CAP 5610: Machine Learning

Lecture 8:
Neural Networks

Instructor: Dr. Gita Sukthankar
Email: gitars@eecs.ucf.edu

Reference Materials From: GuoJun Qi, Ray Mooney, Dean Pomerleau

Reading

Chap 3 and 4 in Marsland's ML: An Algorithmic Approach

Chap 5 in Bishop's PRML
Chap 6 in Goodfellow et al. Deep Learning

3Blue1Brown YouTube video
https://www.youtube.com/watch?v=aircAruvnKk

Recap: linear classifier

- Logistic regression
  - Maximizing the posterior distribution of class Y conditional on the input vector X

- Support vector machines
  - Maximizing the maximum margin, and
    - Hard margin: subject to the constraints that no training error shall be made
    - Soft margin: minimizing the slack variables that represent how much an associated training example violates the classification rule.
  - Extended to nonlinear classifier with kernel trick
    - Mapping input vectors to high dimensional space
    - Linear classifier in high dimensional space, nonlinear in original space.

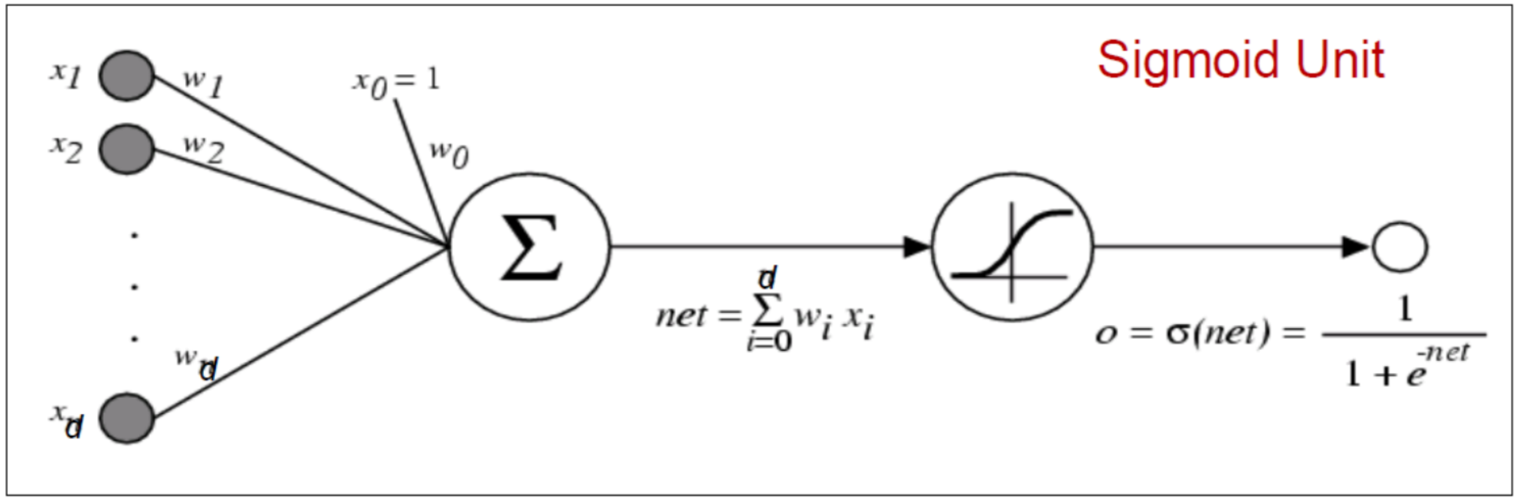
Building nonlinear classifier

- With a network of logistic units?
- A single logistic unit is linear classifier : *f*: X → Y

$$f(X) = \frac{1}{1 + \exp(-W_0 - \sum_{n=1}^{N} W_n X_n)}$$

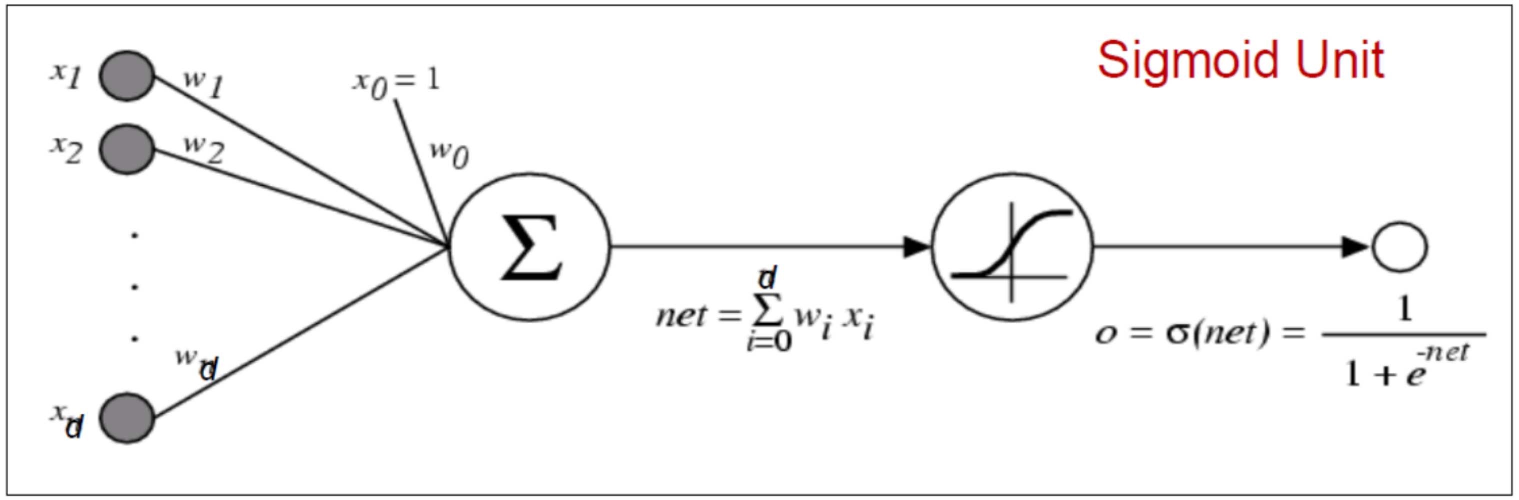
Graph representation of a logistic unit

- Input layer: An input X=(X_1, …, X_n)
- Output: logistic function of the input features


