Neural network

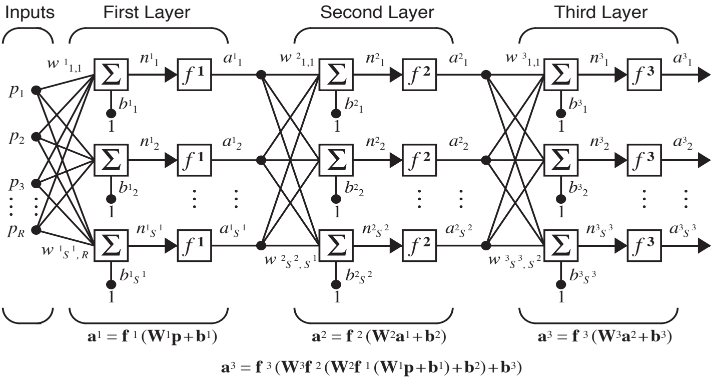
Machine Learning II

Lecture 3-b

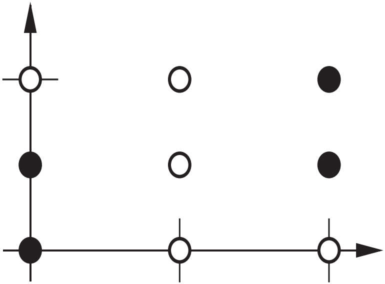
THE GEORGE WASHINGTON UNIVERSITY

WASHINGTON, DC

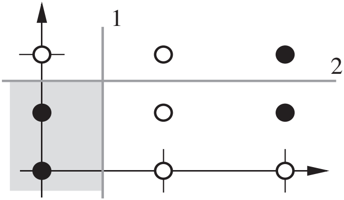
Multilayer Perceptron



$R - S^1 - S^2 - S^3$ Network



Elementary Decision Boundaries



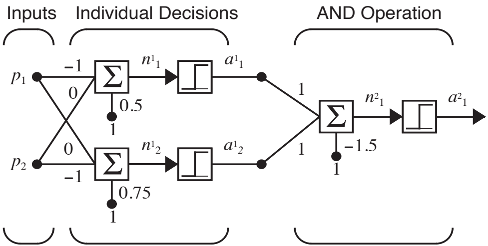
First Boundary:

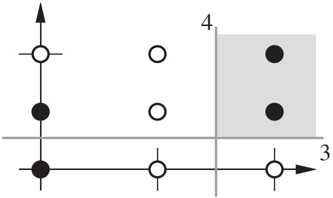
$$a^1_1 = hardlim(\begin{bmatrix} -1 & 0 \end{bmatrix}\mathbf{p} + 0.5)$$

Second Boundary:

$$a^1_2 = hardlim(\begin{bmatrix} 0 & -1 \end{bmatrix}\mathbf{p} + 0.75)$$

First Subnetwork





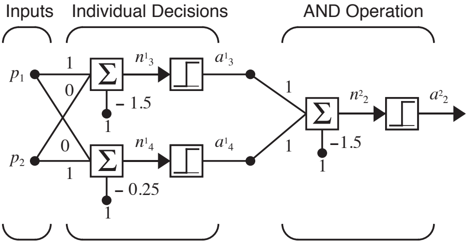
Third Boundary:

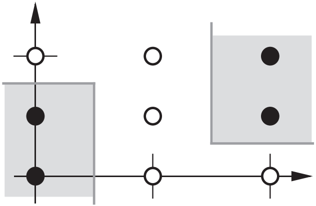
$$a_3^1 = hardlim(\begin{bmatrix}1 & 0\end{bmatrix}\mathbf{p} - 1.5)$$

