Neural Networks

Statistical Learning

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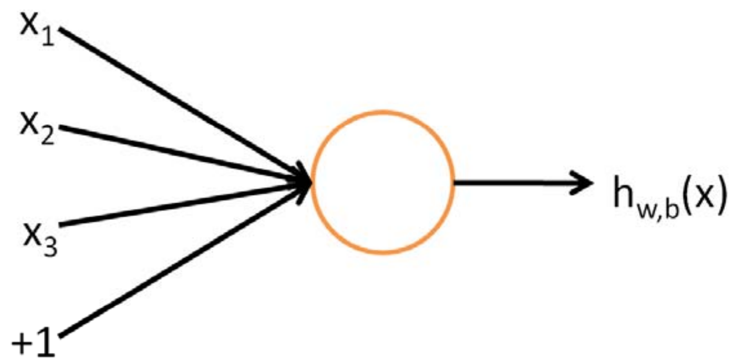
Introduction

- Basic idea:
  - Extract linear combinations of the inputs as derived features
  - Model the target as a nonlinear function of these features
- An example of a single neuron:



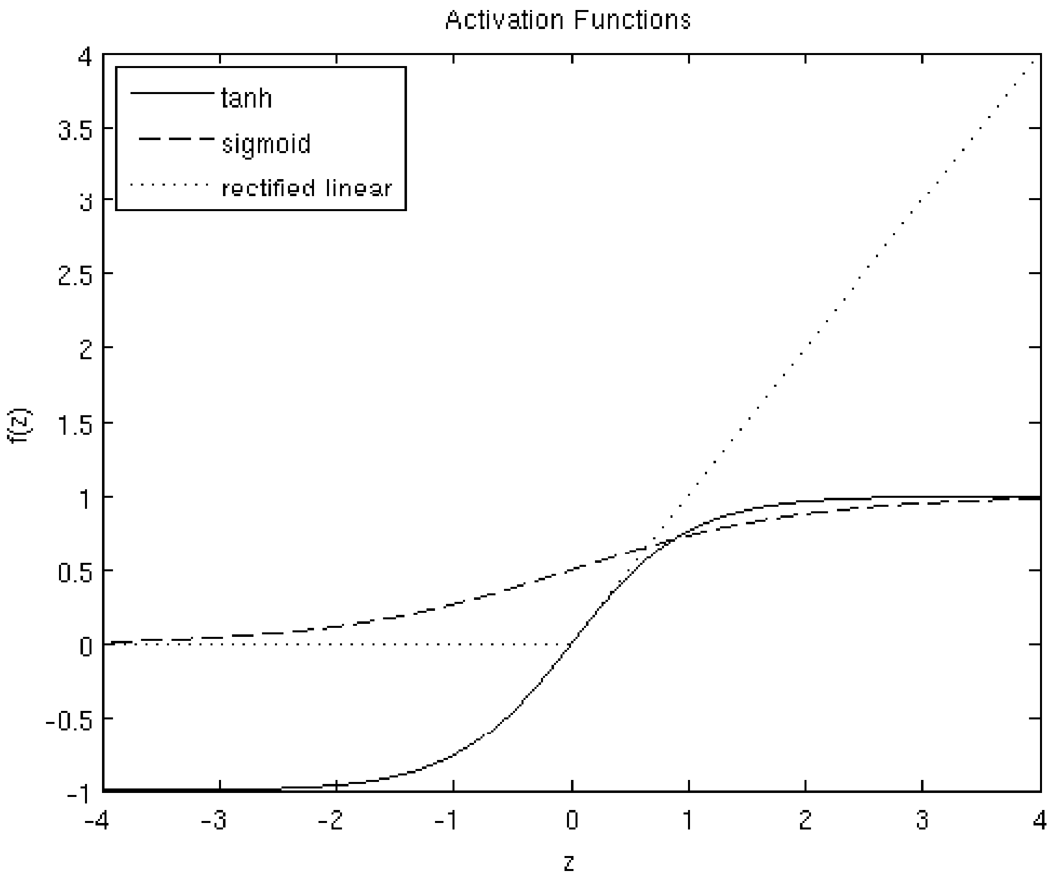
- $h_{W,b}(x) = f(W^T x) = f(\sum_{i=1}^{3} W_i x_i + b)$
  - *f* is the activation function
  - *b* is the bias term

Activation functions

- Sigmoid: [0, 1]

$$f(z) = \frac{1}{1+\exp(-z)}$$

  - Derivative:
    - $f'(z)=f(z)(1-f(z))$



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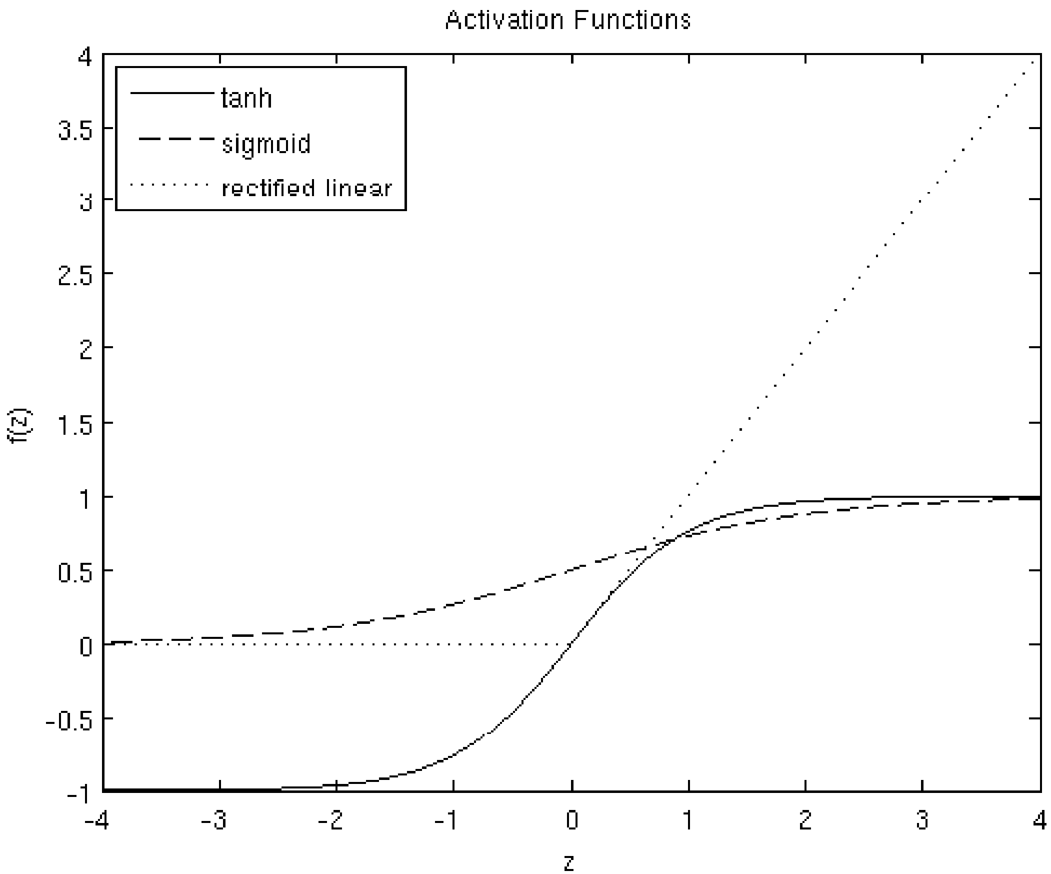
Activation functions (ii)

