class $c$):
    - $\prod_{n=1}^{N}\prod_{c=1}^{C} p_c(x_n)^{y_{nc}} \to \max_w$ equivalent to $\sum_{n=1}^{N}\sum_{c=1}^{C} y_{nc}\ln p_c(x_n) \to \max_w$

# 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.

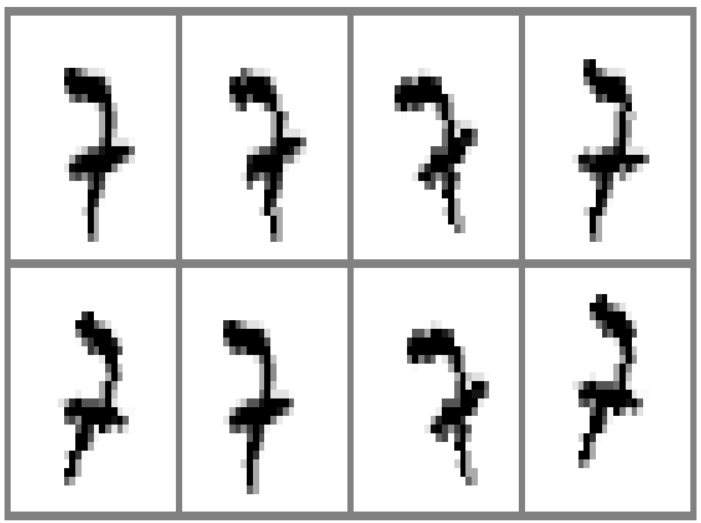
# Multiple minima problem

- Neural network optimization function has multiple minima
- Solution: select lowest minimum from multiple optimizations with different starting values
- Robust solutions:
  - average outputs of neural networks obtained by using different starting values
  - average outputs of neural networks trained on different bootstrap subsamples

# Table of Contents

# 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

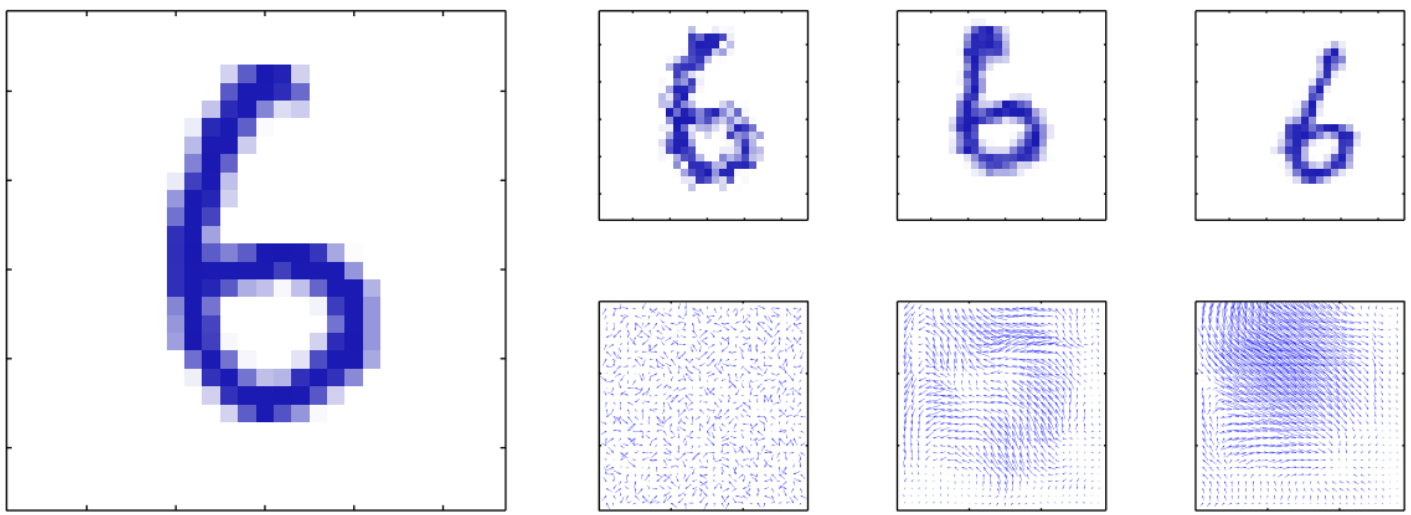


# Invariances

- 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 $\xi$.
- 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:

