Multi-Layer Networks
Multi-Layer Networks

- Generally much more versatile than single neurons

- No linear-separability requirement.

- Training is less obvious and potentially more time consuming.
Multi-Level Networks

Several varieties, the most common of which is known as:

- MLP (Multi-Level Perceptron)

- Backpropagation Network (alluding to a common method of training these networks; other training methods could conceivably be used.)
Note that sometimes the input is counted as a “layer”.
The real layers other than the output are called “hidden” layers.
Bias

\[ b_i = \text{bias} = \text{negative of threshold} \]
Design a network by hand that implements this decision problem.
Elementary Decision Boundaries

First Boundary:
\[ a_1^1 = \text{hardlim} \left( \begin{bmatrix} -1 & 0 \end{bmatrix} p + 0.5 \right) \]

Second Boundary:
\[ a_2^1 = \text{hardlim} \left( \begin{bmatrix} 0 & -1 \end{bmatrix} p + 0.75 \right) \]

First Subnetwork
Elementary Decision Boundaries

Third Boundary:

\[ a_3^1 = hardlim\left( \begin{bmatrix} 1 & 0 \end{bmatrix} p - 1.5 \right) \]

Fourth Boundary:

\[ a_4^1 = hardlim\left( \begin{bmatrix} 0 & 1 \end{bmatrix} p - 0.25 \right) \]

Second Subnetwork
Total Network

\[ W^1 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad b^1 = \begin{bmatrix} 0.5 \\ 0.75 \\ -1.5 \\ -0.25 \end{bmatrix} \]

\[ W^2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \quad b^2 = \begin{bmatrix} -1.5 \\ -1.5 \end{bmatrix} \]

\[ W^3 = \begin{bmatrix} 1 & 1 \end{bmatrix}, \quad b^3 = \begin{bmatrix} -0.5 \end{bmatrix} \]
Demo nnd11f

- Shows a simple 2-level network:
  - 1 input, 1 output
  - 2 neurons in first layer, with 1 weight and 1 bias each, logsig activation function
  - 1 neuron in output layer, with 2 weights and 1 bias
  - Output activation function selectable from: purelin (identity), tansig, logsig

- Plot is network output vs. input
Function Approximation Demo nn11f

\[
f^1(n) = \frac{1}{1 + e^{-n}}
\]

\[
f^2(n) = n
\]

Nominal Parameter Values

\[
w^1_{1,1} = 10 \quad w^1_{2,1} = 10 \quad b^1 = -10 \quad b^1_2 = 10
\]

\[
w^2_{1,1} = 1 \quad w^2_{1,2} = 1 \quad b^2 = 0
\]
Nominal Response
Parameter Variations

\[ 0 \leq b_2^1 \leq 20 \]

\[ -1 \leq w_1, 1 \leq 1 \]

\[ -1 \leq w_1, 2 \leq 1 \]

\[ -1 \leq b_2^2 \leq 1 \]
How to Train a MLP?

- With a single neuron, it is not too hard to see how to adjust the weights based upon the error values. We’ve already seen a couple of ways.

- With a multi-layer network, it is less obvious. For one thing, **what is the “error” for the neurons in non-final layers?** Without these, we don’t know how to adjust.

- This is called the “credit assignment” problem (maybe should be “blame assignment”).
Backpropagation


- Rumelhart and McClelland, in 1985, discovered the method, presumably independently, and popularized it under the current name.

- In mathematics, such methods are in the category of “optimization”.
The technique is gradient descent, as explained for Adalines.

However, the computation of the gradient is less clear.
Backpropagation Training Cycle

- **Forward propagation**: Derive the activation values (the inputs to the activation functions) at each neuron, and the final output.

- **Compute the error** in the output.

- **Backpropagate** the error through the network to get “sensitivities” at each neuron. (The gradient approximation is derivable from the sensitivities.)

- Use the sensitivities to **derive weight changes**.

- Apply the weight changes.
Backpropagation Training Cycle

- Backpropagate is mathematically a lot like forward propagate.
- Sensitivities are used instead of signal values.
- The sensitivities are the partial derivatives of the MSE with respect to the activation values.
- Basically both are iterated matrix multiplications.
How to Train a MLP?

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Multi-Layer Network

Each box has a row-vector of weights and a bias.

Each layer has a matrix of weights and a column vector of biases.
Multi-Layer Network

- Given an input vector, can compute the outputs.
- Given a sample, can compute the errors in output.
- Knowing gradient, can adjust the weights.
- Big Question: How to compute the gradient?
Recall that the gradient consists of components $\frac{\partial J}{\partial w}$ where $J$ is the mean-squared error and $w$ is some weight (or bias) in the network.