Sigmoid Unit
x_1
x_2
x_d
w_1
w_2
w_d
$x_0 = 1$
w_0
Σ
$net = \sum_{i=0}^{d} w_i x_i$
$o = \sigma(net) = \frac{1}{1 + e^{-net}}$

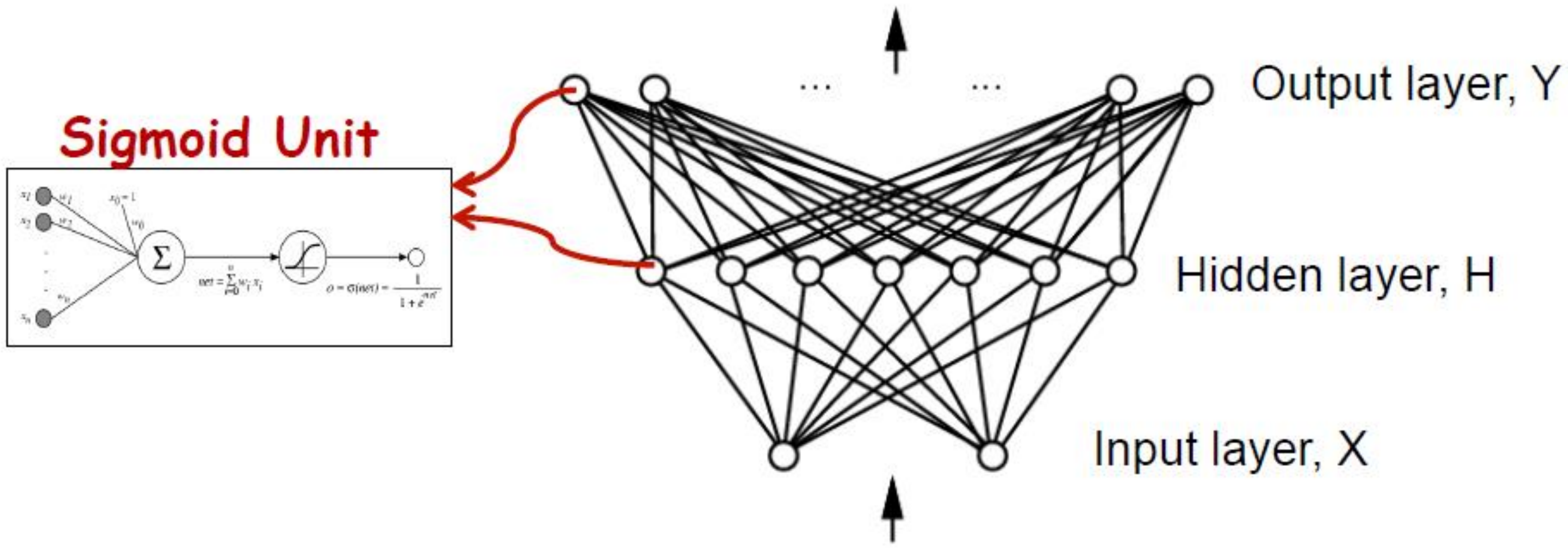
A logistic unit as an neuron:

- Input layer: An input X=(X_1, …, X_n)
- Activation: weighted sum of input features $a = W_0 + \sum_{n=1}^{N} W_n X_n$
- Activation function: logistic function *h* applied to the weighted sum
- Output: $\mathrm{z} = h(a)$


Sigmoid Unit
x_1
x_2
x_d
w_1
w_2
w_d
$x_0 = 1$
w_0
Σ
$net = \sum_{i=0}^{d} w_i x_i$
$o = \sigma(net) = \frac{1}{1 + e^{-net}}$

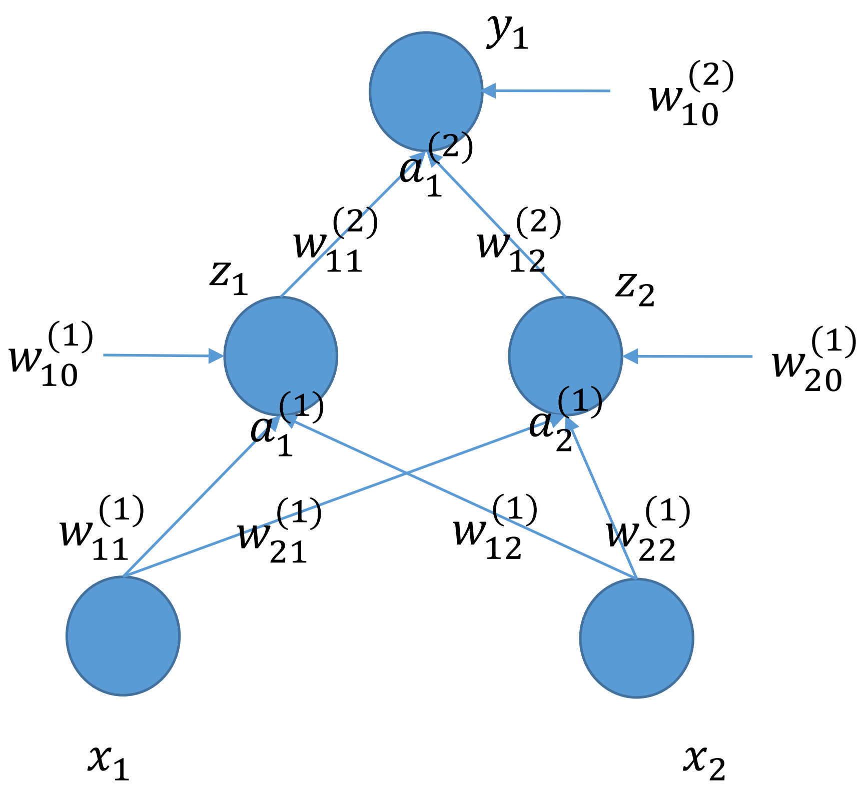
Neural Network: Multiple layers of neurons