Fourth Boundary:

$$a_4^1 = hardlim(\begin{bmatrix}0 & 1\end{bmatrix}\mathbf{p} - 0.25)$$

Second Subnetwork

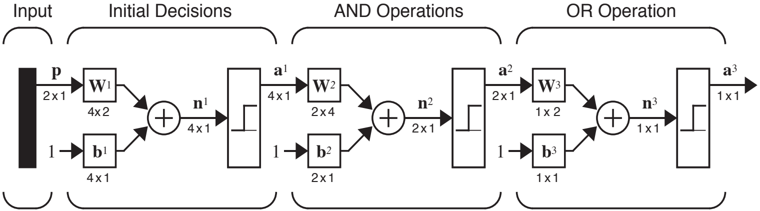




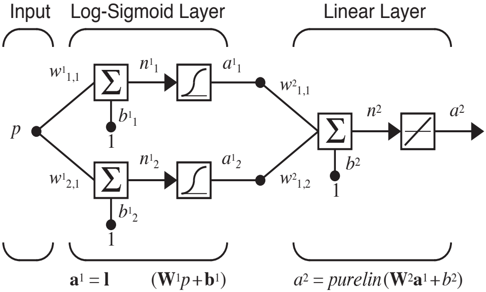
$$\mathbf{W}^1 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \mathbf{b}^1 = \begin{bmatrix} 0.5 \\ 0.75 \\ -1.5 \\ -0.25 \end{bmatrix}$$

$$\mathbf{W}^2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix} \qquad \mathbf{b}^2 = \begin{bmatrix} -1.5 \\ -1.5 \end{bmatrix}$$

$$\mathbf{W}^3 = \begin{bmatrix} 1 & 1 \end{bmatrix} \qquad \mathbf{b}^3 = \begin{bmatrix} -0.5 \end{bmatrix}$$



$$\mathbf{a}^1 = \mathbf{hardlim}(\mathbf{W}^1\mathbf{p} + \mathbf{b}^1) \qquad \mathbf{a}^2 = \mathbf{hardlim}(\mathbf{W}^2\mathbf{a}^1 + \mathbf{b}^2) \qquad \mathbf{a}^3 = \mathbf{hardlim}(\mathbf{W}^3\mathbf{a}^2 + \mathbf{b}^3)$$



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

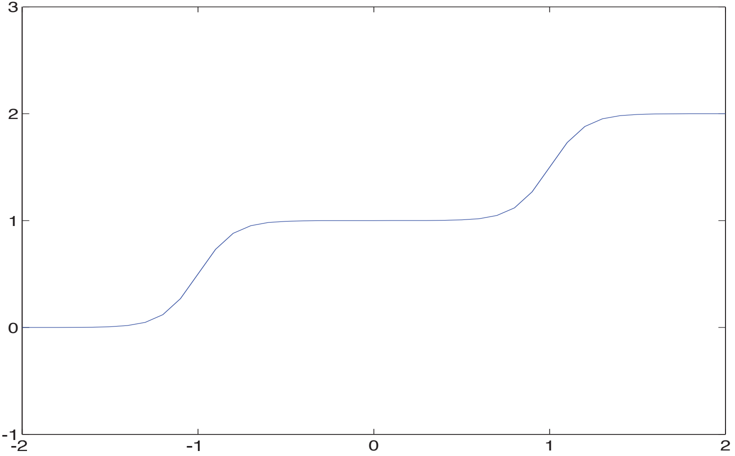
$$f^2(n) = n$$

Nominal Parameter Values

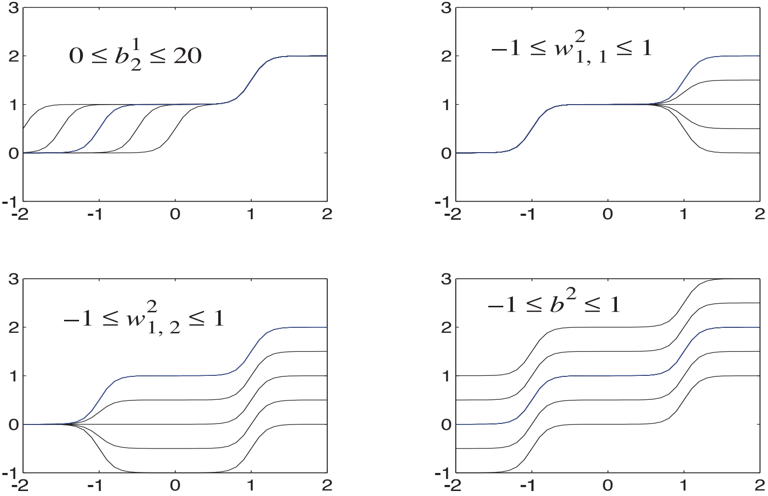
$$w^1_{1,1} = 10 \qquad w^1_{2,1} = 10 \qquad b^1_1 = -10 \qquad b^1_2 = 10$$