For the Adaline, already derived:

$$\frac{\partial J}{\partial w_i} = -2 \overline{x_i} f'(n),$$

where $x_i$ is the input corresponding to weight $w_i$, and $n(\text{net})$ is the weighted sum. This works as is for the multi-layer case at the output layer.
Inside one neuron

\[
\frac{\partial J}{\partial w_i} = \frac{\partial J}{\partial n} \left( \frac{\partial n}{\partial w_i} \right) \\
= \left( \frac{\partial (d-f(n))^2}{\partial n} \right) \left( \frac{\partial n}{\partial w_i} \right) \\
= -2 (d-f(n)) f'(n) x_i \\
= s x_i
\]

where \( s = \frac{\partial J}{\partial n} \) is called the sensitivity
Chain Rule Refresher

\[
\frac{df(n(w))}{dw} = \frac{df(n)}{dn} \cdot \frac{dn(w)}{dw}
\]

Example

\[\begin{align*}
  f(n) &= \cos(n) \quad n = e^{2w} \quad f(n(w)) = \cos(e^{2w}) \\
  \frac{df(n(w))}{dw} &= \frac{df(n)}{dn} \cdot \frac{dn(w)}{dw} = (-\sin(n))(2e^{2w}) = (-\sin(e^{2w}))(2e^{2w})
\end{align*}\]

Application to Gradient Calculation

\[
\frac{\partial J}{\partial w_{i,j}^m} = \frac{\partial J}{\partial n_i^m} \cdot \frac{\partial n_i^m}{\partial w_{i,j}^m}
\]
Last Layer

output = f(n)

n = \text{net}
Utility of Sensitivity

\[ \frac{\partial J}{\partial w_i} = (\frac{\partial J}{\partial n}) (\frac{\partial n}{\partial w_i}) \]
\[ = s x_i \]

*anywhere* in the network, not just at the final layer.
e.g. Next-Last Layer

\[ \frac{\partial J}{\partial w_i} = \frac{\partial J}{\partial n} \left( \frac{\partial n}{\partial w_i} \right) \]
\[ = S x_i \]
Computing of Sensitivity

Unlike at the output, it is less clear how to compute the sensitivity at an *arbitrary* neuron.

The key idea is to use an iterative approach that starts with the sensitivities at the last layer and works backward toward the first layer.
Backward Propagation of Sensitivity

sensitivities known

sensitivities desired

$w_i$
Backward Propagation of Sensitivity

Express desired as a weighted sum of known:

\[ s = f'(n) \prod w_j s_j \]
Express desired as a weighted sum of known:

\[ s = f'(n) \mathbf{w}_j s_j \]

Vector Form for entire layer:

\[ s^m = \mathbf{F}^m(n^m)(\mathbf{W}^{m+1})^T s^{m+1} \]
Correctness

Why should \( s = f'(n) \sum w_j s_j \) ??

\[ s = \frac{\partial J}{\partial n^m} \]

\[ = \left( \frac{\partial n^{m+1}}{\partial n^m} \right) \left( \frac{\partial J}{\partial n^{m+1}} \right) \]

from the *vector* form of the chain rule

\[ s^m = \frac{\partial J}{\partial n^m} = \begin{bmatrix} \frac{\partial n^{m+1}}{\partial n^m} \end{bmatrix}^T \frac{\partial J}{\partial n^{m+1}} \]
In the vector form \( s^m = \frac{\partial J}{\partial n^m} = \frac{\partial n^{m+1}}{\partial n^m} \) \( \frac{\partial J}{\partial n^{m+1}} \)

\[
\begin{bmatrix}
\frac{\partial n_1^{m+1}}{\partial n_1^m} & \frac{\partial n_1^{m+1}}{\partial n_2^m} \\
\frac{\partial n_2^{m+1}}{\partial n_1^m} & \frac{\partial n_2^{m+1}}{\partial n_2^m} \\
\frac{\partial n_{S_1}^{m+1}}{\partial n_1^m} & \frac{\partial n_{S_1}^{m+1}}{\partial n_2^m} \\
\frac{\partial n_{S_2}^{m+1}}{\partial n_1^m} & \frac{\partial n_{S_2}^{m+1}}{\partial n_2^m}
\end{bmatrix}
\]

the Jacobian
Correctness, continued

\[ s = \nabla \left( \frac{\partial n^{m+1}}{\partial n^m} \right) \left( \frac{\partial J}{\partial n^{m+1}} \right) \]

\[ = \left( \frac{\partial}{\partial n^m} \right) \nabla w_j f(n_j^m) \quad s_j \quad \text{by def. of } n^{m+1} \]

