# Neural networks

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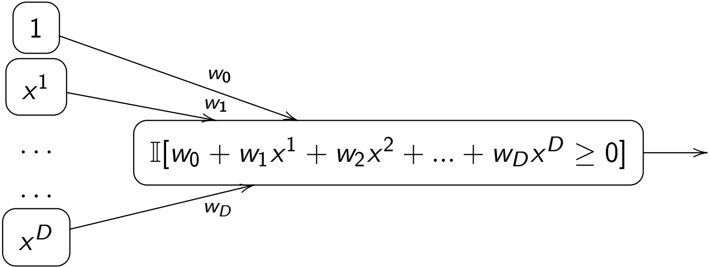
# History

- 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.

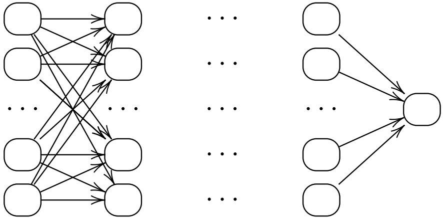
# Simple model of a neuron




- Neuron get's activated in the half-space, defined by $w_0 + w_1x^1 + w_2x^2 + ... + w_Dx^D \geq 0$.
- Each node is called a neuron
- Each edge is associated a weight
- Constant feature 1 stands for bias

# Multilayer perceptron architecture[1]

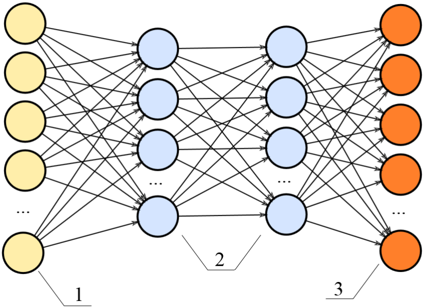
- Hierarchically nested set of neurons.
- Each node has its own weights.




This is structure of multilayer perceptron - acyclic directed graph.

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

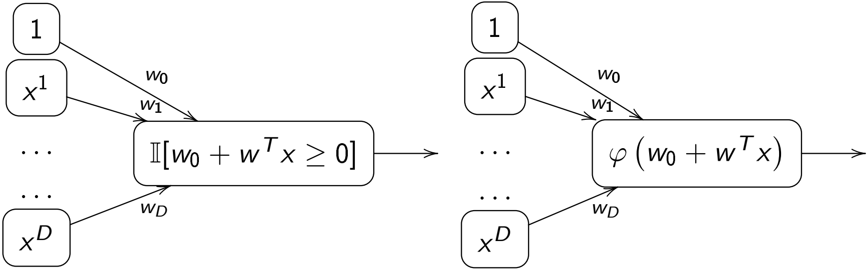
# Layers




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

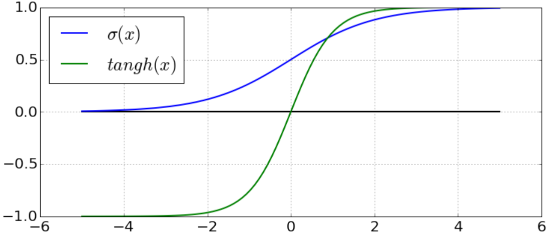
# Continious activations

- 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

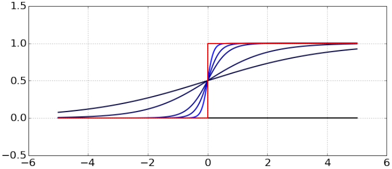
- sigmoidal: $\sigma(x) = \frac{1}{1+e^{-x}}$
  - 1-layer neural network with sigmoidal activation is equivalent to logistic regression
- hyperbolic tangent: $\text{tangh}(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$



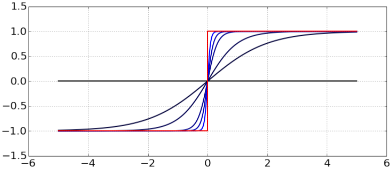

- ReLu: $\varphi(x) = [x]_{+}$.

