Introduction to Neural Networks

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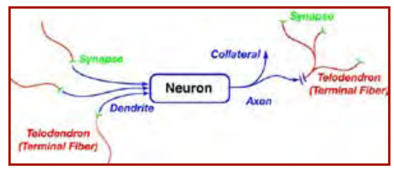
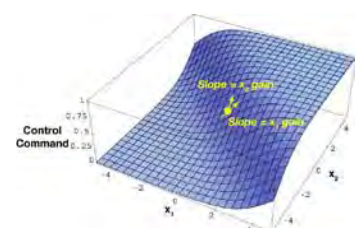
Robotics and Intelligent Systems, MAE 345, Princeton University, 2015

Learning Objectives

- Natural and artificial neurons
- Natural and computational neural networks
  - Linear network
  - Perceptron
  - Sigmoid network
  - Radial basis function
- Applications of neural networks
- Supervised training
  - Left pseudoinverse
  - Steepest descent
  - Back-propagation



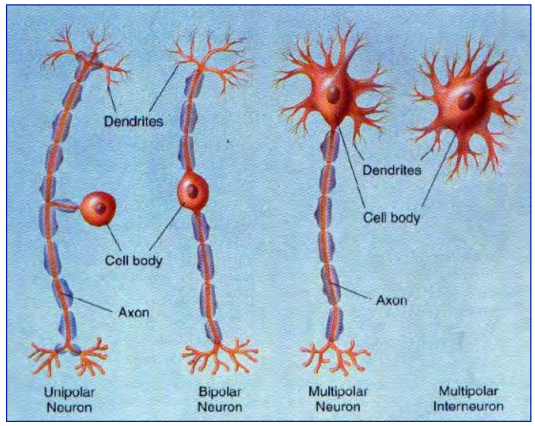
Applications of Computational Neural Networks



- Classification of data sets
- Nonlinear function approximation
  - Efficient data storage and retrieval
  - System identification
- Nonlinear and adaptive control systems

Neurons

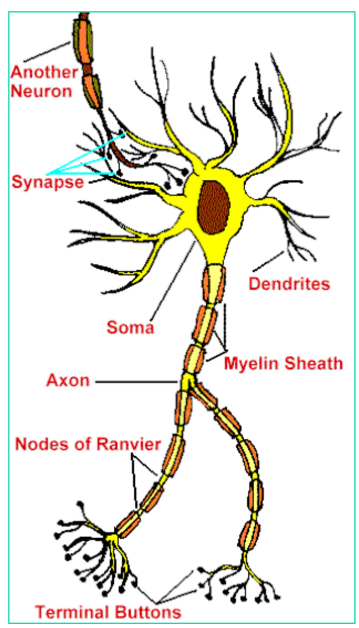
- Biological cells with significant electrochemical activity
- ~10-100 billion neurons in the brain
- Inputs from thousands of other neurons
- Output is scalar, but may have thousands of branches



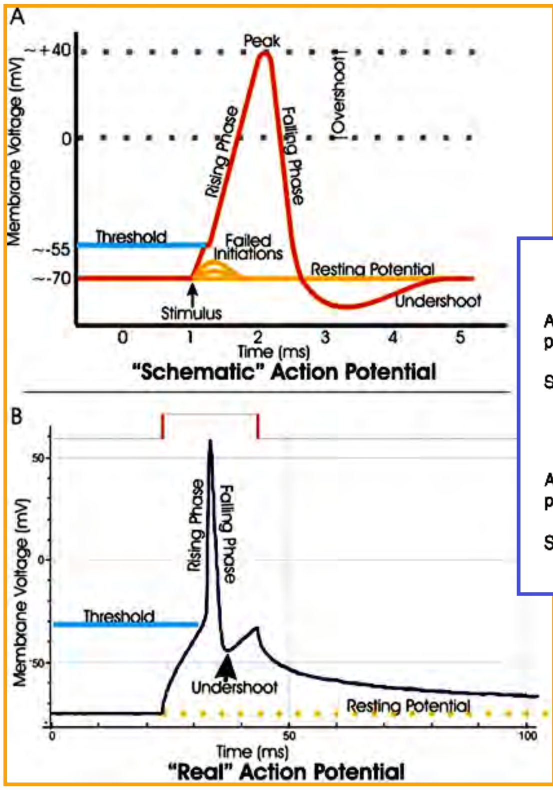
- Afferent (sensor) neurons send signals from organs and the periphery to the central nervous system
- Efferent (motor) neurons issue commands from the CNS to effector (e.g., muscle) cells
- Interneurons send signals between neurons in the central nervous system
- Signals are ionic, i.e., chemical (neurotransmitter atoms and molecules) and electrical (charge)