- Hyperbolic tangent: [-1, 1]

$$f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

  - Derivative:
    - $f'(z) = 1 - (f(z))^2$



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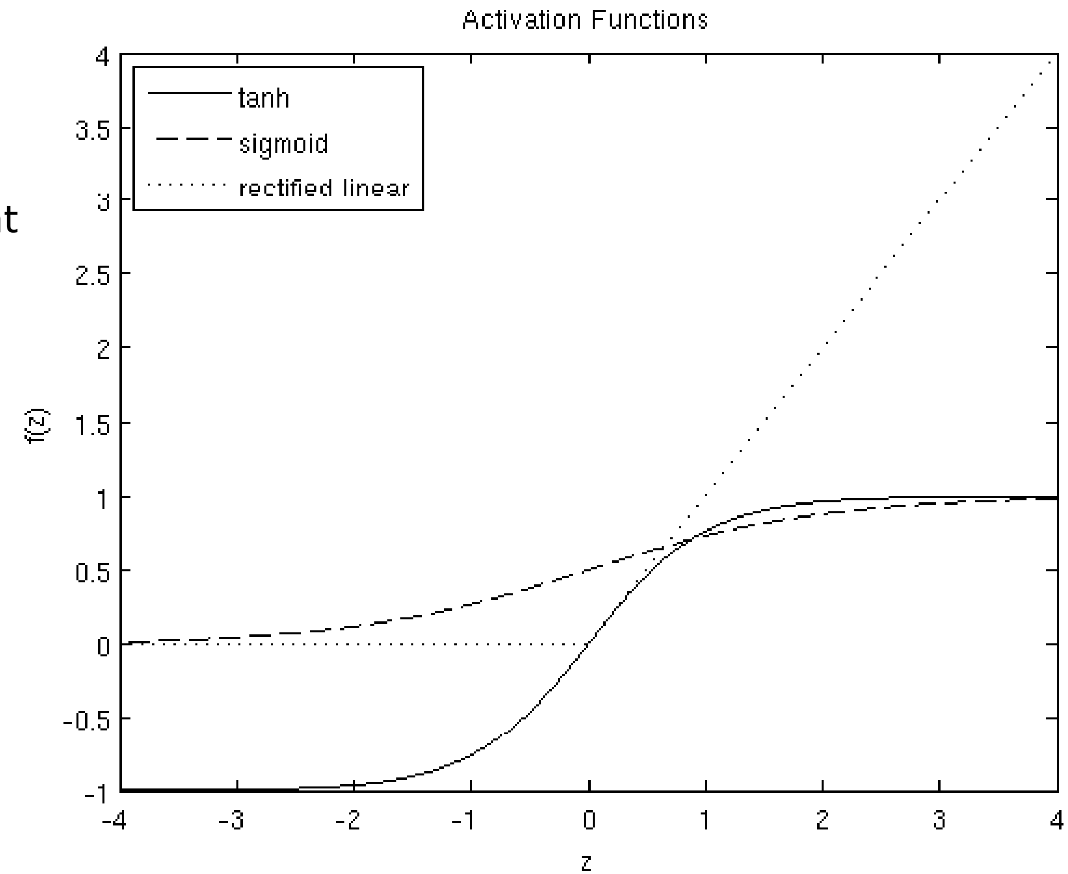
Activation functions (iii)

- Rectified linear unit (ReLU):

  $f(z) = \max(0, z)$

  - Derivative:
    - 0 if $z<0$, 1 otherwise
    - Undefined at $z=0$
      - Average the gradient over many training examples during optimization

- Gaussian radial basis functions
  - RBF networks
  - $f(z) = \exp(-(1/2)(z-c)^T\Sigma^{-1}(z-c))$