\[ = \nabla w_j f'(n^m) \quad s_j \]

\[ = f'(n^m) \nabla w_j \quad s_j \]
Vector Form

\[ s^m = \frac{\partial J}{\partial n^m} = \nabla_n \left[ \begin{array}{c} n^m+1 \\ \end{array} \right]^T \frac{\partial J}{\partial n^m} = F^m(n^m)(W^{m+1})^T \frac{\partial J}{\partial n^{m+1}} \]

\[ s^m = \dot{F}^m(n^m)(W^{m+1})^T s^{m+1} \]

\[ \frac{\partial n^{m+1}}{\partial n^m} = W^{m+1} F^m(n^m) \quad \dot{F}^m(n^m) = \left[ \begin{array}{cccc} f^m(n_1^m) & 0 & \square & 0 \\ 0 & f^m(n_2^m) & \square & 0 \\ \square & \square & \square & \square \\ 0 & 0 & \square & f^m(n_{3m}^m) \end{array} \right] \]
Fully-Subscripted Alternatives to the Vector Forms

\[ n_i^m = \sum_{j=1}^{w_i,j} a_{j}^{m-1} + b_i^m \]

\[ \frac{\partial n_i^m}{\partial w_{i,j}} = a_{j}^{m-1} \]

\[ \frac{\partial n_i^m}{\partial b_i^m} = 1 \]

Sensitivity

\[ s_i^m \equiv \frac{\partial J}{\partial n_i^m} \]

Gradient

\[ \frac{\partial J}{\partial w_{i,j}^m} = s_i^m a_{j}^{m-1} \]

\[ \frac{\partial J}{\partial b_i^m} = s_i^m \]
Fully-Subscripted Alternatives to the Vector Forms

\[
\frac{\partial n^{m+1}_i}{\partial n^m_j} = \frac{\partial}{\partial n^m_j} \left[ \sum_{l=1}^{S^m_i} w_{i,l} a^m + b^{m+1}_i \right] = w_{i,j} \frac{\partial a^m_j}{\partial n^m_j}
\]

\[
\frac{\partial n^{m+1}_i}{\partial n^m_j} = w_{i,j} \frac{\partial f^m(n^m_j)}{\partial n^m_j} = w_{i,j} f^m(n^m_j)
\]

\[
f^m(n^m_j) = \frac{\partial f^m(n^m_j)}{\partial n^m_j}
\]
Vector Form for Last Layer

\[
\begin{align*}
    s_i^M &= \frac{\partial \hat{F}}{\partial n_i^M} = \frac{\partial (\mathbf{t} - \mathbf{a})^T (\mathbf{t} - \mathbf{a})}{\partial n_i^M} = \sum_{j=1}^{S^M} \left( t_j - a_j \right)^2 \\
    \frac{\partial a_i^M}{\partial n_i^M} &= \frac{\partial f^M(n_i^M)}{\partial n_i^M} = f^M(n_i^M) \\
    s_i^M &= -2(t_i - a_i) f^M(n_i^M)
\end{align*}
\]
Backpropagation Training Cycle

- **Forward propagation**: Derive the activation values (the inputs to the activation functions) at each neuron, and the final output.
- **Compute the error** in the output.
- **Backpropagate** the error through the network to get “sensitivities” at each neuron. (The gradient approximation is derivable from the sensitivities.)
- Use the sensitivities to **derive weight changes**.
- Apply the weight changes.
Backpropagation (Sensitivities)

The sensitivities are computed by starting at the last layer, and then propagating backwards through the network to the first layer.

\[ s^M \quad s^{M-1} \quad \cdots \quad s^2 \quad s^1 \]

\[ s^M = -2F^M (n^M) (t - a) \quad \text{basis} \]

\[ s^m = F^m (n^m) (W^m+1)^T s^{m+1} \quad \text{induction step} \]

diagonal matrix of activation function derivative values

\[
F^m (n^m) = \begin{bmatrix}
0 & 0 & \cdots & 0 \\
0 & f'(n_2^m) & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & f'(n_{S^m}^m)
\end{bmatrix}
\]
Weight and Bias Update

Here we are using $\alpha$ instead of $\eta$ for the learning rate.