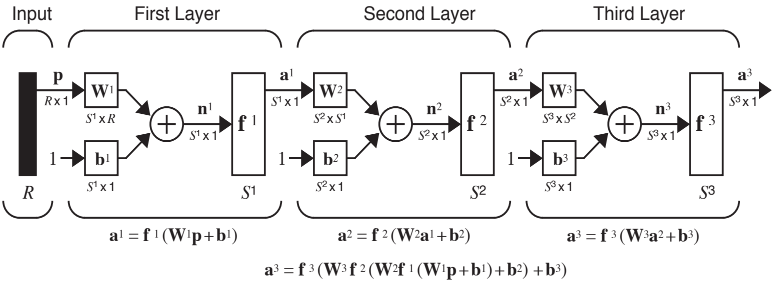
$$w^2_{1,1} = 1 \qquad w^2_{1,2} = 1 \qquad b^2 = 0$$

Nominal Response



Parameter Variations





$$\mathbf{a}^{m+1} = \mathbf{f}^{m+1}(\mathbf{W}^{m+1}\mathbf{a}^{m} + \mathbf{b}^{m+1}) \qquad m = 0, 2, \ldots, M-1$$

$$\mathbf{a}^{0} = \mathbf{p}$$

$$\mathbf{a} = \mathbf{a}^{M}$$

Training Set

$$\{\mathbf{p}_1, \mathbf{t}_1\}, \{\mathbf{p}_2, \mathbf{t}_2\}, \ldots, \{\mathbf{p}_Q, \mathbf{t}_Q\}$$

Mean Square Error

$$F(\mathbf{x}) = E[e^2] = E[(\quad - \quad)^2]$$

Vector Case

$$F(\mathbf{x}) = E[\mathbf{e}^T\mathbf{e}] = E[(\mathbf{t} - \mathbf{a})^T(\mathbf{t} - \mathbf{a})]$$

Approximate Mean Square Error (Single Sample)

$$\hat{F}(\mathbf{x}) = (\mathbf{t}(k) - \mathbf{a}(k))^T(\mathbf{t}(k) - \mathbf{a}(k)) = \mathbf{e}^T(k)\mathbf{e}(k)$$

Approximate Steepest Descent

$$w_{i,j}^m(k+1) = w_{i,j}^m(k) - \alpha\frac{\partial\hat{F}}{\partial w_{i,j}^m} \qquad b_i^m(k+1) = b_i^m(k) - \alpha\frac{\partial\hat{F}}{\partial b_i^m}$$

$$\frac{df(n(w))}{dw} = \frac{df(n)}{dn} \times \frac{dn(w)}{dw}$$

Example

$$f(n) = \cos(n) \qquad n = \mathrm{e}^{2w} \qquad f(n(w)) = \cos(e^{2w})$$

$$\frac{df(n(w))}{dw} = \frac{df(n)}{dn} \times \frac{dn(w)}{dw} = (-\sin(n))(2e^{2w}) = (-\sin(e^{2w}))(2e^{2w})$$