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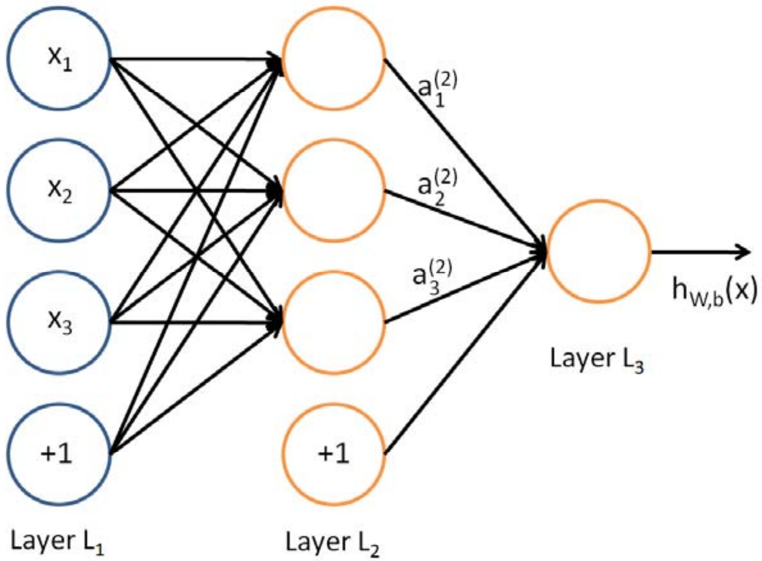
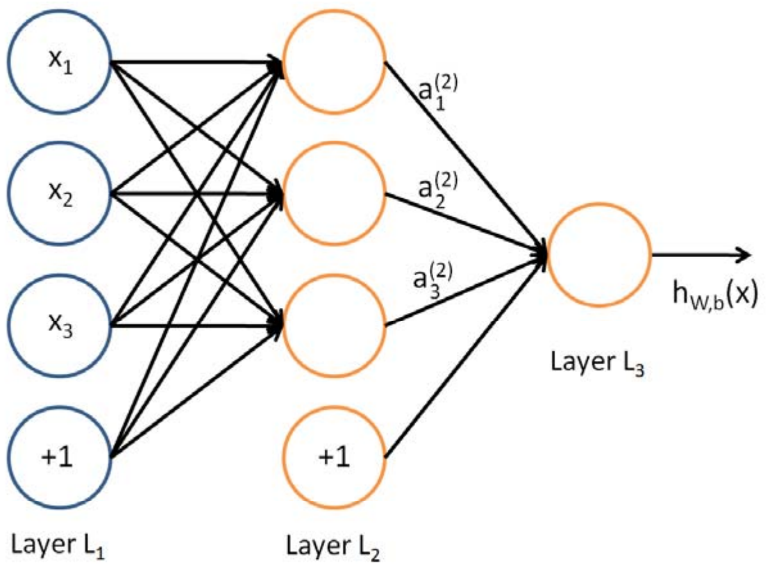
Neural Network Model

- A single hidden layer feed-forward neural network:



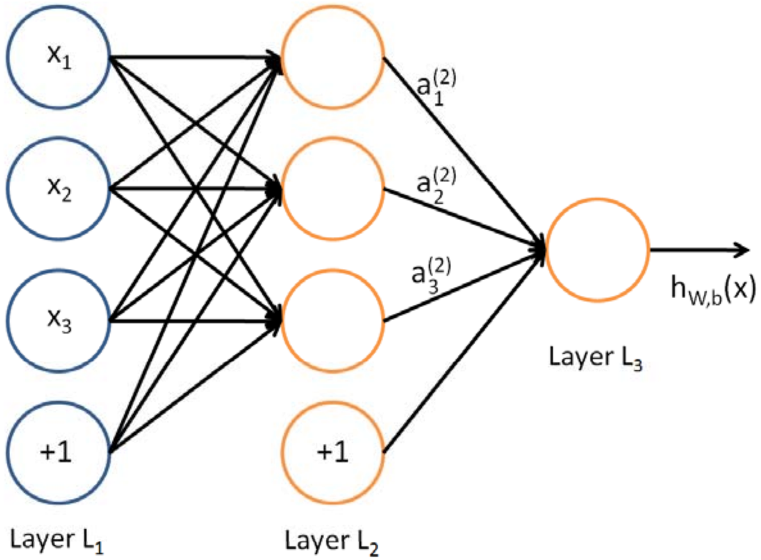
- Input layer, hidden layer, output layer
- Parameters: $(W,b)=(W^{(1)},b^{(1)},W^{(2)},b^{(2)})$
  - $W_{ij}^{(l)}$: weight associated with the connection between unit j in layer l and unit i in layer l+1
    - $W^{(1)} \in R^{3\times3}$, and $W^{(2)} \in R^{1\times3}$
  - $b_i^{(l)}$ is the bias associated with unit i in layer l+1
    - Bias units do not have inputs or connections going into them

Neural Network Model (ii)



- $a_i^{(l)}$: activation (output value) of unit *i* in layer *l*
  - $a_i^{(1)} = x_i$
- s_l: number of nodes in layer *l* (not counting the bias unit)

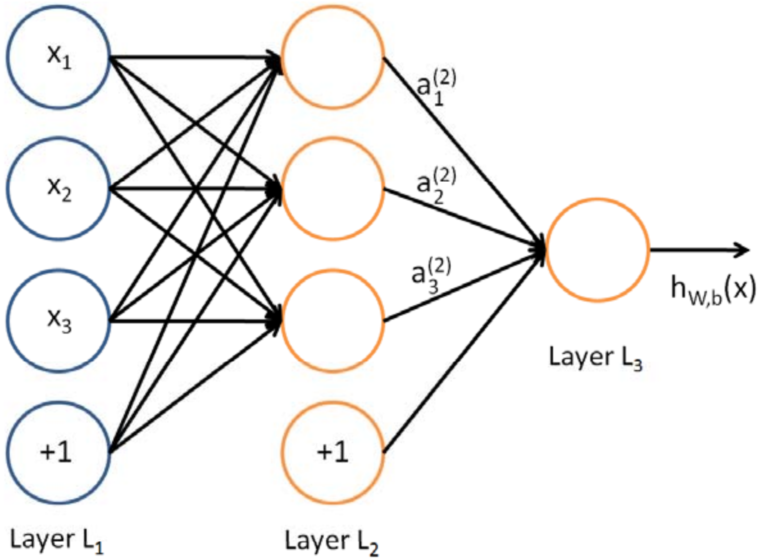
Neural Network Model (iii)



- Computation:

$$
\begin{aligned}
a_1^{(2)} &= f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)}) \\
a_2^{(2)} &= f(W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + b_2^{(1)}) \\
a_3^{(2)} &= f(W_{31}^{(1)}x_1 + W_{32}^{(1)}x_2 + W_{33}^{(1)}x_3 + b_3^{(1)}) \\
h_{W,b}(x) = a_1^{(3)} &= f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_1^{(2)})
\end{aligned}
$$

Neural Network Model (iv)