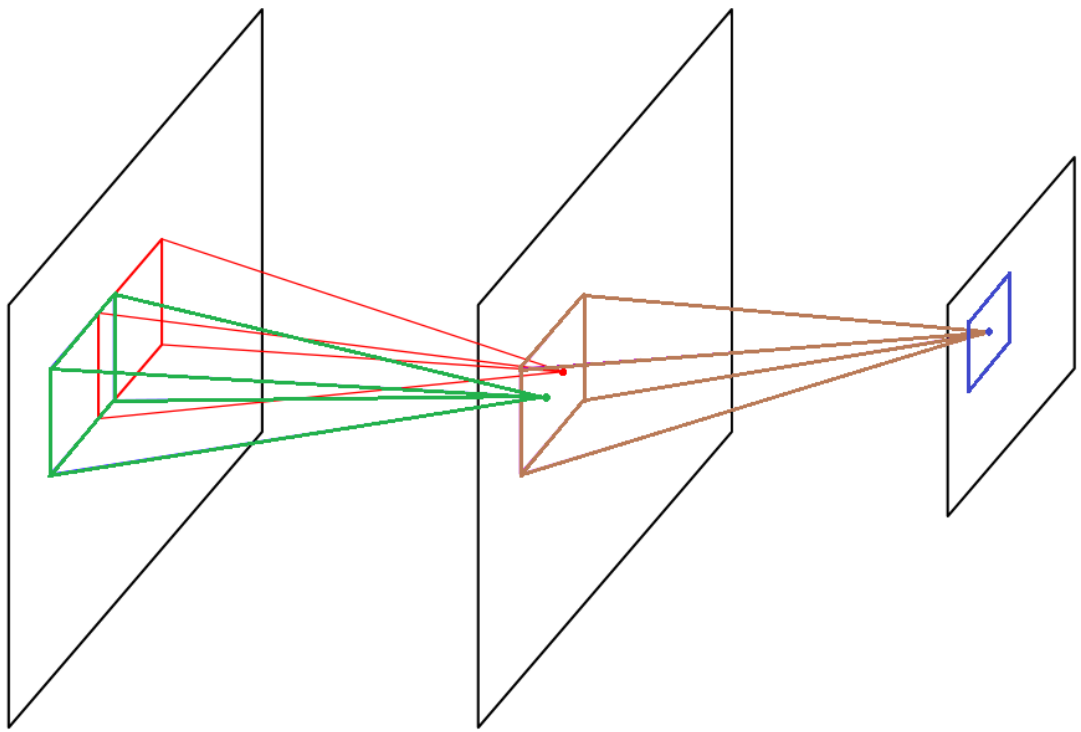
$$\left.\frac{\partial y_k}{\partial \xi}\right|_{\xi=0} = \sum_{i=1}^{D} \frac{\partial y_k}{\partial x_i}\frac{\partial x_i}{\partial \xi} = \sum_{i=1}^{D} J_{ki}\tau_i$$