Application to Gradient Calculation

$$\frac{\partial \hat{F}}{\partial w_{i,}^{m}} = \frac{\partial \hat{F}}{\partial n_{i}^{m}} \times \frac{\partial n_{i}^{m}}{\partial w_{i,}^{m}} \qquad \frac{\partial \hat{F}}{\partial b_{i}^{m}} = \frac{\partial \hat{F}}{\partial n_{i}^{m}} \times \frac{\partial n_{i}^{m}}{\partial b_{i}^{m}}$$

$$n_i^m = \sum_{j=1}^{S^{m-1}} w_{i,}^m \; a_j^{m-1} + b_i^m$$

$$\frac{\partial n_i^m}{\partial w_{i,}^m} = a_j^{m-1} \qquad\qquad \frac{\partial n_i^m}{\partial b_i^m} = 1$$

Sensitivity

$$s_i^m \equiv \frac{\partial \hat{F}}{\partial n_i^m}$$

Gradient

$$\frac{\partial \hat{F}}{\partial w_{i,}^m} = s_i^m a_j^{m-1} \qquad\qquad \frac{\partial \hat{F}}{\partial b_i^m} = s_i^m$$

$$w_{i,j}^{m}(k+1) = w_{i,j}^{m}(k) - \alpha s_i^m a_j^{m-1} \qquad b_i^m(k+1) = b_i^m(k) - \alpha s_i^m$$

$$\boxed{\mathbf{W}^m(k+1) = \mathbf{W}^m(k) - \alpha \mathbf{s}^m (\mathbf{a}^{m-1})^T \qquad \mathbf{b}^m(k+1) = \mathbf{b}^m(k) - \alpha \mathbf{s}^m}$$

$$\mathbf{s}^m \equiv \frac{\partial \hat{F}}{\partial \mathbf{n}^m} = \begin{bmatrix} \frac{\partial \hat{F}}{\partial n_1^m} \\ \frac{\partial \hat{F}}{\partial n_2^m} \\ \vdots \\ \frac{\partial \hat{F}}{\partial n_{S^m}^m} \end{bmatrix}$$

Next Step: Compute the Sensitivities (Backpropagation)

$$\frac{\partial \mathbf{n}^{m+1}}{\partial \mathbf{n}^m} \equiv \begin{bmatrix} \frac{\partial n_1^{m+1}}{\partial n_1^m} & \frac{\partial n_1^{m+1}}{\partial n_2^m} & \cdots & \frac{\partial n_1^{m+1}}{\partial n_{S^m}^m} \\ \frac{\partial n_2^{m+1}}{\partial n_1^m} & \frac{\partial n_2^{m+1}}{\partial n_2^m} & \cdots & \frac{\partial n_2^{m+1}}{\partial n_{S^m}^m} \\ \vdots & \vdots & & \vdots \\ \frac{\partial n_{S^{m+1}}^{m+1}}{\partial n_1^m} & \frac{\partial n_{S^{m+1}}^{m+1}}{\partial n_2^m} & \cdots & \frac{\partial n_{S^{m+1}}^{m+1}}{\partial n_{S^m}^m} \end{bmatrix}$$

$$\frac{\partial n_i^{m+1}}{\partial n_j^m} = \frac{\partial\left(\sum_{l=1}^{S^m} w_{i,l}^{m+1} a_l^m + b_i^{m+1}\right)}{\partial n_j^m} = w_{i,j}^{m+1} \frac{\partial a_j^m}{\partial n_j^m}$$

$$\frac{\partial n_i^{m+1}}{\partial n_j^m} = w_{i,j}^{m+1} \frac{\partial f^m(n_j^m)}{\partial n_j^m} = w_{i,j}^{m+1} \dot{f}^m(n_j^m)$$

$$\dot{f}^m(n_j^m) = \frac{\partial f^m(n_j^m)}{\partial n_j^m}$$

$$\frac{\partial \mathbf{n}^{m+1}}{\partial \mathbf{n}^m} = \mathbf{W}^{m+1} \dot{\mathbf{F}}^m(\mathbf{n}^m)$$

$$\dot{\mathbf{F}}^m(\mathbf{n}^m) = \begin{bmatrix} \dot{f}^m(n_1^m) & 0 & \cdots & 0 \\ 0 & \dot{f}^m(n_2^m) & & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \dot{f}^m(n_{S^m}^m) \end{bmatrix}$$