- Output of a layer is the input into the upper layer



An example

- A three layer neural network



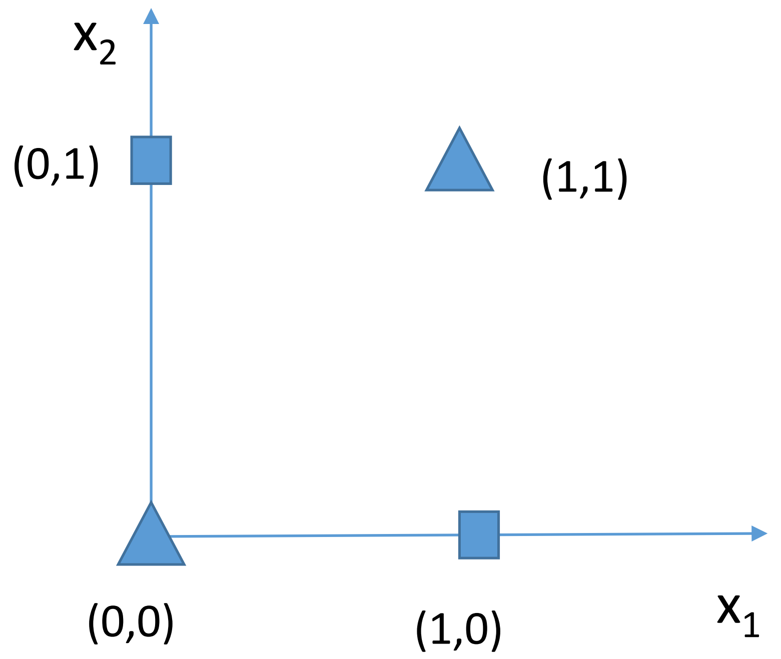
$$a_1^{(1)} = w_{11}^{(1)} x_1 + w_{12}^{(1)} x_2 + w_{10}^{(1)}$$
$$z_1 = h(a_1^{(1)})$$

$$a_2^{(1)} = w_{21}^{(1)} x_1 + w_{22}^{(1)} x_2 + w_{20}^{(1)}$$
$$z_2 = h(a_2^{(1)})$$

$$a_1^{(2)} = w_{11}^{(2)} z_1 + w_{12}^{(2)} x_2 + w_{10}^{(2)}$$
$$y_1 = f(a_1^{(2)})$$

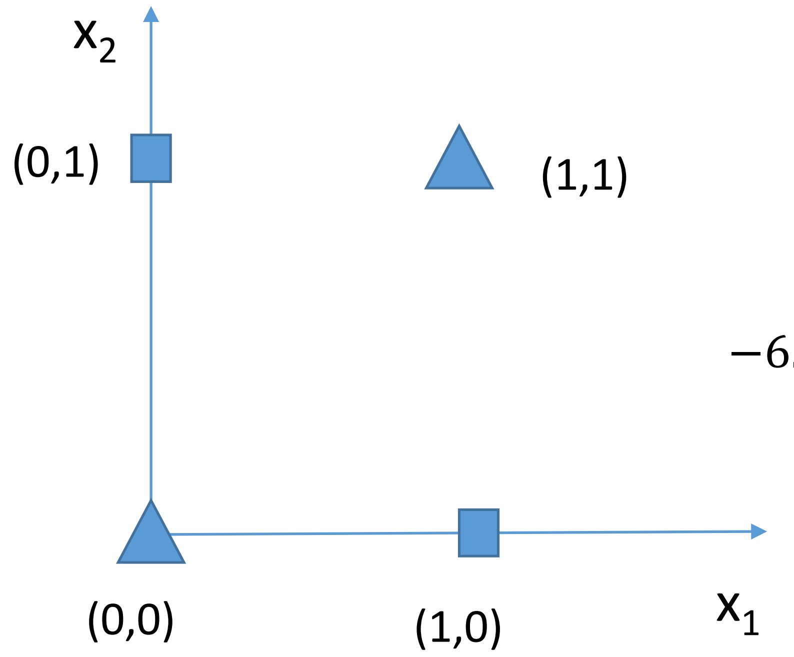
XOR Problem

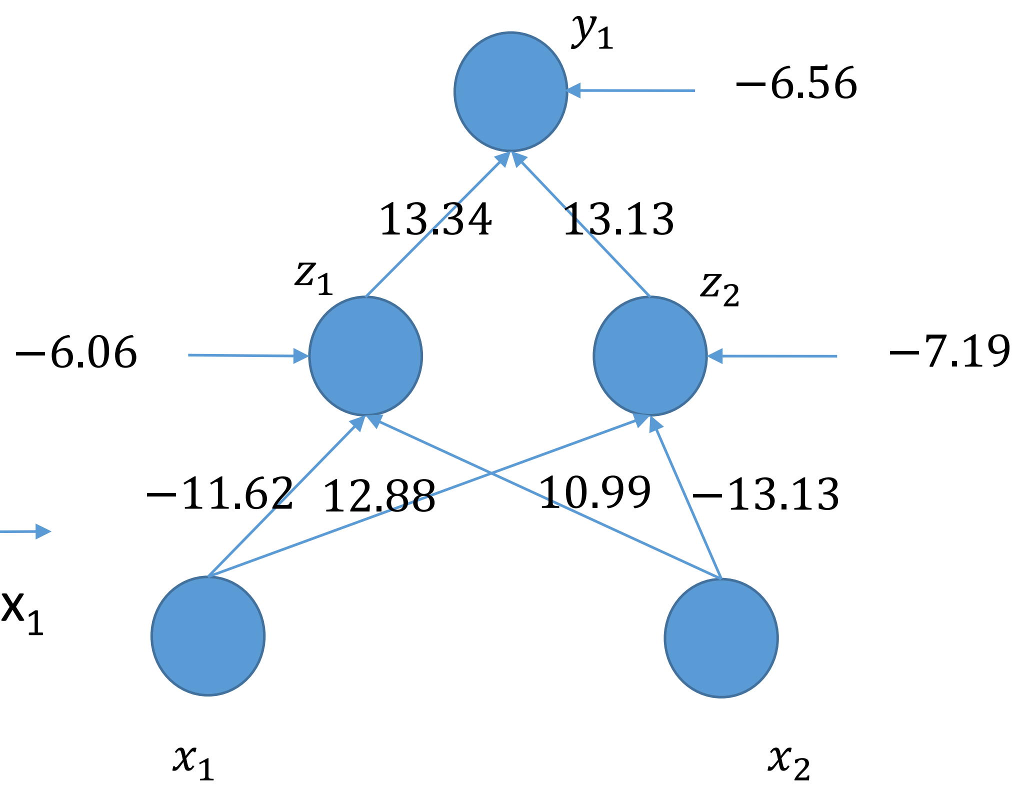
- It is impossible to linearly separate these two classes