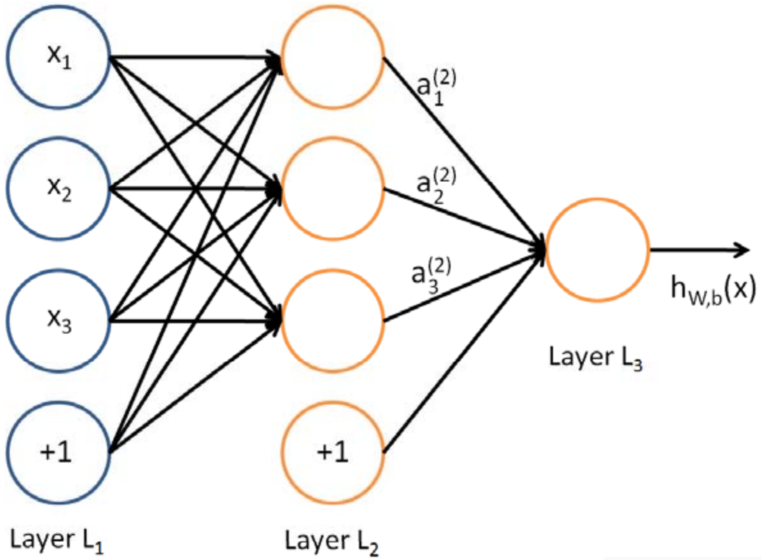


- If $z_i^{(l+1)}$ is the total weighted sum of inputs to unit i in layer l+1:

$$z_i^{(l+1)} = \sum_{j=1}^{s_l} W_{ij}^{(l)} a_j^{(l)} + b_i^{(l)}$$

- $a_i^{(l)}=f(z_i^{(l)})$

Neural Network Model (v)



- Computation: forward propagation

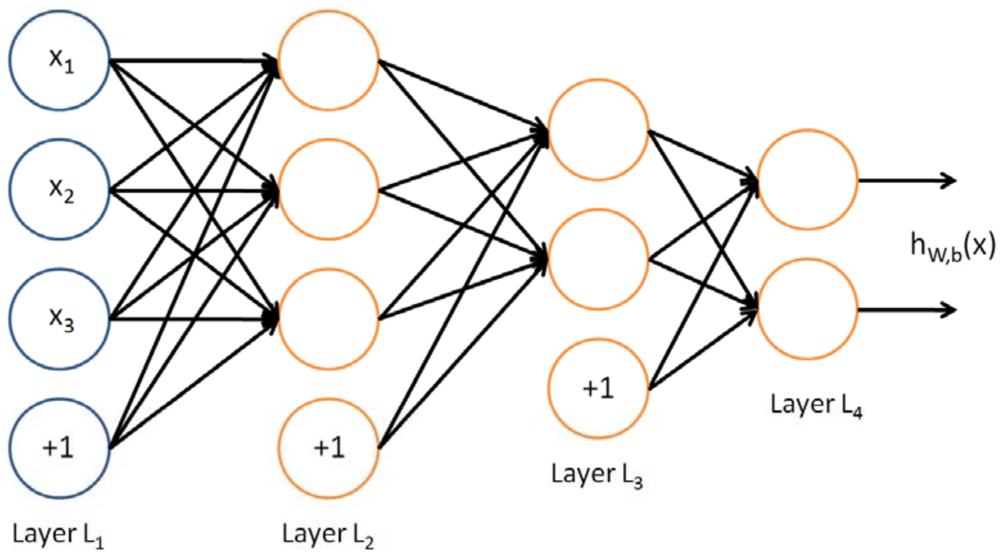
$$
\begin{aligned}
z^{(2)} &= W^{(1)}x + b^{(1)} \\
a^{(2)} &= f(z^{(2)}) \\
z^{(3)} &= W^{(2)}a^{(2)} + b^{(2)} \\
h_{W,b}(x) &= a^{(3)} = f(z^{(3)})
\end{aligned}
$$

- In general (matrix-vector operations):

$$
\begin{aligned}
z^{(l+1)} &= W^{(l)}a^{(l)} + b^{(l)} \\
a^{(l+1)} &= f(z^{(l+1)})
\end{aligned}
$$

Architectures

- Patterns of connectivity between neurons
  - Multiple hidden layers
  - Fully (densely) vs. locally connected
  - Weight sharing (locally connected)
  - feed-forward (no loops)
- Most common choice: multilayer feed-forward neural network (multilayer perceptron network)
  - Forward propagation step to calculate outputs of each layer



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Architectures (ii)

- Regression:
  - Typically, one output unit, except when there are several outputs
  - The output function is typically the identity function
- Classification:
  - For K-class classification, K units in the output layer

E.g. $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

pedestrian car motorcycle truck

  - Output function: *softmax*

$$f(z_i^{(l)}) = \frac{e^{z_i^{(l)}}}{\sum_{j=1}^{K} e^{z_j^{(l)}}}$$

Architectures (iii)

- An example of the output of *softmax*
  - Three categories (K=3): bike, car, truck

$$f(z_i^{(l)}) = \frac{e^{z_i^{(l)}}}{\sum_{j=1}^{K} e^{z_j^{(l)}}}$$

	z_i	$\exp(z_i)$	$f(z_i)$	Correct probs.
Bike	-0.2	0.8	0.02 (2%)	0.00
Car	**3.6**	**36.6**	**0.75 (75%)**	**1.00**
Truck	2.4	11.0	0.23 (23%)	0.00

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Fitting Neural Networks

- Backpropagation algorithm
  - Training examples: $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$
  - For a single example:
    - Regression and classification:

$$J(W, b; x, y) = \frac{1}{2} \left\| h_{W,b}(x) - y \right\|^2$$

    - For classification (mutually exclusive classes), cross-entropy is also valid:

$$J(W, b, x, y) = -\sum_{k=1}^{K} y_k \log\left(h_{W,b}(x)\right)_k$$

- For classification:
  - Sigmoid, *softmax*: y=0, 1; output in [0, 1]
  - tanh: y=-1, 1; output in [-1, 1]
- For regression: scale the outputs (range depends on the activation function)

Fitting Neural Networks (ii)

- Overall cost function:

$$J(W,b) = \left[\frac{1}{m}\sum_{i=1}^{m} J(W,b;x^{(i)},y^{(i)})\right] + \frac{\lambda}{2}\sum_{l=1}^{n_l-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}\left(W_{ji}^{(l)}\right)^2$$
$$= \left[\frac{1}{m}\sum_{i=1}^{m}\left(\frac{1}{2}\left\|h_{W,b}(x^{(i)}) - y^{(i)}\right\|^2\right)\right] + \frac{\lambda}{2}\sum_{l=1}^{n_l-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}\left(W_{ji}^{(l)}\right)^2$$

  - Regularization term (weight decay): prevent overfitting
    - Not applied to the bias terms
- Minimize *J* through backpropagation
  - *J* is non-convex: local minima
  - Gradient descent: usually works fairly well