- 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

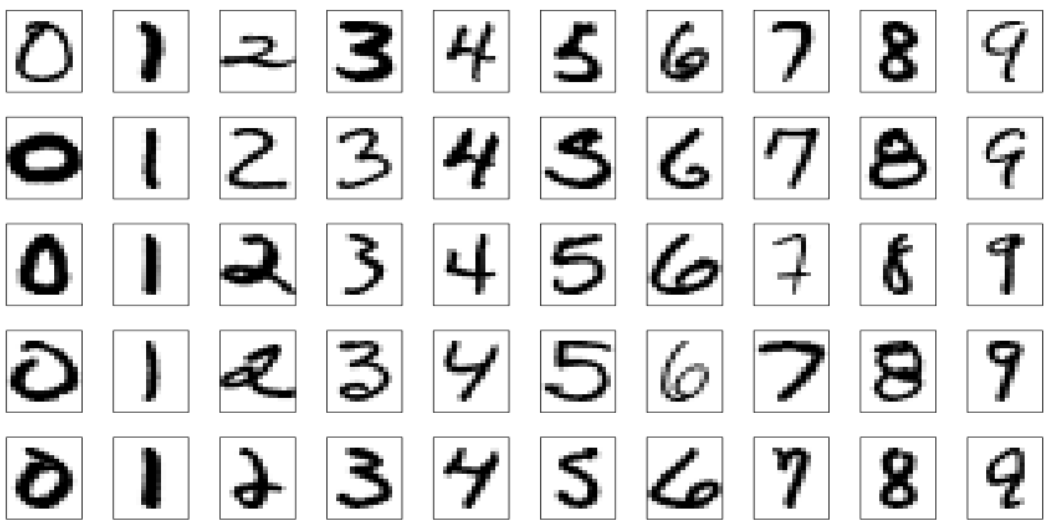
# Convolutional neural networks

- 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

# Table of Contents

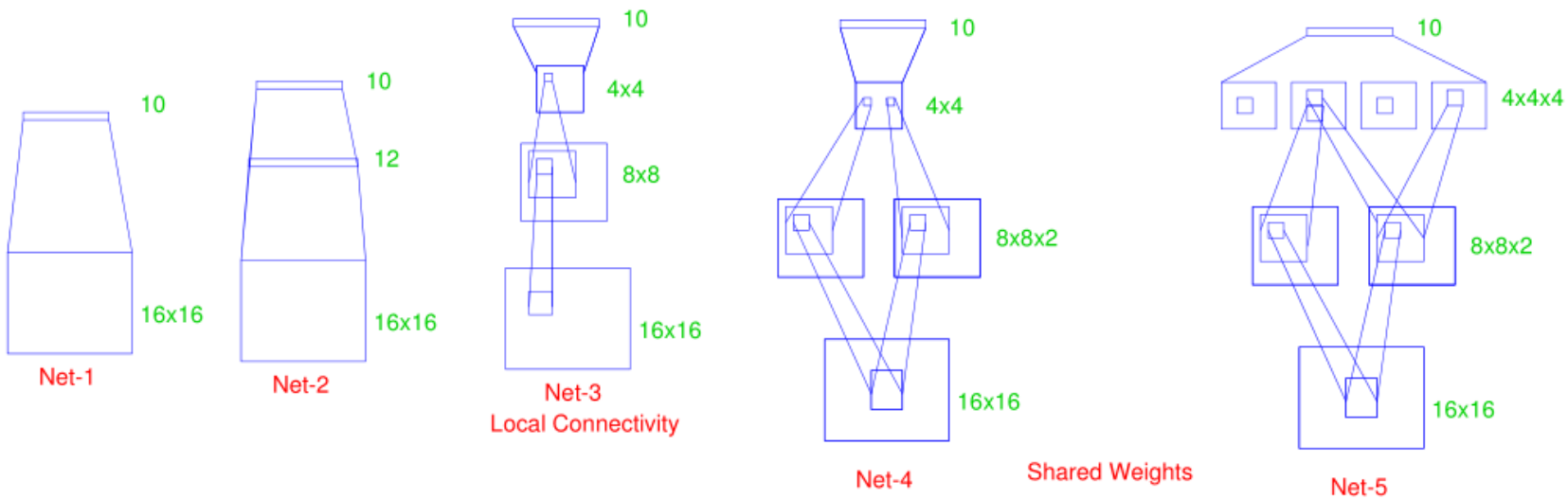
# Case study (due to Hastie et al. The Elements of Statistical Learning)