XOR Problem

- Two classes become separable by putting a threshold 0.5 to the output y_1

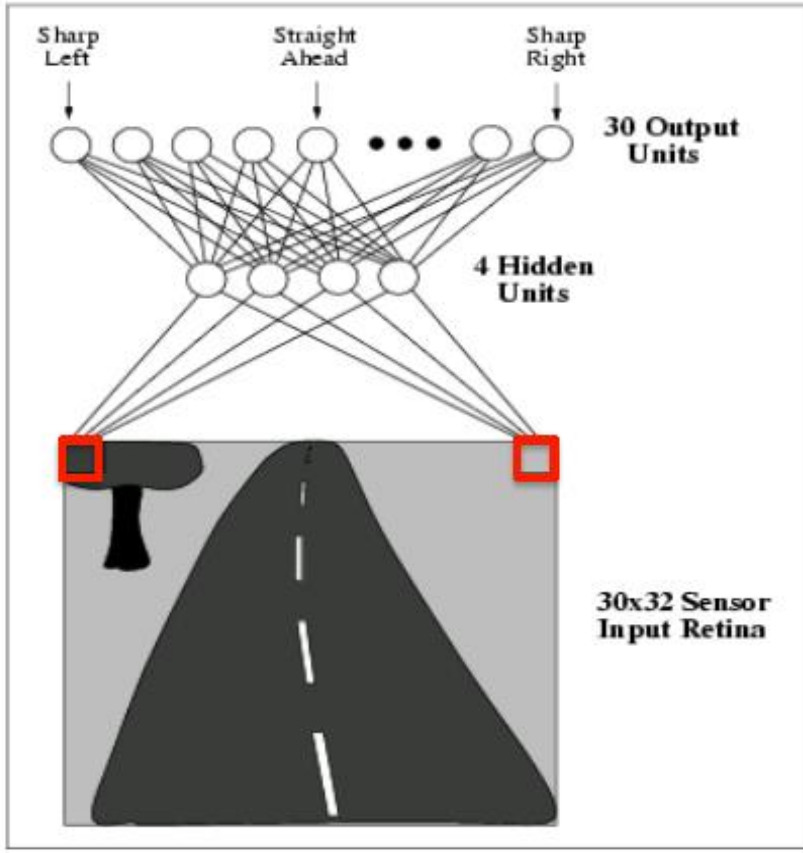




Input	Output
(0,0)	0.057
(1,0)	0.949
(0,1)	0.946
(1,1)	0.052

Application: Autonomous Driving

- Input: real-time videos captured by a camera
- Output: signals that steer a car
  - From the sharp left, straight to sharp right



ALVINN (Pomerleau, 1989),

Training Neural Network

- Given a training set of *M* examples $\{(x^{(i)},t^{(i)})|i=1,\ldots,M\}$
- Training neural network is equivalent to minimizing the least square error between the network output and the true value

$$\min_w L(w) = \frac{1}{2}\sum_{i=1}^{M}(y^{(i)} - t^{(i)})^2$$

Where $y^{(i)}$ is the output depending on the network parameters w.

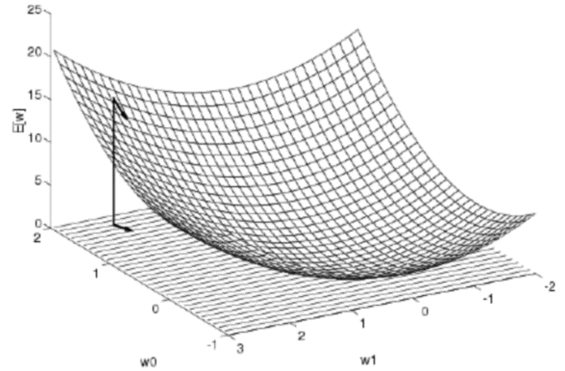
Recap: Gradient Ascent/Descent Method

- Gradient descent method is an iterative algorithm
  - Hill climbing method to find the peak point of a "mountain"
  - At each point, compute its gradient

$$\nabla L = \left[\frac{\partial L}{\partial w_0}, \frac{\partial L}{\partial w_1}, \ldots, \frac{\partial L}{\partial w_N} \right]$$

  - Gradient is a vector that points to the steepest direction climbing up the mountain.
  - At each point, w is updated so it moves a size of step λ in the gradient direction (or away)

$$w \leftarrow w + \lambda \nabla L(w)$$



Stochastic Gradient Descent Method

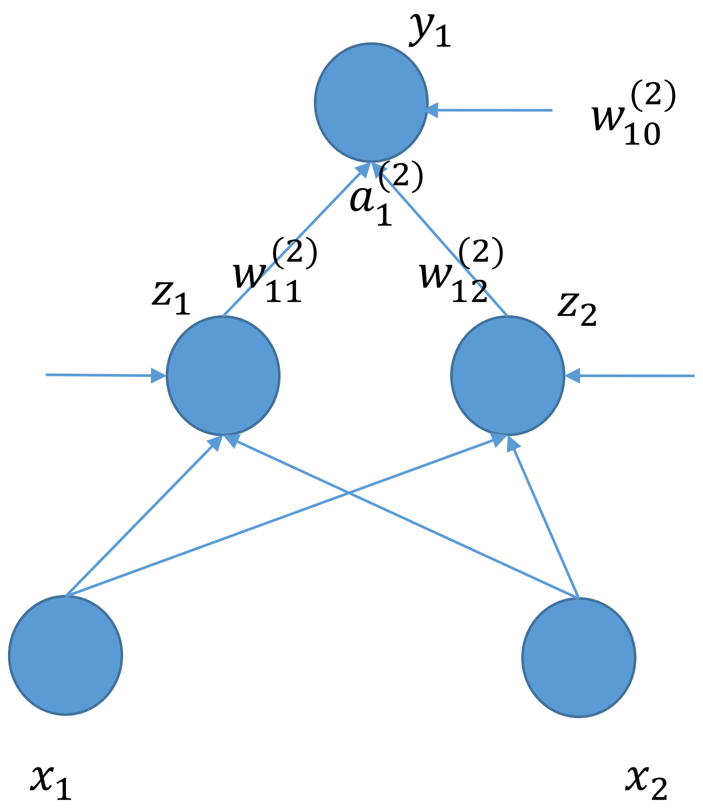
- Making the learning algorithm scalable to big data
- Computing the gradient of square error for only one example

$$L(w) = \sum_{i=1}^{M} (y^{(i)} - t^{(i)})^2 \qquad \nabla L = \left[\frac{\partial L}{\partial w_0}, \frac{\partial L}{\partial w_1}, \dots, \frac{\partial L}{\partial w_N} \right]$$

$$\Big\Downarrow$$

$$L^{(i)}(w) = (y^{(i)} - t^{(i)})^2 \qquad \nabla L^{(i)} = \left[\frac{\partial L^{(i)}}{\partial w_0}, \frac{\partial L^{(i)}}{\partial w_1}, \dots, \frac{\partial L^{(i)}}{\partial w_N} \right]$$

