Lecture 9: Neural Networks

Machine Learning

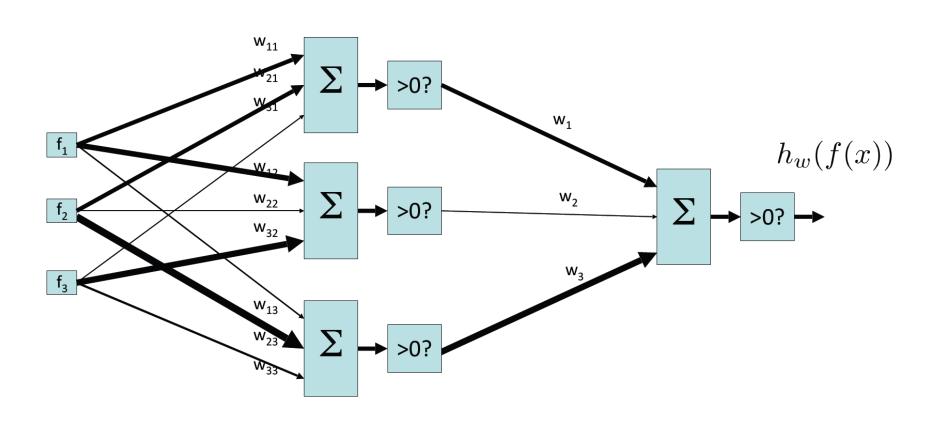
Spring Semester '2022

Multi-Layer Perceptron

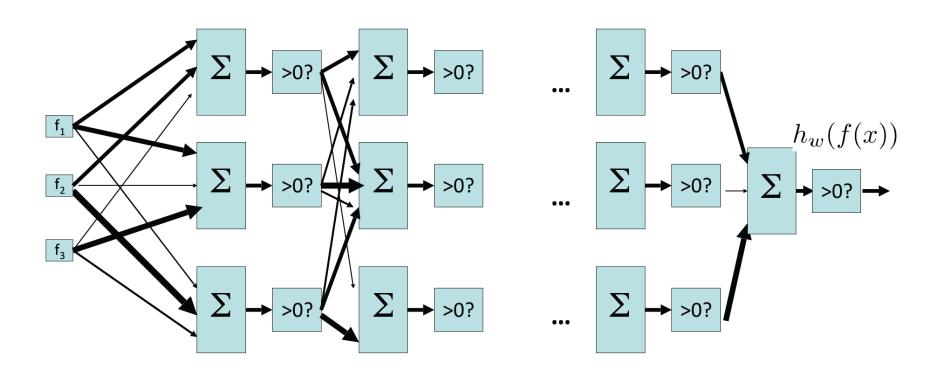
Higher representational power

Structure	Regions	XOR	Meshed regions
single layer	Half plane bounded by hyper- plane	A B A	B
two layer	Convex open or closed regions	A B	B
three layer	Arbitrary (limited by # of nodes)	A B A	B

Two-layer perceptron network

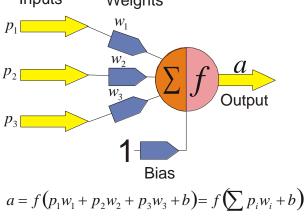


N-layer perceptron network



The Key Elements of Neural Networks

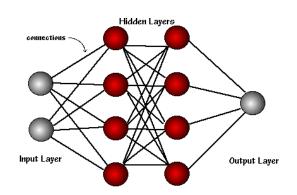
 Neural computing requires a number of neurons, to be connected together into a neural network. Neurons are arranged in layers.

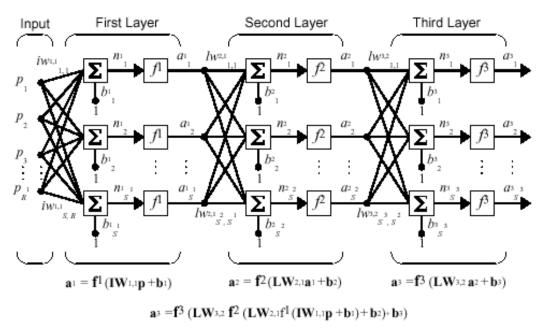


 Each neuron within the network is usually a simple processing unit which takes one or more inputs and produces an output. At each neuron, every input has an associated weight which modifies the strength of each input. The neuron simply adds together all the inputs and calculates an output to be passed on.