Fitting Neural Networks (iii)

- One iteration of gradient descent updates *W*, *b*: Widrow-Hoff rule

$$W_{ij}^{(l)} = W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b)$$

$$b_i^{(l)} = b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W,b)$$

  - α: learning rate

- Compute the partial derivatives: backpropagation algorithm

$$\frac{\partial J(W,b)}{\partial W_{ij}^{(l)}} = \left[\frac{1}{m} \sum_{e=1}^{m} \frac{\partial J\left(W,b;x^{(e)},y^{(e)}\right)}{\partial W_{ij}^{(l)}} \right] + \lambda W_{ij}^{(l)}$$

$$\frac{\partial J(W,b)}{\partial b_i^{(l)}} = \frac{1}{m} \sum_{e=1}^{m} \frac{\partial J\left(W,b;x^{(e)},y^{(e)}\right)}{\partial b_i^{(l)}}$$

Backpropagation algorithm

1. Perform a feedforward pass, computing the activations for layers L_2, L_3, and so on up to the output layer L_{n_l}.

2. For each output unit i in layer n_l (the output layer), set

$$\delta_i^{(n_l)} = \frac{\partial}{\partial z_i^{(n_l)}} \frac{1}{2} \|y - h_{W,b}(x)\|^2 = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$

3. For $l = n_l - 1, n_l - 2, n_l - 3, \ldots, 2$

   For each node i in layer l, set

$$\delta_i^{(l)} = \left(\sum_{j=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)} \right) f'(z_i^{(l)})$$

Intuition:
$\delta_i^{(l)}$ = error of node *i* in layer *l*

4. Compute the desired partial derivatives, which are given as:

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b; x, y) = a_j^{(l)} \delta_i^{(l+1)}$$

$$\frac{\partial}{\partial b_i^{(l)}} J(W, b; x, y) = \delta_i^{(l+1)}.$$

How much error changes with modifications in $W_{ij}^{(l)}$:
[activation of node *j* in layer *l*] times [error of node *i* in layer *l+1*]

Backpropagation algorithm (ii)

- Matrix-vectorial notation

1. Perform a feedforward pass, computing the activations for layers L_2, L_3, up to the output layer L_{n_l}, using the equations defining the forward propagation steps

2. For the output layer (layer n_l), set

$$\delta^{(n_l)} = -(y - a^{(n_l)}) \bullet f'(z^{(n_l)})$$

3. For $l = n_l - 1, n_l - 2, n_l - 3, \ldots, 2$, set

$$\delta^{(l)} = \left((W^{(l)})^T \delta^{(l+1)}\right) \bullet f'(z^{(l)})$$

4. Compute the desired partial derivatives:

$$\nabla_{W^{(l)}} J(W,b;x,y) = \delta^{(l+1)} (a^{(l)})^T,$$
$$\nabla_{b^{(l)}} J(W,b;x,y) = \delta^{(l+1)}.$$

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Full gradient descent algorithm

1. Set $\Delta W^{(l)} := 0$, $\Delta b^{(l)} := 0$ (matrix/vector of zeros) for all l.

2. For $i = 1$ to m,

   1. Use backpropagation to compute $\nabla_{W^{(l)}} J(W, b; x, y)$ and $\nabla_{b^{(l)}} J(W, b; x, y)$.
   2. Set $\Delta W^{(l)} := \Delta W^{(l)} + \nabla_{W^{(l)}} J(W, b; x, y)$.
   3. Set $\Delta b^{(l)} := \Delta b^{(l)} + \nabla_{b^{(l)}} J(W, b; x, y)$.

3. Update the parameters:

$$W^{(l)} = W^{(l)} - \alpha \left[\left(\frac{1}{m} \Delta W^{(l)} \right) + \lambda W^{(l)} \right]$$

$$b^{(l)} = b^{(l)} - \alpha \left[\frac{1}{m} \Delta b^{(l)} \right]$$

Training Neural Networks

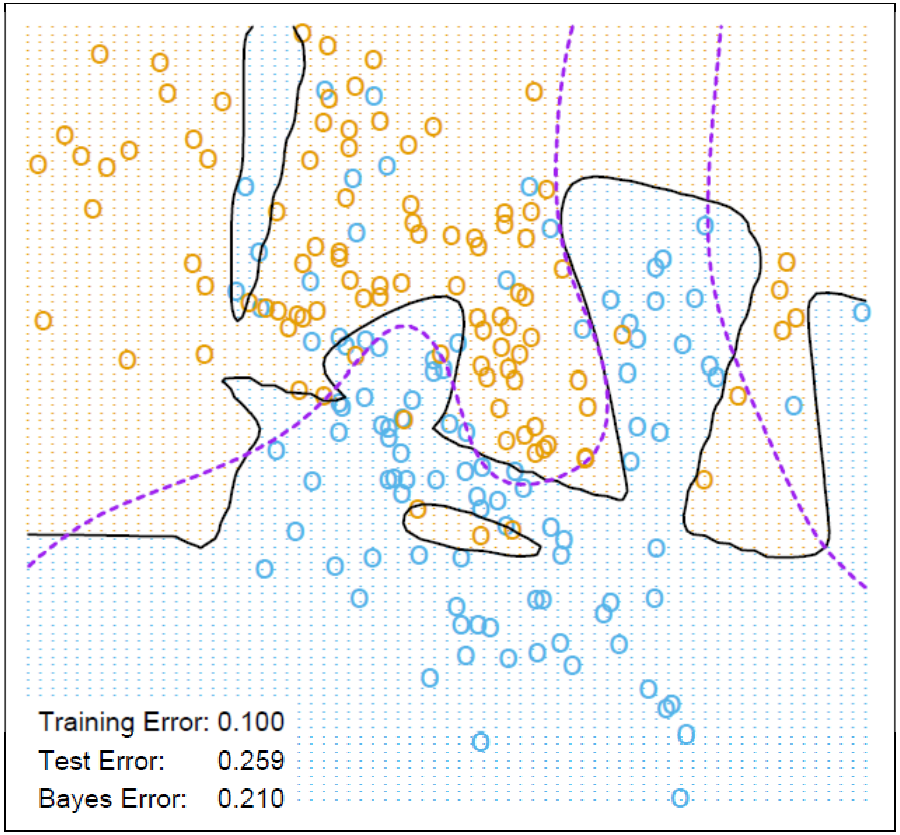
- Over-parametrized model, non-convex and unstable optimization problem