Computing the gradient



Square loss: $L = \frac{1}{2}(\mathrm{y}_k - \mathrm{t}_k)^2$

$$\mathrm{y}_k = f(a_k), a_k^{(2)} = \sum_j w_{kj}^{(2)} z_j$$

Derivative to the activation in the second layer:

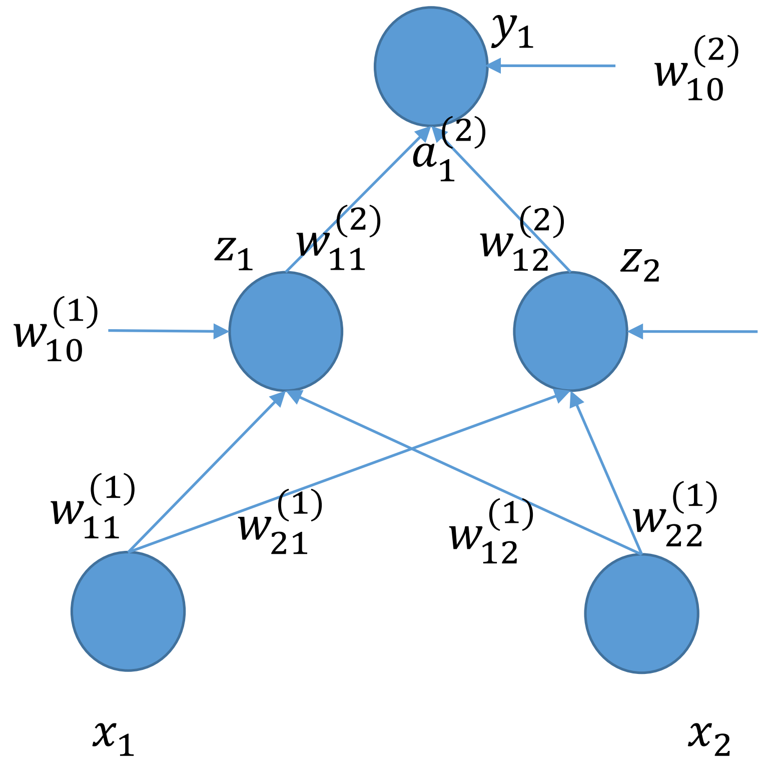
$$\delta_k^{(2)} \triangleq \frac{\partial L}{\partial a_k^{(2)}} = (\mathrm{y}_k - t_k)\frac{\partial y_k}{\partial a_k^{(2)}} = (\mathrm{y}_k - t_k) f'(a_k^{(2)})$$

Derivative to the parameter in the second layer:

$$\frac{\partial L}{\partial w_{ki}^{(2)}} = \frac{\partial L}{\partial a_k^{(2)}} \frac{\partial a_k}{\partial w_{ki}^{(2)}} = \delta_k^{(2)} z_i$$

Computing the gradient

- Computing the derivatives to the parameters in the first layer



Relation between activations of the first and second layers

$$a_k^{(2)} = \sum_j w_{kj}^{(2)} h(a_j^{(1)})$$

By chain rule: $$\frac{\partial L}{\partial a_j^{(1)}} = \sum_k \frac{\partial L}{\partial a_k^{(2)}} \frac{\partial a_k^{(2)}}{\partial a_j^{(1)}}$$

$$= h'(a_j^{(1)}) \sum_k \delta_k^{(2)} w_{kj}^{(2)} \triangleq \delta_j^{(1)}$$

The derivative to the parameter in the first layer:

$$a_j^{(1)} = \sum_n w_{jn}^{(1)} x_n \qquad \frac{\partial L}{\partial w_{jn}^{(1)}} = \frac{\partial L}{\partial a_j^{(1)}} \frac{\partial a_j^{(1)}}{\partial w_{jn}^{(1)}} = \delta_j^{(1)} x_n$$