\[
W^m(k + 1) = W^m(k) - \alpha s^m (a^{m-1})^T
\]

input of layer m = output of layer m-1

\[
b^m(k + 1) = b^m(k) - \alpha s^m
\]
Fully-Subscripted Version of Weight Update

\[
\begin{align*}
  w_{i,j}^m(k+1) &= w_{i,j}^m(k) - \nabla s_i a_j^m - 1 \\
  b_i^m(k+1) &= b_i^m(k) - \nabla s_i
\end{align*}
\]

\[
\begin{align*}
  W^m(k+1) &= W^m(k) - \nabla s^m (a^{m-1})^T \\
  b^m(k+1) &= b^m(k) - \nabla s^m
\end{align*}
\]

\[
\mathbf{s}^m = \frac{\partial J}{\partial \mathbf{n}^m} = \begin{bmatrix}
  \frac{\partial J}{\partial n_1^m} \\
  \frac{\partial J}{\partial n_2^m} \\
  \vdots \\
  \frac{\partial J}{\partial n_S^m} \\
\end{bmatrix}
\]
Summary

Forward Propagation

\[ a^0 = p \]
\[ a^{m+1} = f^{m+1}(W^{m+1}a^m) \quad m = 0, 2, \ldots, M - 1 \]
\[ a = a^M \]

Backpropagation

\[ s^M = -2\dot{F}^{M}(n^{M})(t - a) \]
\[ s^m = \dot{F}^m(n^m)(W^{m+1})^Ts^{m+1} \quad m = M - 1, \ldots, 2, 1 \]

Weight Update

\[ W^m(k + 1) = W^m(k) - \delta s^m(a^{m-1})^T \quad b^m(k + 1) = b^m(k) - \delta s^m \]
Exercise

- Derive the backprop equations symbolically for a simple network.
- Then use the equations to train the network.
A simple network
Label the Levels

0 1 M = 2
Label the Signal Vectors or Lines

\[ a^0 \quad a^1 \quad a^2 \]

Vectors, superscript = level
Label the Signal Vectors or Lines

\[ a^0_1 \to a^1_1 \to a^2_1 \]

Lines, superscript = level,
Label the Net (Activation) Values
Label the Weights and Biases
Write the forward equations for activations

\[ n_{1}^{1} = w_{11}^{1} a_{0}^{1} + w_{12}^{1} a_{0}^{2} + b_{1}^{1} \]
\[ a_{1}^{1} = f(n_{1}^{1}) \]

\[ n_{1}^{2} = w_{11}^{2} a_{1}^{1} + w_{12}^{2} a_{1}^{2} + b_{1}^{2} \]
\[ a_{1}^{2} = f(n_{1}^{2}) \]

\[ n_{2}^{1} = w_{21}^{1} a_{1}^{1} + w_{22}^{1} a_{1}^{2} + b_{2}^{1} \]
\[ a_{2}^{1} = f(n_{2}^{1}) \]
Write the backward equations for sensitivities

\[ s_{11} = w_{11}^2 s_{1} f'(n_{11}) \]

\[ s_{12} = w_{12}^2 s_{1} f'(n_{12}) \]

\[ s_{21} = -2(d_{1}^2 - a_{1}^2) f'(n_{21}) \]
Note

- The summations for the backpropagated sensitivities have only one term in this example, since the following layer has only one neuron.
Write the Equations for Weight and Bias Update

\[ \Delta w_{11} = -\Delta s_1 \cdot a_0 \]
\[ \Delta w_{12} = -\Delta s_1 \cdot a_2 \]
\[ \Delta b_1 = -\Delta s_1 \]

\[ \Delta w_{21} = -\Delta s_2 \cdot a_1 \]
\[ \Delta w_{22} = -\Delta s_2 \cdot a_2 \]
\[ \Delta b_2 = -\Delta s_2 \]
Exercise

- Use the derivation to train the network to realize xor, where the first layer activations are logsig and the second layer is a hardlim.

- Carry out the preceding type of derivation for a 2-3-2 network (2 inputs, 3 middle neurons, 2 outputs).
Discontinuous functions such as hardlim, hardlims, etc. don’t have derivatives.

Therefore we train the network with continuous approximations to these functions, then replace them with the discontinuous versions during usage:

- usage: hardlim, hardlims
- train with: logsig, tansig
Numeric Example

1-2-1 Network

(Input) \( p \) \( \rightarrow \) Log-Sigmoid Layer \( \rightarrow \) Linear Layer \( \rightarrow \) \( a \)
Initial Conditions

\[
\begin{align*}
W^1(0) &= \begin{bmatrix} -0.27 \\ -0.41 \end{bmatrix} & b^1(0) &= \begin{bmatrix} -0.48 \\ -0.13 \end{bmatrix} & W^2(0) &= \begin{bmatrix} 0.09 & -0.17 \end{bmatrix} & b^2(0) &= \begin{bmatrix} 0.48 \end{bmatrix}
\end{align*}
\]
Forward Propagation

\[ a^0 = p = 1 \]