Feedforword NNs

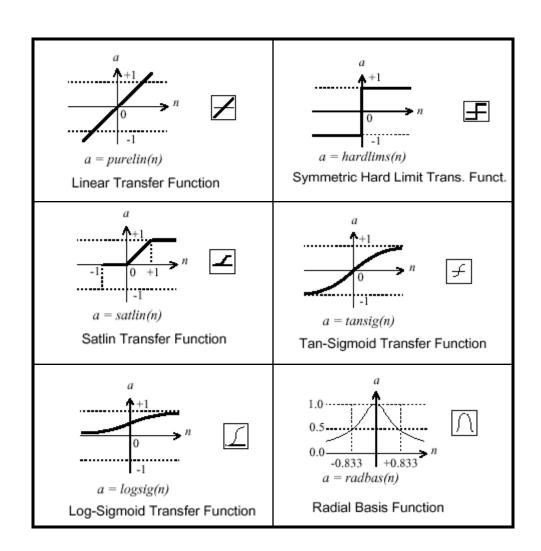
- The basic structure of a feedforward Neural Network
- The learning rule modifies the weights according to the input patterns that it is presented with. In a sense, NNs learn by example as do their biological counterparts.
- When the desired output are known we have supervised learning or learning with a teacher.





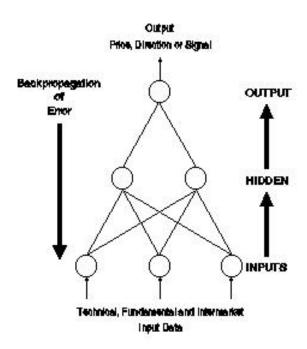
Activation functions

 The activation function is generally nonlinear.



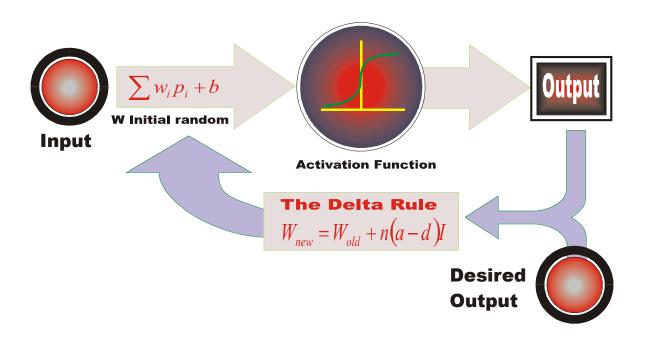
An overview of the backpropagation

- Problem statement defined
 - input into the network and desired output from the network
- Set of training samples assembled
- Input data entered into network via the input layer.
- Each neuron processes input data with resultant values steadily "percolating" through the network, layer by layer, until result is generated by the output layer
- 5. Actual output of the network compared to expected output for that particular input
 - Results in error value
- 6. Connection weights gradually adjusted working backwards from output layer, through hidden layer, and to input layer, until correct output is produced, i.e. the network *learns*.



The Learning Rule

The delta rule is often utilized by the most common class of NNs.



Learning to approximate

Error measure:

$$E = \frac{1}{N} \sum_{t=1}^{N} (F(x_t; W) - y_t)^2$$

Rule for changing the synaptic weights:

$$\Delta w_i^j = -c \cdot \frac{\partial E}{\partial w_i^j}(W)$$

$$w_i^{j,new} = w_i^j + \Delta w_i^j$$

c is the learning parameter (usually a constant)

Sigmoidal Neurons

$$f_i(net_i(t)) = \frac{1}{1 + e^{-(net_i(t) - \theta)/\tau}}$$

$$f_i(net_i(t))$$

$$\tau = 0.1$$

$$\tau = 1$$

$$1 \quad net_i(t)$$

• In backpropagation networks, we typically choose $\tau = 1$ and $\theta = 0$.

Sigmoidal Neurons

•This leads to a simplified form of the sigmoid function:

$$S(net) = \frac{1}{1 + e^{(-net)}}$$

We do not need a modifiable threshold Θ , because we will use "dummy" inputs as we did for perceptrons.

The choice $\tau = 1$ works well in most situations and results in a very simple derivative of S(net).