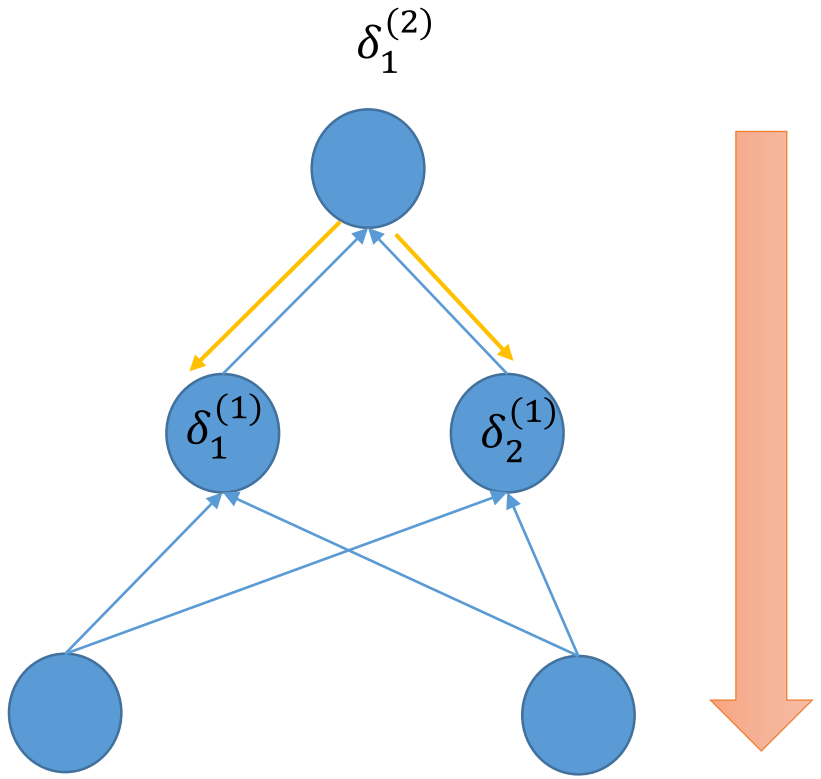
Summary: Back propagation

- For each training example (x,y),
  - For each output unit *k*

$$\delta_k^{(2)} = (y_k - t_k) f'(a_k^{(2)})$$

  - For each hidden unit *j*

$$\delta_j^{(1)} = h'(a_j^{(1)}) \sum_k \delta_k^{(2)} w_{kj}^{(2)}$$



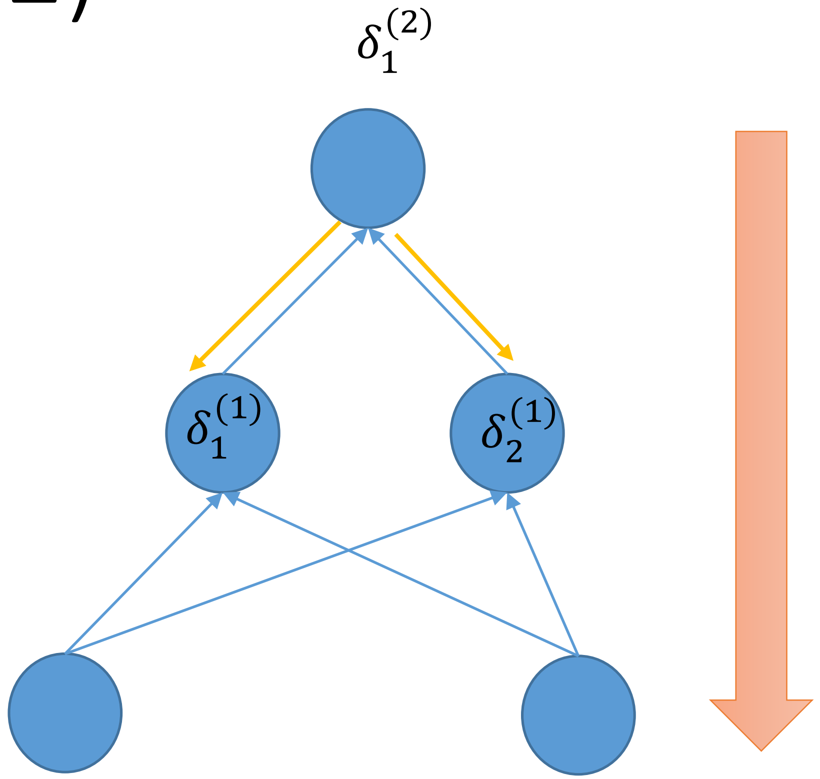
Summary: Back propagation (2)

- For each training example (x,y),
  - For each weight $w_{ki}^{(2)}$: $\frac{\partial L}{\partial w_{ki}^{(2)}} = \delta_k^{(2)} z_i$
    - Update

$$w_{ki}^{(2)} \leftarrow w_{ki}^{(2)} - \delta_k^{(2)} z_i$$

  - For each weight $w_{jn}^{(1)}$: $\frac{\partial L}{\partial w_{jn}^{(1)}} = \delta_j^{(1)} x_n$
    - Update

$$w_{jn}^{(1)} \leftarrow w_{jn}^{(1)} - \delta_j^{(1)} x_n$$



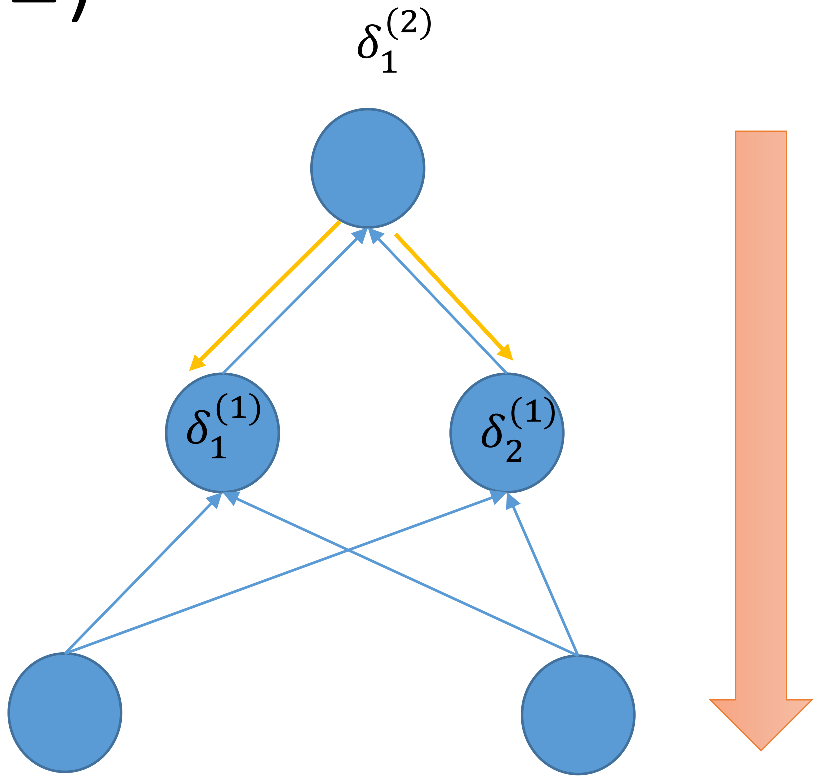
Regularized Square Error

- Add a zero mean Gaussian prior on the weights $w_{ij}^{(l)} \sim N(0, \sigma^2)$
- MAP estimate of w

$$L^{(i)}(w) = \frac{1}{2}(y^{(i)} - t^{(i)})^2 + \frac{\gamma}{2}\sum (w_{ij}^{(l)})^2$$

Summary: Back propagation (2)