ZIP code recognition task

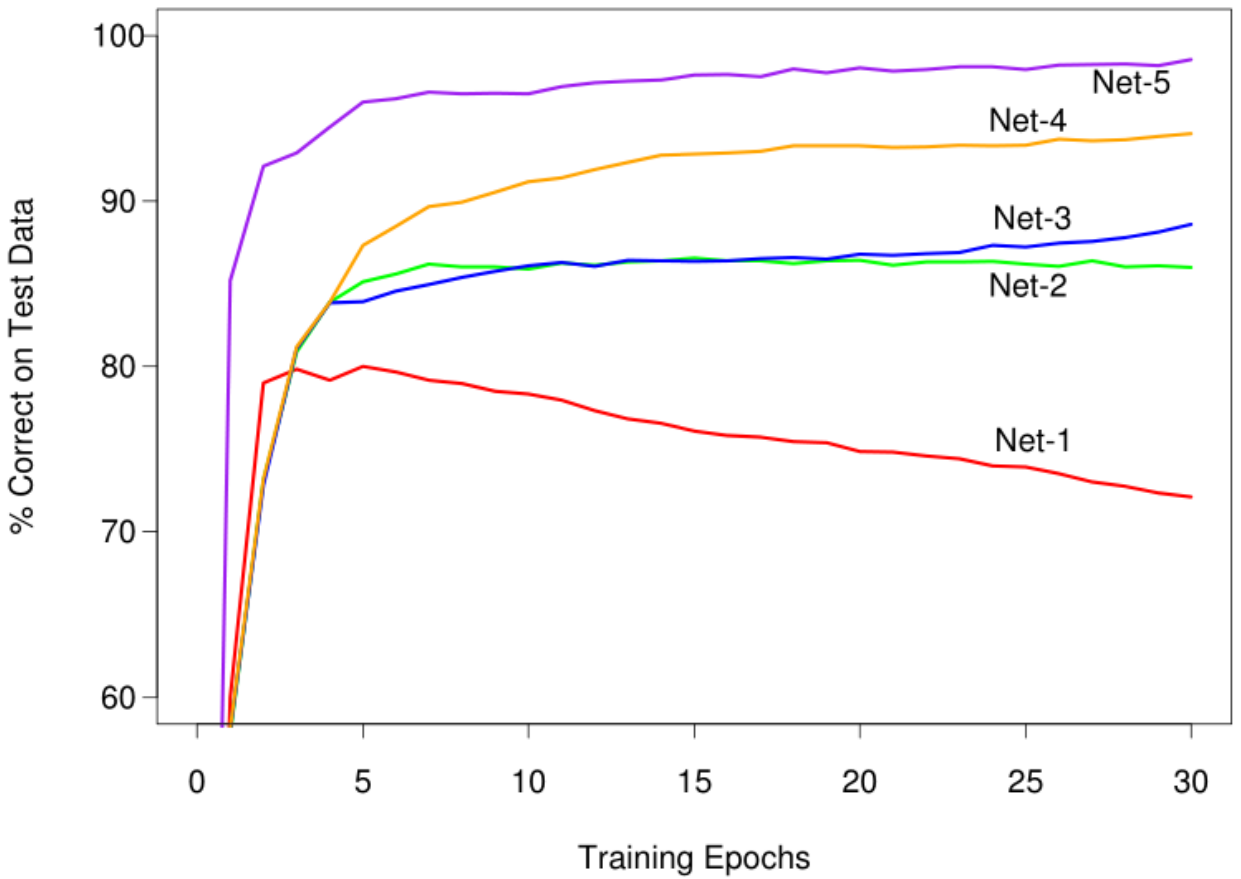


# Neural network structures

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

- Neural networks weights may be constrained to belong to mixture density
  - $\tilde{E} \leftarrow E - P(w)$, 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