- Starting values:
  - Random values near 0 for W, biases to 0
    - With standardized inputs, random uniform weights in [-0.7, 0.7]
      - Ok for small networks
    - Xavier initialization: random() * sqrt(1/n)
      - random(): mean 0, variance 1
      - n: number of inputs
  - Model starts out nearly linear, and becomes nonlinear as weights increase
  - 0 weights give perfect symmetry, large weights lead poor solutions

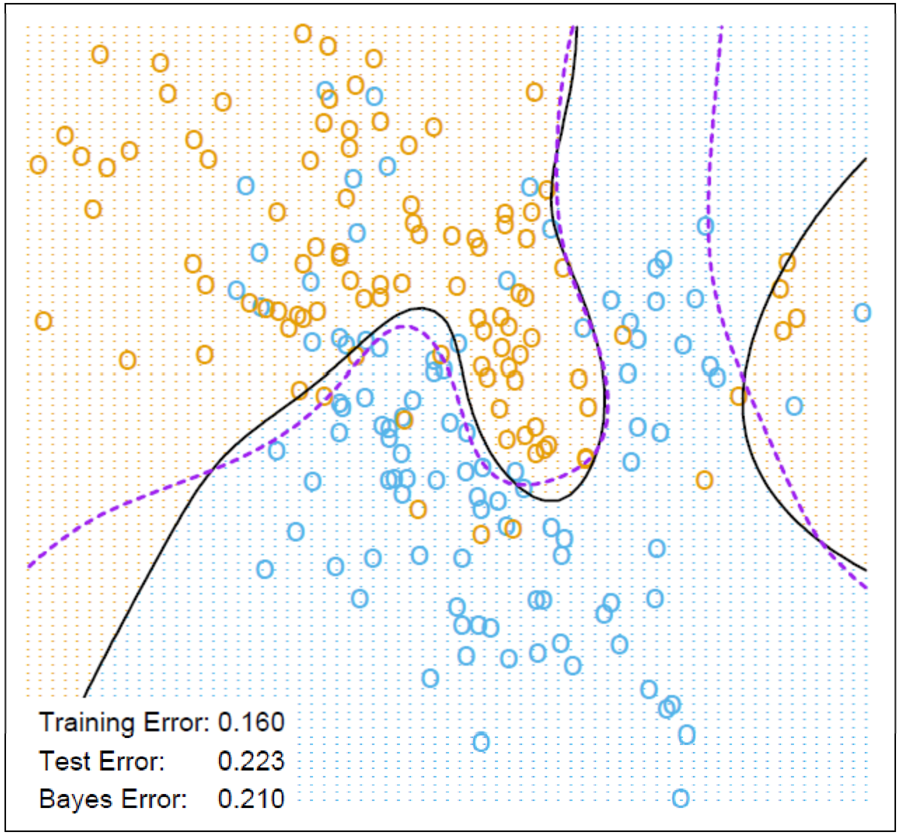
Training Neural Networks (ii)

- Overfitting: regularization term (weight decay)
  - Cross-validation to estimate the regularization parameter

Neural Network - 10 Units, No Weight Decay



Neural Network - 10 Units, Weight Decay=0.02



Training Neural Networks (iii)

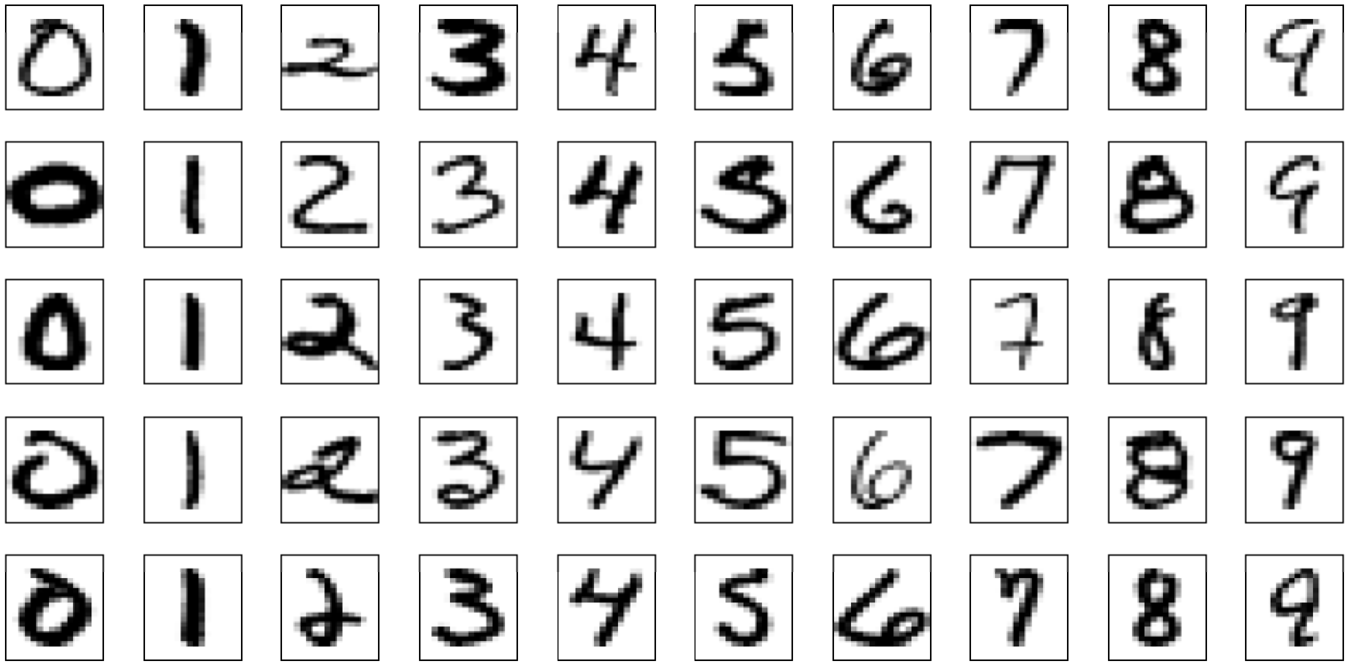
- Scaling of the inputs:
  - Can have a large effect in the quality of the final solution: scaling of the weights
  - Standardize inputs (and outputs) to have mean zero and standard deviation one:
    - Treat all inputs equally: regularization
    - Choose a meaningful range for the starting weights
- Number of hidden units:
  - Better to have too many hidden units than too few
    - Too few: not enough flexibility to capture nonlinearities
    - Too many: extra weights can be shrunk toward zero with regularization
  - Typical number of hidden units: 5 to 100 (per layer)
    - Number increasing with number of inputs and number of training cases
    - Same number in every layer (reasonable default)