Sigmoidal Neurons

$$S(x) = \frac{1}{1 + e^{-x}}$$

$$S'(x) = \frac{dS(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2}$$

$$= \frac{1+e^{-x}-1}{(1+e^{-x})^2} = \frac{1}{1+e^{-x}} - \frac{1}{(1+e^{-x})^2}$$

$$= S(x)(1-S(x))$$

This result will be very useful when we develop the backpropagation algorithm.

The goal of the Backpropagation learning algorithm is to modify the network's weights so that its output vector

$$o_p = (o_{p,1}, o_{p,2}, ..., o_{p,K})$$

is as close as possible to the desired output vector

$$\mathbf{d}_p = (d_{p,1}, d_{p,2}, ..., d_{p,K})$$

for *K* output neurons and input patterns p = 1, ..., P.

The set of input-output pairs (exemplars)

 $\{(\boldsymbol{x}_p, \boldsymbol{d}_p) \mid p = 1, ..., P\}$ constitutes the training set.

Also, we need a cumulative error function that is to be minimized:

$$Error = \sum_{p=1}^{P} Err(\mathbf{o}_{p}, \mathbf{d}_{p})$$

We can choose the mean square error (MSE) once again (but the 1/P factor does not matter):

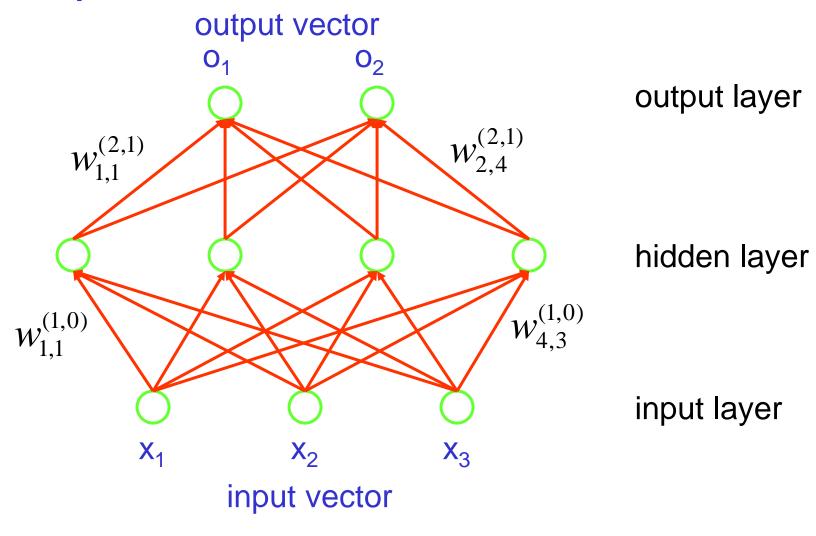
$$MSE = \frac{1}{P} \sum_{p=1}^{P} \sum_{j=1}^{K} (l_{p,j})^{2}$$

where

$$l_{p,j} = o_{p,j} - d_{p,j}$$

Terminology

•Example: Network function f: $\mathbb{R}^3 \to \mathbb{R}^2$



For input pattern p, the i-th input layer node holds $x_{p,i}$.

Net input to j-th node in hidden layer:
$$net_j^{(1)} = \sum_{i=0}^n w_{j,i}^{(1,0)} x_{p,i}$$

Output of j-th node in hidden layer:
$$x_{p,j}^{(1)} = S\left(\sum_{i=0}^{n} w_{j,i}^{(1,0)} x_{p,i}\right)$$

Net input to k-th node in output layer:
$$net_k^{(2)} = \sum_j w_{k,j}^{(2,1)} x_{p,j}^{(1)}$$

Output of k-th node in output layer:
$$o_{p,k} = S \left(\sum_{j} w_{k,j}^{(2,1)} x_{p,j}^{(1)} \right)$$

Network error for p:
$$E_{p} = \sum_{k=1}^{K} (l_{p,k})^{2} = \sum_{k=1}^{K} (d_{p,k} - o_{p,k})^{2}$$

- As E is a function of the network weights, we can use gradient descent to find those weights that result in minimal error.
- For individual weights in the hidden and output layers, we should move against the error gradient (omitting index p):

$$\Delta w_{k,j}^{(2,1)} \propto \frac{-\partial E}{\partial w_{k,j}^{(2,1)}}$$
 Output layer: Derivative easy to calculate

$$\Delta w_{j,i}^{(1,0)} \propto \frac{-\partial E}{\partial w_{i,i}^{(1,0)}}$$
 Hidden layer: Derivative difficult to calculate

When computing the derivative with regard to $w_{k,j}^{(2,1)}$, we can disregard any output units except o_k :

$$E = \sum_{i \neq k} l_i^2 + (d_k - o_k)^2$$
$$\frac{\partial E}{\partial o_k} = -2(d_k - o_k)$$

Remember that o_k is obtained by applying the sigmoid function S to $net_k^{(2)}$, which is computed by:

$$net_k^{(2)} = \sum_j w_{k,j}^{(2,1)} x_j^{(1)}$$

Therefore, we need to apply the chain rule twice.