# 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 $j$: $I_j = \sum_{k \in inc(j)} w_{kj} O_k + w_{0j}$,
    - $w_{0j}$ 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

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

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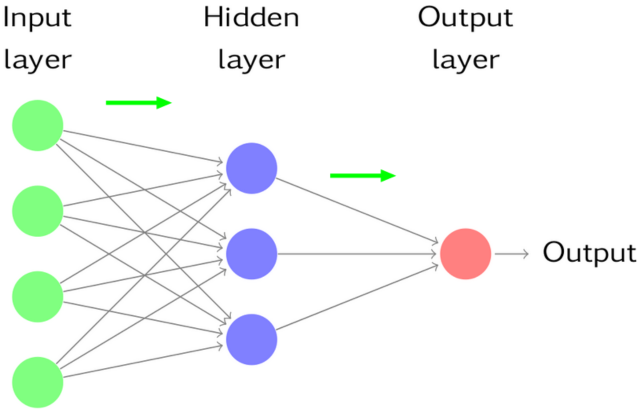
# Output generation

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



# Activations at output layer

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

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

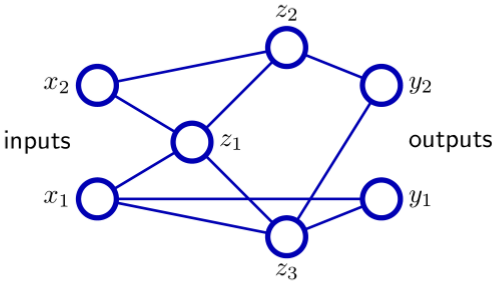
  - multiclass: $y \in 1, 2, ...C$

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

where $O_1, ...O_C$ are outputs of output layer.

## Generalizations

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

# 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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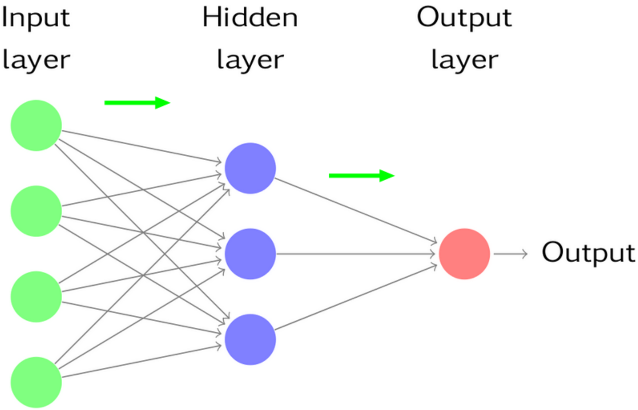
# Weight space symmetries

- 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

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

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

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

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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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- 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:

$k = 0$
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)
- Denote $W$ - total number of edges (and weights) in the neural net.

# Gradient calculation

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

$$\frac{\partial E}{\partial w_i} = \frac{E(w+\varepsilon_i) - E(w)}{\varepsilon} + O(\varepsilon) \tag{1}$$

or better

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

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.

# 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 $\varphi$ 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:

$$\delta_j = \frac{\partial E}{\partial O_j}\frac{\partial O_j}{\partial I_j} = \frac{\partial E}{\partial O_j}\varphi'(I_j) \tag{3}$$

- 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 sigmoid $\varphi(I) = \sigma(I)$:
  $$\varphi'(I_j) = \sigma(I_j)\left(1 - \sigma(I_j)\right) = O_j(1 - O_j)$$
  - 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 of neuron $j$ as their input.
- 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:

$$\delta_j = \frac{\partial E}{\partial I_j} = \frac{\partial E}{\partial O_j} \frac{\partial O_j}{\partial I_j} = \sum_{k \in out(j)} (\delta_k w_{jk}) \varphi'(I_j) \tag{4}$$

- Weight derivatives are calculated using errors and outputs:

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial I_j} \frac{\partial I_j}{\partial w_{ij}} = \delta_j O_i \tag{5}$$

# 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 $\delta_i$ for all $i \in$output layer using (3).
  3. Backpropagate $\delta_i$ from final layer backwards layer by layer using (4).
  4. Using calculated deltas and outputs calculate $\frac{\partial E}{\partial w_{ij}}$ with (5).

# Backpropagation

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  1. Forward propagate $x_n$ to the neural network, store all inputs $I_i$ and outputs $O_i$ for each neuron.
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  3. Backpropagate $\delta_i$ from final layer backwards layer by layer using (4).
  4. Using calculated deltas and outputs calculate $\frac{\partial E}{\partial w_{ij}}$ with (5).
- Let be $W$ is total number of edges.
- Calculating complexity: $O(W)$
- Memory complexity: $O(W)$
  - need to store inputs and outputs for each node

# Backpropagation - optimization

- Optimization updates:
  - batch (only for small $N$)
  - stochastic
    - using minibatches of objects
    - minibatches - iterative traversal of shuffled training set
    - minibatch size $\propto$ parallelization of CPU

# Backpropagation - comments

- Backpropagation correctness is checked by comparing results with (1), (2).
- Allows to finetune neurons on previous layers
    - all network is optimized
    - in contrast:
        - boosting keeps previous trees fixed
        - stacking keeps base learners fixed.