Training Neural Networks (iv)

- Number of hidden layers:
  - background knowledge and experimentation
  - Allow the construction of hierarchical features at different levels of resolution
- Multiple minima: non-convex error function
  - Try a number of random starting configurations: choose the best solution
  - Better approach: average the predictions over a collection of networks
  - Another approach: bagging
- Batch learning: all the examples
  - Stochastic Gradient Descent (SGD): 1 example
- Advanced optimization methods:
  - Conjugate gradient
  - Quasi-Newton: Broyden–Fletcher–Goldfard–Shanno (BFGS) and L-BFGS

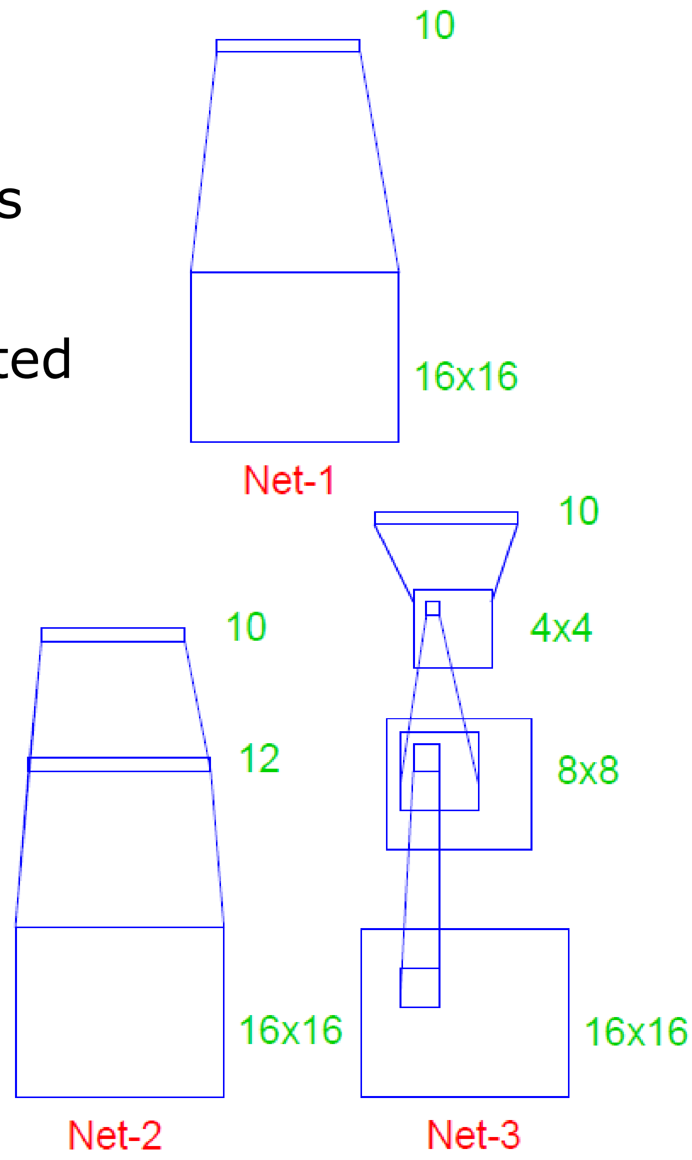
Example: ZIP Code Data

- Le Cun, 1989
- 16x16 grayscale images
- Training with 320 digits, test with 160
- Five different networks: sigmoidal output units, sum-of-squares error function



Example: ZIP Code Data (ii)

- Net-1: no hidden layer, equivalent to multinomial logistic regression
- Net-2: one hidden layer, 12 hidden units fully connected
- Net-3: two hidden layers locally connected
  - First hidden layer:
    - Inputs from a 3x3 patch
    - Units 1 unit apart are 2 pixels apart
  - Second hidden layer:
    - Inputs from a 5x5 patch
    - Units 1 unit apart are 2 pixels apart
  - Local connectivity:
    - Each unit extracts local features from the previous layer
    - Lower number of weights



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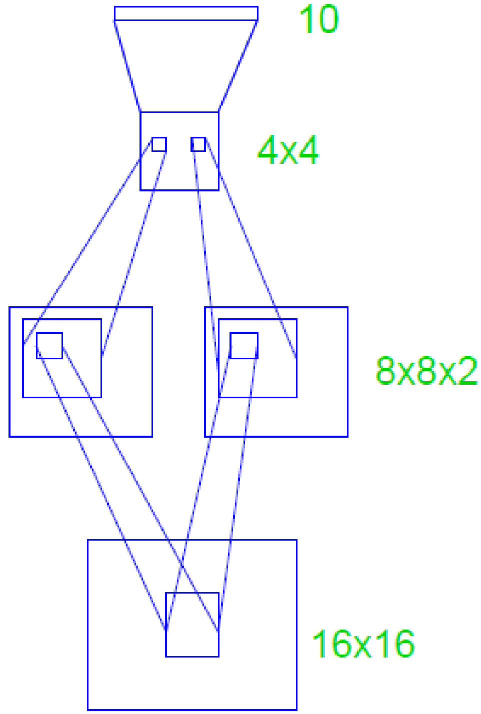
Example: ZIP Code Data (iii)