$$\mathbf{s}^m = \frac{\partial \hat{F}}{\partial \mathbf{n}^m} = \left(\frac{\partial \mathbf{n}^{m+1}}{\partial \mathbf{n}^m}\right)^T \frac{\partial \hat{F}}{\partial \mathbf{n}^{m+1}} = \dot{\mathbf{F}}^m(\mathbf{n}^m)(\mathbf{W}^{m+1})^T \frac{\partial \hat{F}}{\partial \mathbf{n}^{m+1}}$$

$$\boxed{\mathbf{s}^m = \dot{\mathbf{F}}^m(\mathbf{n}^m)(\mathbf{W}^{m+1})^T \mathbf{s}^{m+1}}$$

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

$$\mathbf{s}^M \to \mathbf{s}^{M-1} \to \ldots \to \mathbf{s}^2 \to \mathbf{s}^1$$

$$s_i^M = \frac{\partial \hat{F}}{\partial n_i^M} = \frac{\partial (\mathbf{t}-\mathbf{a})^T(\mathbf{t}-\mathbf{a})}{\partial n_i^M} = \frac{\partial \sum_{j=1}^{S^M} (t_j - a_j)^2}{\partial n_i^M} = -2(t_i - a_i)\frac{\partial a_i}{\partial n_i^M}$$

$$\frac{\partial a_i}{\partial n_i^M} = \frac{\partial a_i^M}{\partial n_i^M} = \frac{\partial f^M(n_i^M)}{\partial n_i^M} = \dot{f}^M(n_i^M)$$

$$s_i^M = -2(t_i - a_i)\dot{f}^M(n_i^M)$$

$$\boxed{\mathbf{s}^M = -2\dot{\mathbf{F}}^M(\mathbf{n}^M)(\mathbf{t}-\mathbf{a})}$$

Forward Propagation

$$\mathbf{a}^0 = \mathbf{p}$$

$$\mathbf{a}^{m+1} = \mathbf{f}^{m+1}(\mathbf{W}^{m+1}\mathbf{a}^m + \mathbf{b}^{m+1}) \qquad m = 0, 2, \ldots, M-1$$

$$\mathbf{a} = \mathbf{a}^M$$

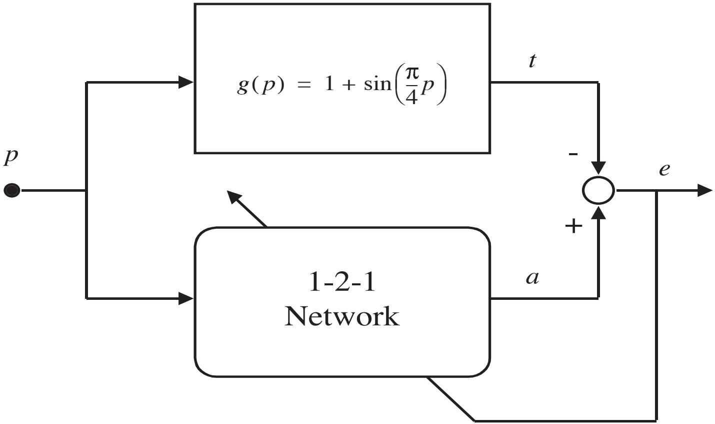
Backpropagation

$$\mathbf{s}^M = -2\dot{\mathbf{F}}^M(\mathbf{n}^M)(\mathbf{t} - \mathbf{a})$$

$$\mathbf{s}^m = \dot{\mathbf{F}}^m(\mathbf{n}^m)(\mathbf{W}^{m+1})^T\mathbf{s}^{m+1} \qquad m = M-1, \ldots, 2, 1$$