- For each training example (x,y),
  - For each weight $w_{ki}^{(2)}$: $\frac{\partial L}{\partial w_{ki}^{(2)}} = \delta_k^{(2)} z_i + \gamma w_{ki}^{(2)}$
    - Update $w_{ki}^{(2)} \leftarrow w_{ki}^{(2)} - \delta_k^{(2)} z_i - \gamma w_{ki}^{(2)}$
  - For each weight $w_{jn}^{(1)}$: $\frac{\partial L}{\partial w_{jn}^{(1)}} = \delta_j^{(1)} x_n + \gamma w_{jn}^{(1)}$
    - Update $w_{jn}^{(1)} \leftarrow w_{jn}^{(1)} - \delta_j^{(1)} x_n - \gamma w_{jn}^{(1)}$



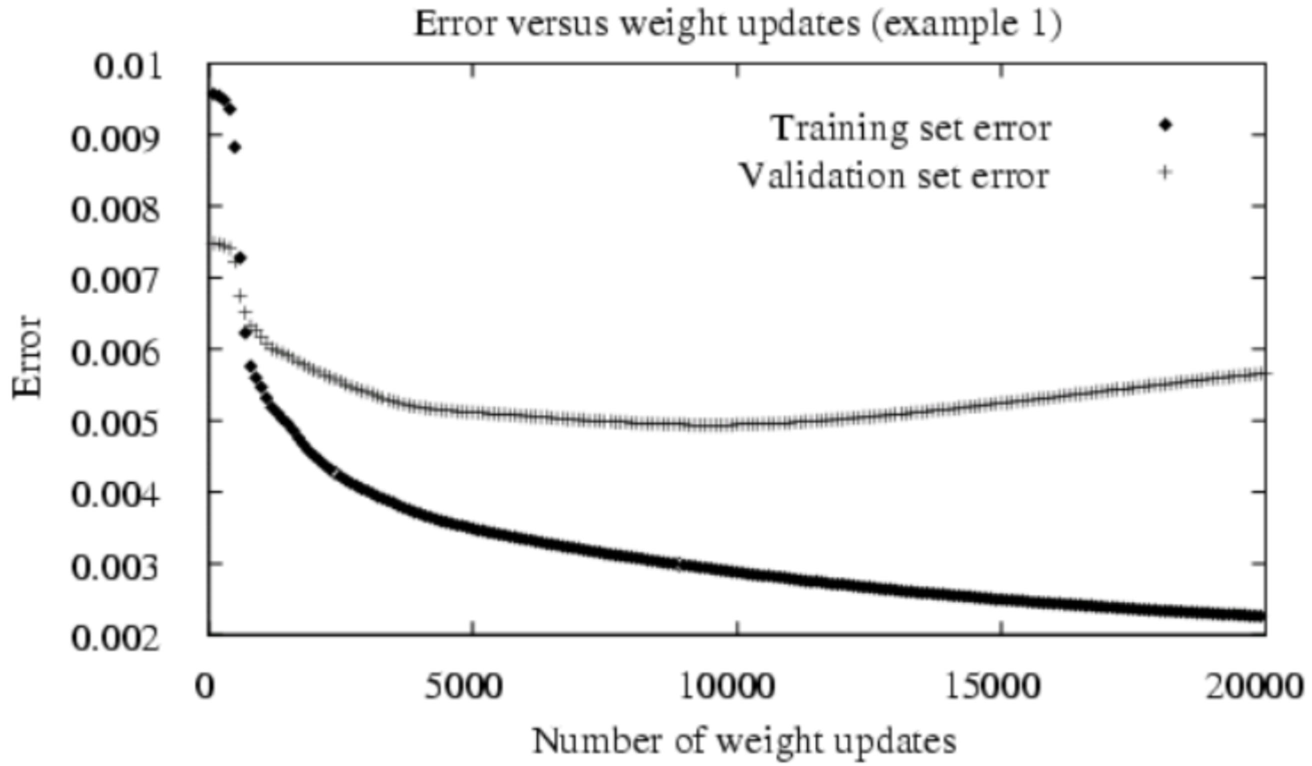
Multiple outputs encoding multiple classes

- MNIST: ten classes of digits
- Encoding multiple classes as multiple outputs:
  - An output variable is set to 1 if the corresponding class is positive for the example
  - Otherwise, the output is set to 0.
- The posterior probability of an example belonging to class k

$$P(\text{Class}_k|\mathbf{x}) = \frac{y_k}{{}_{k'=1}^{K} y_{k'}}$$

Overfitting

- Tuning the number of update iterations on validation set



How expressive is NN?

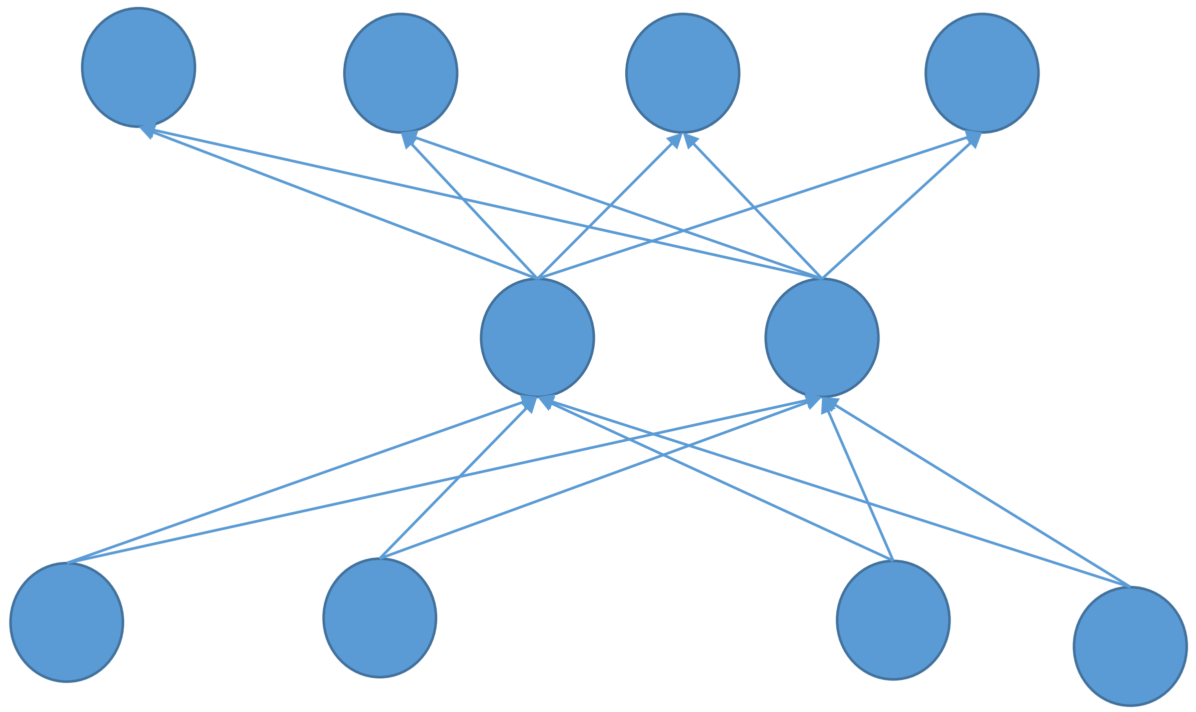
- Boolean functions:
  - Every Boolean function can be represented by network with single hidden layer
  - But might require exponential number of hidden units
- Continuous functions:
  - Every bounded continuous function can be approximated with arbitrarily small error by neural network with one hidden layer
  - Any function can be approximated to arbitrary accuracy by a network with two hidden layers