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Backpropagation Learning

$$\frac{\partial E}{\partial w_{k,j}^{(2.1)}} = \frac{\partial E}{\partial o_k} \frac{\partial o_k}{\partial net_k^{(2)}} \frac{\partial net_k^{(2)}}{\partial w_{k,j}^{(2.1)}}$$

We know that: $\frac{\partial o_k}{\partial net_k^{(2)}} = S'(net_k^{(2)})$

Since
$$net_k^{(2)} = \sum_j w_{k,j}^{(2,1)} x_j^{(1)}$$

We have: $\frac{\partial net_k^{(2)}}{\partial w_{k,i}^{(2,1)}} = x_j^{(1)}$

Which gives us: $\frac{\partial E}{\partial w_{k,j}^{(2.1)}} = -2(d_k - o_k)S' \left(net_k^{(2)}\right) x_j^{(1)}$

For the derivative with regard to $w_{j,i}^{(1,0)}$, notice that E depends on it through $net_j^{(1)}$, which influences each o_k with k = 1, ..., K:

$$o_k = S(net_k^{(2)}), \quad x_j^{(1)} = S(net_j^{(1)}), \quad net_j^{(1)} = \sum_i w_{j,i}^{(1,0)} x_i$$

Using the chain rule of derivatives again:

$$\frac{\partial E}{\partial w_{j,i}^{(1,0)}} = \sum_{k=1}^{K} \frac{\partial E}{\partial o_k} \frac{\partial o_k}{\partial net_k^{(2)}} \frac{\partial net_k^{(2)}}{\partial x_j^{(1)}} \frac{\partial x_j^{(1)}}{\partial net_j^{(1)}} \frac{\partial net_j^{(1)}}{\partial w_{j,i}^{(1,0)}}$$

$$\frac{\partial E}{\partial w_{j,i}^{(1,0)}} = \sum_{k=1}^{K} \left[-2(d_k - o_k)S'(net_k^{(2)})w_{k,j}^{(2,1)}S'(net_j^{(1)})x_i \right]$$

This gives us the following weight changes at the output layer:

$$\Delta w_{k,j}^{(2.1)} = \eta \cdot \delta_k \cdot x_j^{(1)} \quad with$$
$$\delta_k = (d_k - o_k) S'(net_k^{(2)})$$

... and at the inner layer:

$$\Delta w_{j,i}^{(1,0)} = \eta \cdot \mu_j \cdot x_i \quad with$$

$$\mu_j = \left(\sum_{k=1}^K \delta_k w_{k,j}^{(2,1)}\right) S'(net_j^{(1)})$$

As you surely remember from a few minutes ago:

$$S'(x) = S(x)(1 - S(x))$$

Then we can simplify the generalized error terms:

$$\delta_k = (d_k - o_k)S'(net_k^{(2)}) \Longrightarrow \delta_k = (d_k - o_k)o_k(1 - o_k)$$

And:

$$\mu_{j} = \left(\sum_{k=1}^{K} \delta_{k} w_{k,j}^{(2,1)}\right) S'(net_{j}^{(1)})$$

$$\Rightarrow \mu_{j} = \sum_{k=1}^{K} \delta_{k} w_{k,j}^{(2,1)} x_{j}^{(1)} \left(1 - x_{j}^{(1)}\right)$$

- The simplified error terms δ_k and μ_j use variables that are calculated in the feedforward phase of the network and can thus be calculated very efficiently.
- Now let us state the final equations again and reintroduce the subscript p for the p-th pattern:

$$\Delta w_{k,j}^{(2.1)} = \eta \cdot \delta_{p,k} \cdot x_{p,j}^{(1)} \quad with$$

$$\delta_{p,k} = (d_{p,k} - o_{p,k}) o_{p,k} (1 - o_{p,k})$$

$$\Delta w_{j,i}^{(1,0)} = \eta \cdot \mu_{p,j} \cdot x_{p,i} \quad with$$

$$\mu_{p,j} = \sum_{i=1}^{K} \delta_{p,k} w_{k,j}^{(2,1)} x_{p,j}^{(1)} \left(1 - x_{p,j}^{(1)}\right)$$