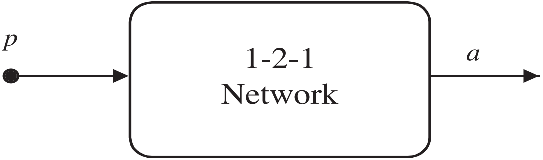
Weight Update

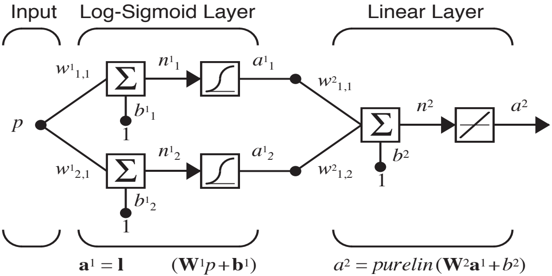
$$\mathbf{W}^m(k+1) = \mathbf{W}^m(k) - \alpha\mathbf{s}^m(\mathbf{a}^{m-1})^T \qquad \mathbf{b}^m(k+1) = \mathbf{b}^m(k) - \alpha\mathbf{s}^m$$



$g(p) = 1 + \sin\left(\frac{\pi}{4}p\right)$
t
p
-
e
+
a
1-2-1
Network

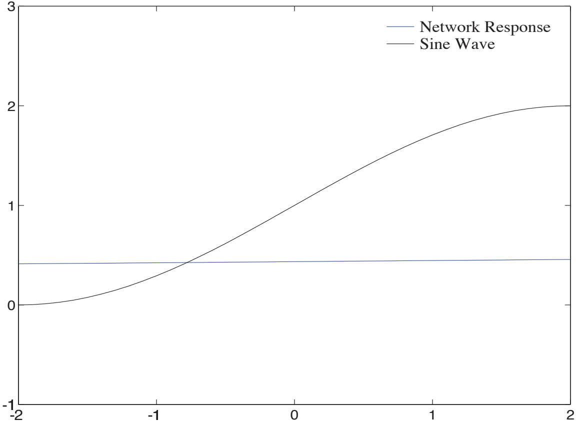
Network


p
1-2-1
Network
a


Input
Log-Sigmoid Layer
Linear Layer
$w^1_{1,1}$
$w^1_{2,1}$
n^1_1
n^1_2
a^1_1
a^1_2
b^1_1
b^1_2
$w^2_{1,1}$
$w^2_{1,2}$
n^2
a^2
b^2
p
1
$\mathbf{a}^1 = \mathbf{l} \quad (\mathbf{W}^1 p + \mathbf{b}^1)$
$a^2 = purelin(\mathbf{W}^2\mathbf{a}^1 + b^2)$

Initial Conditions

$$\mathbf{W}^1(0) = \begin{bmatrix} -0.27 \\ -0.41 \end{bmatrix} \quad \mathbf{b}^1(0) = \begin{bmatrix} -0.48 \\ -0.13 \end{bmatrix} \quad \mathbf{W}^2(0) = \begin{bmatrix} 0.09 & -0.17 \end{bmatrix} \quad \mathbf{b}^2(0) = \begin{bmatrix} 0.48 \end{bmatrix}$$



$$a^0 = p = 1$$

$$\mathbf{a}^1 = \mathbf{f}^1(\mathbf{W}^1\mathbf{a}^0 + \mathbf{b}^1) = \mathbf{logsig}\left(\begin{bmatrix}-0.27\\-0.41\end{bmatrix}\begin{bmatrix}1\end{bmatrix} + \begin{bmatrix}-0.48\\-0.13\end{bmatrix}\right) = \mathbf{logsig}\left(\begin{bmatrix}-0.75\\-0.54\end{bmatrix}\right)$$

$$\mathbf{a}^1 = \begin{bmatrix}\dfrac{1}{1+e^{0.75}}\\[2ex]\dfrac{1}{1+e^{0.54}}\end{bmatrix} = \begin{bmatrix}0.321\\0.368\end{bmatrix}$$

$$a^2 = \mathrm{f}^2(\mathbf{W}^2\mathbf{a}^1 + \mathbf{b}^2) = purelin\left(\begin{bmatrix}0.09 & -0.17\end{bmatrix}\begin{bmatrix}0.321\\0.368\end{bmatrix} + \begin{bmatrix}0.48\end{bmatrix}\right) = \begin{bmatrix}0.446\end{bmatrix}$$

$$e = t - a = \left\{1 + \sin\left(\frac{\pi}{4}p\right)\right\} - a^2 = \left\{1 + \sin\left(\frac{\pi}{4}1\right)\right\} - 0.446 = 1.261$$