Learning feature representation by neural networks

- A compact representation for high dimensional input vectors
  - A large image with thousands of pixels
  - High dimensional input vectors
    - Trigger the curse of dimensionality
      - Needs more examples for training (in lecture 1)
    - Might not capture the intrinsic variations
      - An arbitrary point in a high dimensional space probably does not represent a valid real object.
  - A meaningful low dimensional space is preferred!

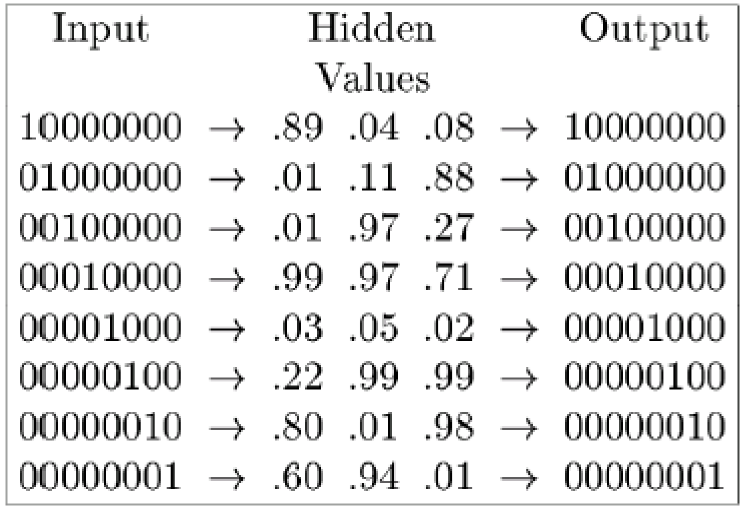
Autoencoder

- Set output to input
- Hidden layers as feature representation, since it contains sufficient information to reconstruct the input in the output layer

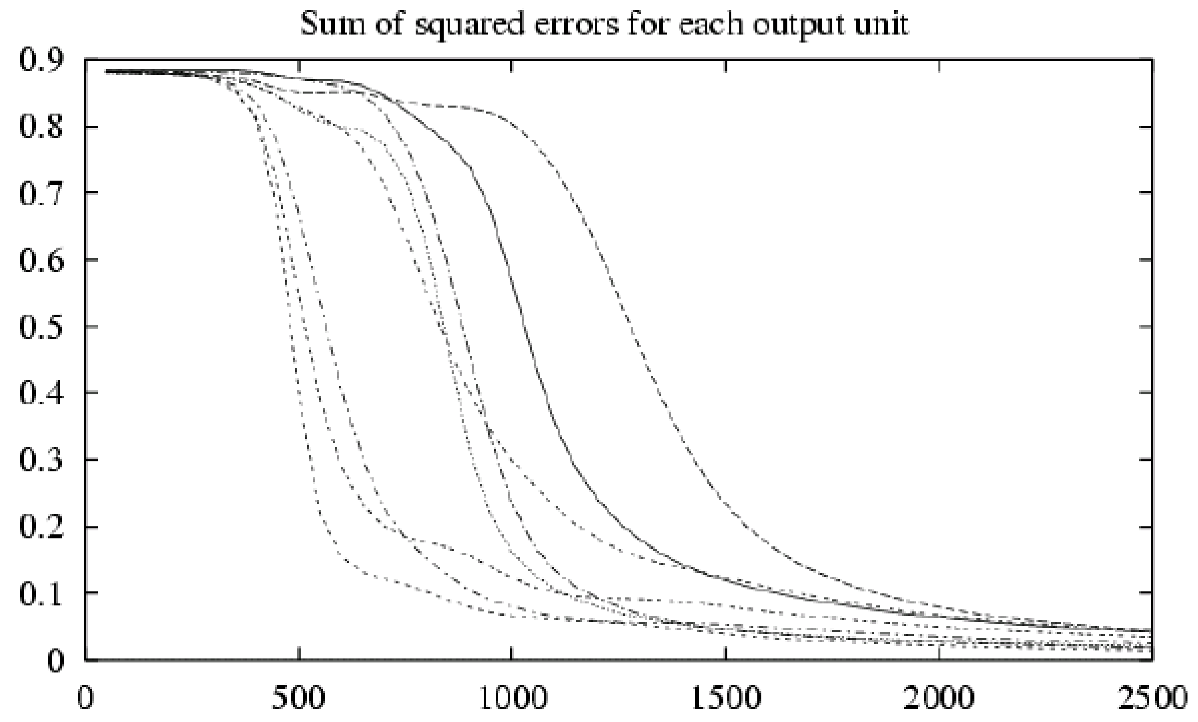


This trick enables us to train networks even when we don't have laeled data!

An example



Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001



Deep Learning: A Deep Feature Representation

- If you build multiple layers to reconstruct the input at the output layer

Summary

- Neural Networks: Multiple layers of neurons
  - Each upper layer neuron encodes weighted sum of inputs from the other neurons at a lower layer by an activation function
- Back propagation training: a stochastic gradient descent method
  - From the output layer down to the hidden and input layers
- Autoencoder: feature representation