# 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

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

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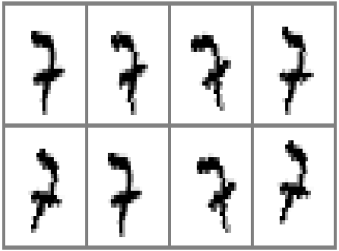
# Invariances

- 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

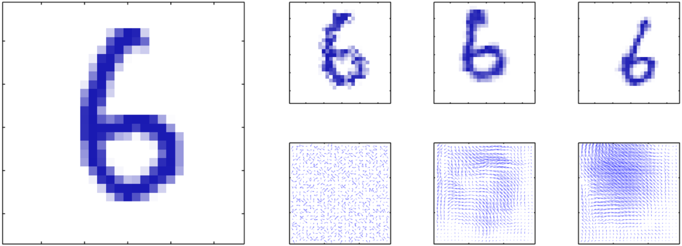


# Invariances

- 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 $\xi$.
- 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:

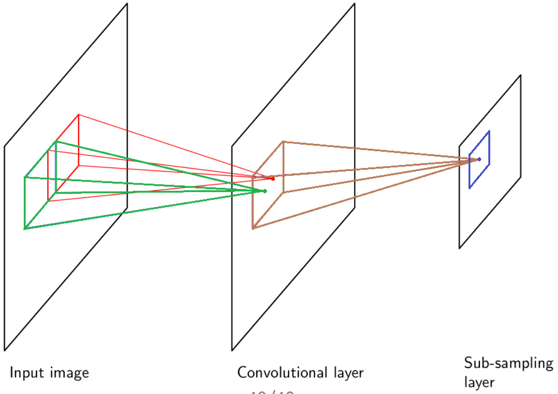
$$\left.\frac{\partial y_k}{\partial \xi}\right|_{\xi=0} = \sum_{i=1}^{D} \frac{\partial y_k}{\partial x_i}\frac{\partial x_i}{\partial \xi} = \sum_{i=1}^{D} J_{ki}\tau_i$$

- 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

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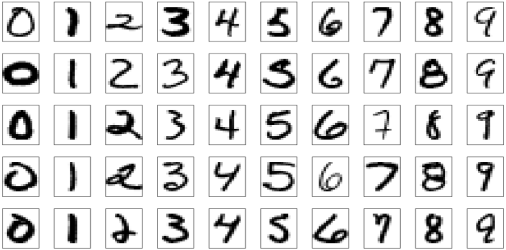
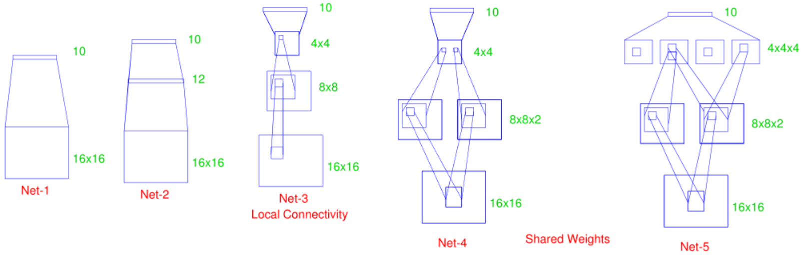
# Case study (due to Hastie et al. The Elements of Statistical Learning)

ZIP code recognition task

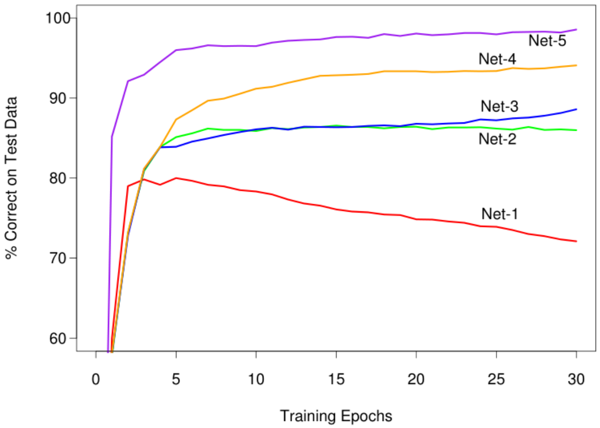


# Neural network structures

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


% Correct on Test Data
Training Epochs
100
90
80
70
60
0
5
10
15
20
25
30
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