Transfer Function Derivatives

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

$$\dot{f}^2(n) = \frac{d}{dn}(n) = 1$$

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

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

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

$$\mathbf{s}^1 = \begin{bmatrix} 0.218 & 0 \\ 0 & 0.233 \end{bmatrix} \begin{bmatrix} -0.227 \\ 0.429 \end{bmatrix} = \begin{bmatrix} -0.0495 \\ 0.0997 \end{bmatrix}$$

$$\alpha = 0.1$$

$$\mathbf{W}^2(1) = \mathbf{W}^2(0) - \alpha\mathbf{s}^2(\mathbf{a}^1)^T = \begin{bmatrix} 0.09 & -0.17 \end{bmatrix} - 0.1\begin{bmatrix} -2.522 \end{bmatrix}\begin{bmatrix} 0.321 & 0.368 \end{bmatrix}$$

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

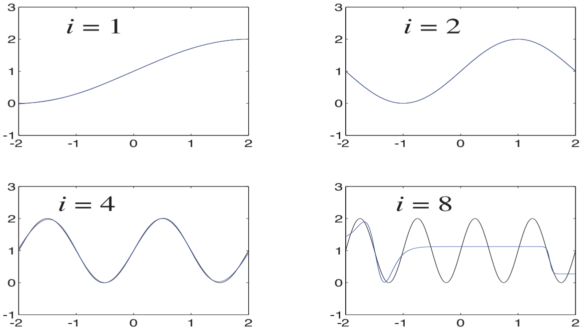
$$\mathbf{b}^2(1) = \mathbf{b}^2(0) - \alpha\mathbf{s}^2 = \begin{bmatrix} 0.48 \end{bmatrix} - 0.1\begin{bmatrix} -2.522 \end{bmatrix} = \begin{bmatrix} 0.732 \end{bmatrix}$$

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

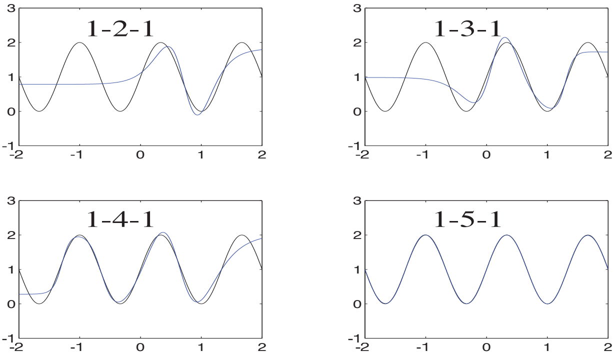
$$\mathbf{b}^1(1) = \mathbf{b}^1(0) - \alpha\mathbf{s}^1 = \begin{bmatrix} -0.48 \\ -0.13 \end{bmatrix} - 0.1\begin{bmatrix} -0.0495 \\ 0.0997 \end{bmatrix} = \begin{bmatrix} -0.475 \\ -0.140 \end{bmatrix}$$