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Algorithm Backpropagation;
  Start with randomly chosen weights;
  while MSE is above desired threshold and computational
    bounds are not exceeded, do
    for each input pattern \mathbf{x}_p, 1 \le p \le P,
       Compute hidden node inputs;
       Compute hidden node outputs;
       Compute inputs to the output nodes;
       Compute the network outputs;
       Compute the error between output and desired output;
       Modify the weights between hidden and output nodes;
       Modify the weights between input and hidden nodes;
    end-for
  end-while
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Improving Backpropagation Performance

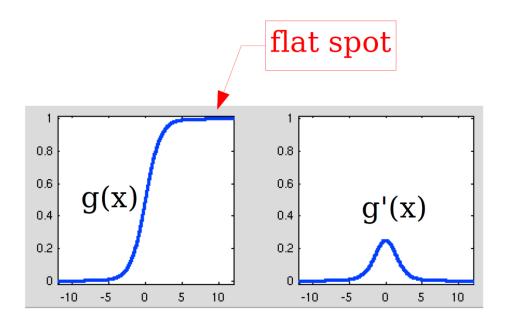
- Avoiding local minima
- Keep derivatives from going to zero
- For classifiers, use reachable targets
- Compensate for error attenuation in deep layers
- Compensate for fan-in effects
- Use momentum to speed learning
- Reduce learning rate when weights oscillate

Avoiding Local Minima

- One problem with backprop is that the error surface is no longer bowl-shaped.
- Gradient descent can get trapped in local minima.
 - In practice, this does not usually prevent learning.
- "Noise" can get us out of local minima:
 - Stochastic update (one pattern at a time).
 - Add noise to training data, weights, or activations.
 - Large learning rates can be a source of noise due to overshooting

Flat Spots

- If weights become large, net_j becomes large, derivative of g() goes to zero.
 - Fahlman's trick: add a small constant to g'(x) to keep the derivative from going to zero. Typical value is 0.1.



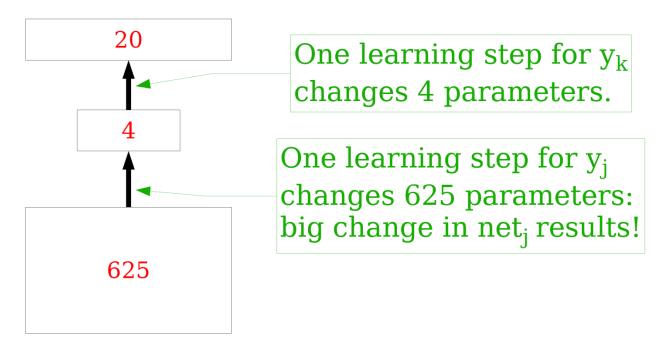
Reachable Targets for Classifiers

- Targets of 0 and 1 are unreachable by the logistic or tanh functions.
- Weights get large as the algorithm tries to force each output unit to reach its asymptotic value.
- Trying to get a "correct" output from 0.95 up to 1.0 wastes time and resources that should be concentrated elsewhere.
- Solution: use "reachable targets" of 0.1 and 0.9 instead of 0/1. And don't penalize the network for overshooting these targets.

Error Signal Attenuation

- The error signal gets attenuated as it moves backward through multiple layers.
 - Input-to-hidden weights learn more slowly than hidden-tooutput weights.
- Solution: have different learning rates for different layers.
 - Or use Deep Learning

Fan-In Affects Learning Rate



• Solution: scale learning rate by fan-in.

Momentum

- Learning is slow if the learning rate is set too low.
- Gradient may be steep in some directions but shallow in others.
- Solution: add a momentum term α .

$$\Delta w_{ij}(t) = -\eta \frac{\partial E}{\partial w_{ii}(t)} + \alpha \cdot \Delta w_{ij}(t-1)$$

- Typical value for α is 0.5.
- If the direction of the gradient remains constant, the algorithm will take increasingly large steps.