\[ a^1 = f^1(W^1a^0 + b^1) = \text{logsig} \left[ \begin{array}{c}
-0.27 \\
-0.41 \\
\end{array} \right] + \left[ \begin{array}{c}
-0.48 \\
-0.13 \\
\end{array} \right] = \text{logsig} \left[ \begin{array}{c}
-0.75 \\
-0.54 \\
\end{array} \right] \]

\[ a^1 = \left[ \begin{array}{c}
\frac{1}{1 + e^{-0.75}} \\
\frac{1}{1 + e^{-0.54}} \\
\end{array} \right] = \left[ \begin{array}{c}
0.321 \\
0.368 \\
\end{array} \right] \]

\[ a^2 = f^2(W^2a^1 + b^2) = \text{purelin} \left( \left[ \begin{array}{cc}
0.09 & -0.17 \\
0.368 & 0.48 \\
\end{array} \right] + \left[ \begin{array}{c}
0.321 \\
0.368 \\
\end{array} \right] \right) = \left[ \begin{array}{c}
0.446 \\
\end{array} \right] \]

\[ e = t - a = \left[ \begin{array}{c}
1 + \sin \frac{\pi}{4}p\right] - a^2 = \left[ \begin{array}{c}
1 + \sin \frac{\pi}{4} \right] - 0.446 = 1.261 \]
Transfer Function Derivatives

\[
f^1(n) = \frac{d}{dn} \left( \frac{1}{1 + e^{-n}} \right) = \frac{e^{-n}}{(1 + e^{-n})^2} = \left[ 1 - \frac{1}{1 + e^{-n}} \right] \frac{1}{1 + e^{-n}} = (1 - a^1)(a^1)
\]

\[
f^2(n) = \frac{d}{dn}(n) = 1
\]
Backpropagation

\[ s^2 = -2F^2(n^2)(t - a) = -2 \left[ f^2(n^2) \right](1.261) = -2 \left[ 1 \right](1.261) = -2.522 \]

\[ s^1 = F^1(n^1)(W^2)^T s^2 = \begin{bmatrix} (1-a_1^1)(a_1^1) & 0 \\ 0 & (1-a_2^1)(a_2^1) \end{bmatrix} \begin{bmatrix} 0.09 \\ -0.17 \end{bmatrix} \begin{bmatrix} -2.522 \end{bmatrix} \]

\[ s^1 = \begin{bmatrix} (1-0.321)(0.321) & 0 \\ 0 & (1-0.368)(0.368) \end{bmatrix} \begin{bmatrix} 0.09 \\ -0.17 \end{bmatrix} \begin{bmatrix} -2.522 \end{bmatrix} \]

\[ s^1 = \begin{bmatrix} 0.218 & 0 \\ 0 & 0.233 \end{bmatrix} \begin{bmatrix} -0.227 \\ 0.429 \end{bmatrix} = \begin{bmatrix} -0.0495 \\ 0.0997 \end{bmatrix} \]
Weight Update

\( \Delta = 0.1 \)

\[
W^2(1) = W^2(0) - \Delta s^2(a^1)^T = \begin{bmatrix} 0.09 & -0.17 \end{bmatrix} - 0.1 \begin{bmatrix} -2.522 \\ 0.321 \end{bmatrix} = \begin{bmatrix} 0.171 & -0.0772 \end{bmatrix}
\]

\[
W^2(1) = \begin{bmatrix} 0.171 & -0.0772 \end{bmatrix}
\]

\[
b^2(1) = b^2(0) - \Delta s^2 = \begin{bmatrix} 0.48 \end{bmatrix} - 0.1 \begin{bmatrix} -2.522 \end{bmatrix} = \begin{bmatrix} 0.732 \end{bmatrix}
\]

\[
b^2(1) = \begin{bmatrix} 0.732 \end{bmatrix}
\]

\[
W^1(1) = W^1(0) - \Delta s^1(a^0)^T = \begin{bmatrix} -0.27 \\ -0.41 \end{bmatrix} - 0.1 \begin{bmatrix} -0.0495 \\ 0.0997 \end{bmatrix} = \begin{bmatrix} -0.265 \\ -0.420 \end{bmatrix}
\]

\[
b^1(1) = b^1(0) - \Delta s^1 = \begin{bmatrix} -0.48 \\ -0.13 \end{bmatrix} - 0.1 \begin{bmatrix} -0.0495 \\ 0.0997 \end{bmatrix} = \begin{bmatrix} -0.475 \\ -0.140 \end{bmatrix}
\]

\[
b^1(1) = \begin{bmatrix} -0.475 \\ -0.140 \end{bmatrix}
\]