$$g(p) = 1 + \sin\left(\frac{i\pi}{4}p\right)$$

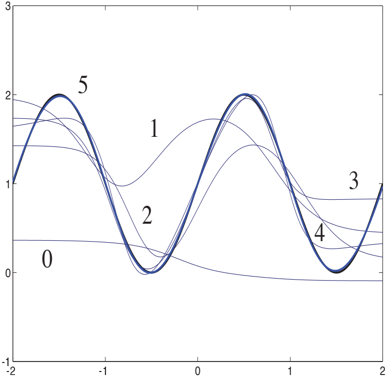
1-3-1 Network

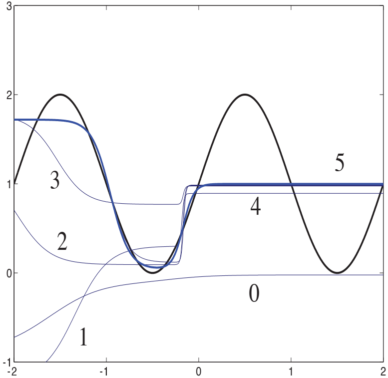


$$g(p) = 1 + \sin\left(\frac{6\pi}{4}p\right)$$



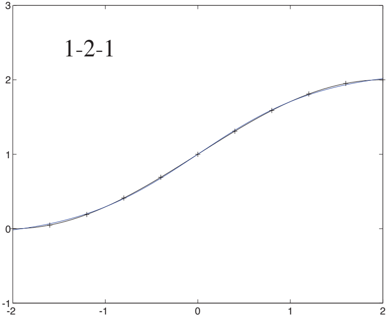
$$g(p) = 1 + \sin(\pi p)$$

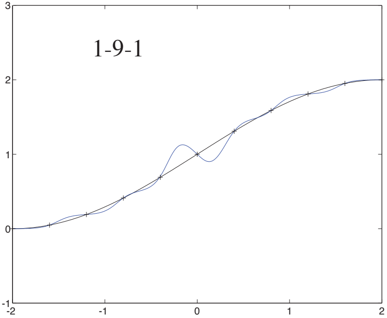




$$\{\mathbf{p}_1, \mathbf{t}_1\}, \{\mathbf{p}_2, \mathbf{t}_2\}, \dots, \{\mathbf{p}_Q, \mathbf{t}_Q\}$$

$$g(\;) = 1 + \sin\left(\frac{\pi}{4} p\right) \qquad p = -2, -1.6, -1.2, \dots, 1.6, 2$$



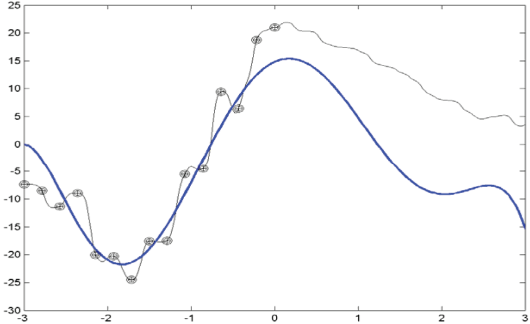


- A cat that once sat on a hot stove will never again sit on a hot stove or on a cold one either.

Mark Twain

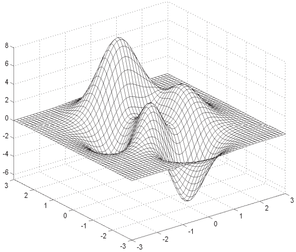
- The network input-output mapping is accurate for the training data and for test data never seen before.
- The network interpolates well.
- Poor generalization is caused by using a network that is too complex (too many neurons/parameters). To have the best performance we need to find the least complex network that can represent the data (Ockham's Razor).
- Find the simplest model that explains the data.

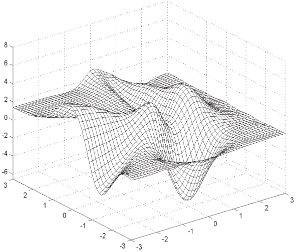
Overfitting Extrapolation



Interpolation

Extrapolation in 3-D





- Part of the available data is set aside during the training process.
- After training, the network error on the test set is used as a measure of generalization ability.
- The test set must never be used in any way to train the network, or even to select one network from a group of candidate networks.
- The test set must be representative of all situations for which the network will be used.

Methods for Improving Generalization

- Pruning (removing neurons) until the performance is degraded.
- Growing (adding neurons) until the performance is adequate.
- Validation Methods
- Regularization

Early Stopping

- Break up data into training, validation, and test sets.
- Use only the training set to compute gradients and determine weight updates.
- Compute the performance on the validation set at each iteration of training.
- Stop training when the performance on the validation set goes up for a specified number of iterations.
- Use the weights which achieved the lowest error on the validation set.

Early Stopping Example