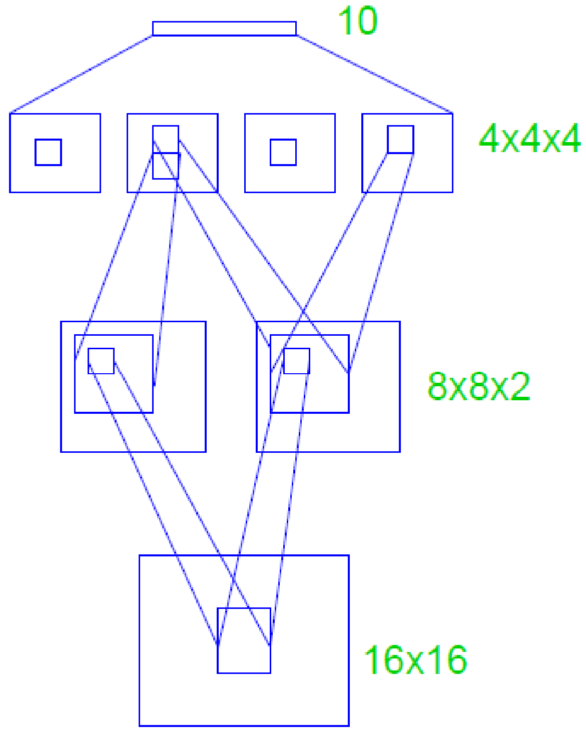
- Net-4: two hidden layers, locally connected, weight sharing
  - First hidden layer: two 8x8 feature maps
    - Input from 3x3 patch
    - Units in the same 8x8 feature map share the same set of 9 weights (bias not shared)
    - Extracted features in different parts of the image are computed with the same linear functional: **convolutional networks**
  - Second hidden layer: no weight sharing
- The gradient of the error for a shared weight is the sum of the gradients to each connection controlled by the weight



Net-4

Example: ZIP Code Data (iv)

- Net-5: two hidden layers, locally connected, two levels of weight sharing
  - First hidden layer: same as Net-4
  - Second hidden layer: four 4x4 feature maps
    - Input from a 5x5 patch
    - Weights shared in each of the feature maps



Net-5

- Features of handwritten style should appear in more than one part of a digit
- Subject matter knowledge should be used to improve performance

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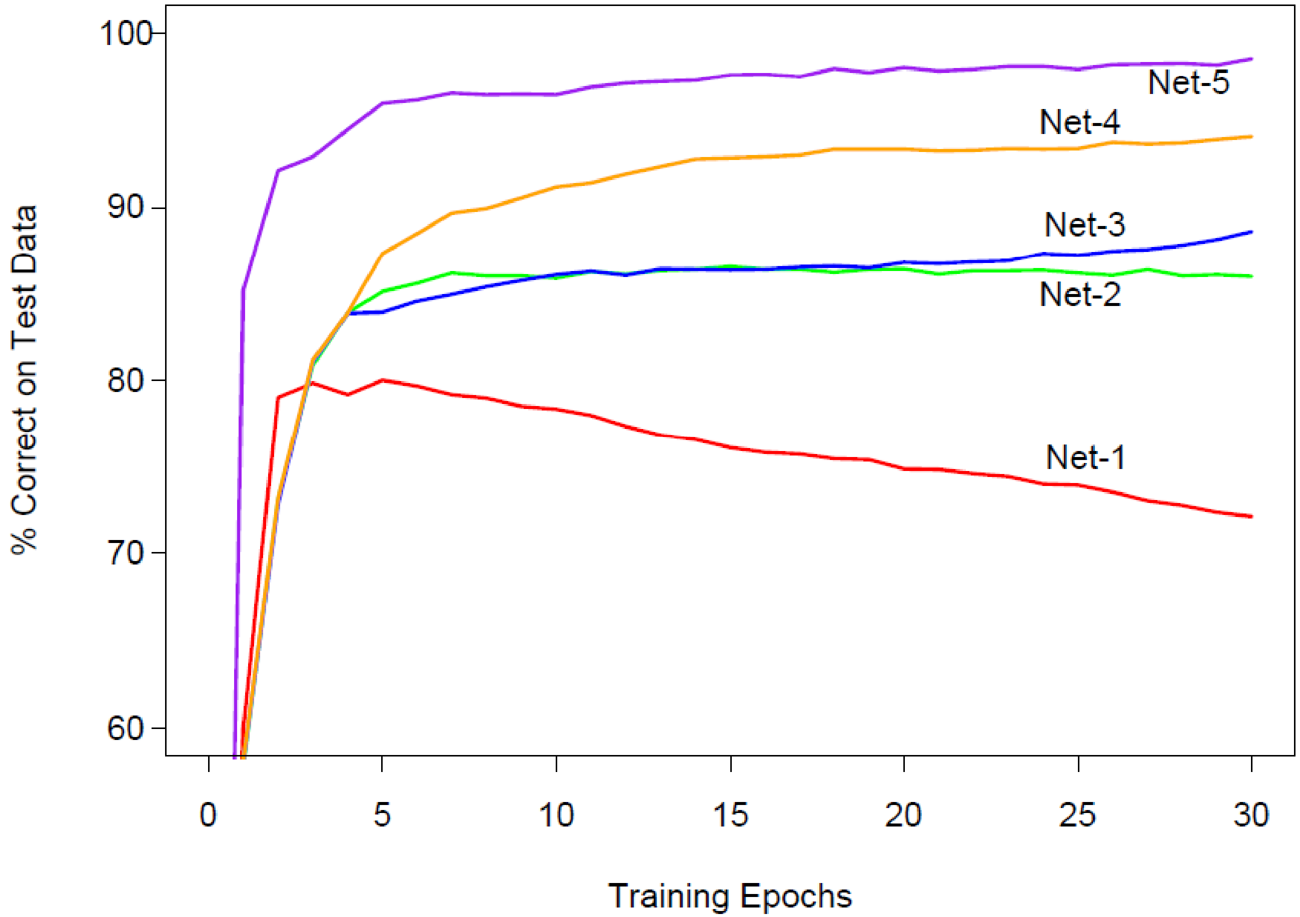
Example: ZIP Code Data (v)

- Training error was 0% in all the cases
  - More parameters than training observations



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Example: ZIP Code Data (vi)

	Network Architecture	Links	Weights	% Correct
Net-1:	Single layer network	2570	2570	80.0%
Net-2:	Two layer network	3214	3214	87.0%
Net-3:	Locally connected	1226	1226	88.5%
Net-4:	Constrained network 1	2266	1132	94.0%
Net-5:	Constrained network 2	5194	1060	98.4%

- Best results on a large database: Le Cun et al., 1998
  - 60,000 training and 10,000 test examples
  - LeNet-5: a more complex convolutional network
    - 99.2% correct
  - Boosted LeNet-4: boosting with a predecesor of LeNet-5
    - 99.3% correct

Bibliography

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