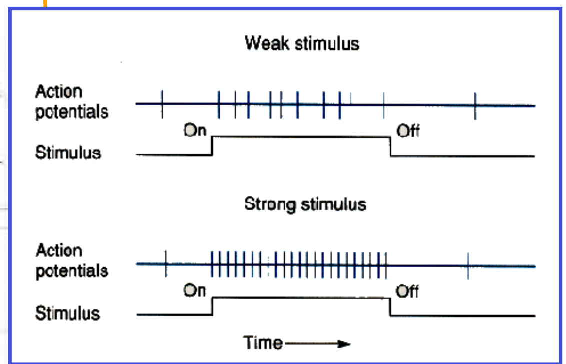
Activation Input to Soma Causes Change in Output Potential

- Stimulus from
  - Receptors
  - Other neurons
  - Muscle cells
  - Pacemakers (c.g. cardiac sino-atrial node)
- When membrane potential of neuronal cell exceeds a threshold
  - Cell is polarized
  - Action potential pulse is transmitted from the cell
  - Activity measured by amplitude and firing frequency of pulses
  - Saltatory conduction along axon
    - Myelin Schwann cells insulate axon
    - Signal boosted at Nodes of Ranvier
- Cell depolarizes and potential returns to rest



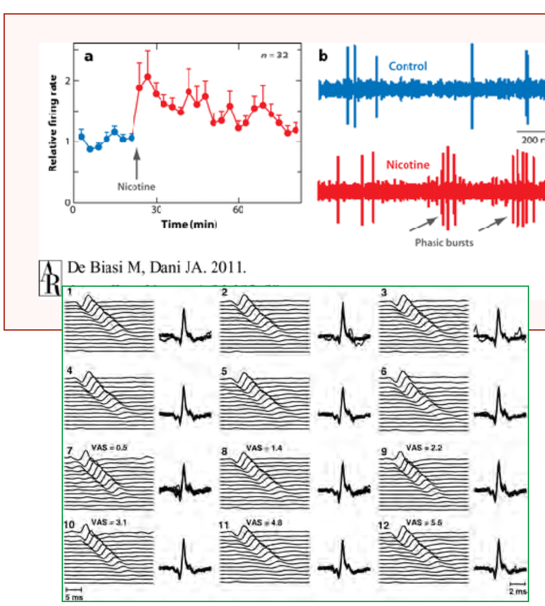
Neural Action Potential

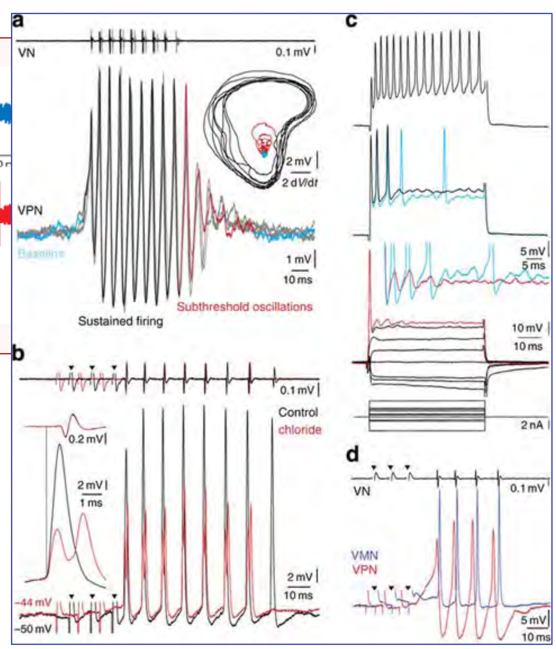




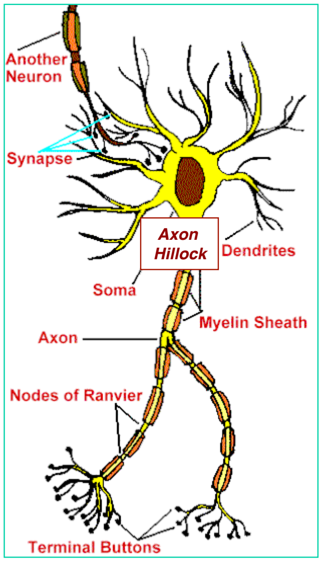
- **Maximum Firing Rate**: 500/sec
- **Refractory Period**: Minimum time increment between action potential firing ~ 1-2 msec

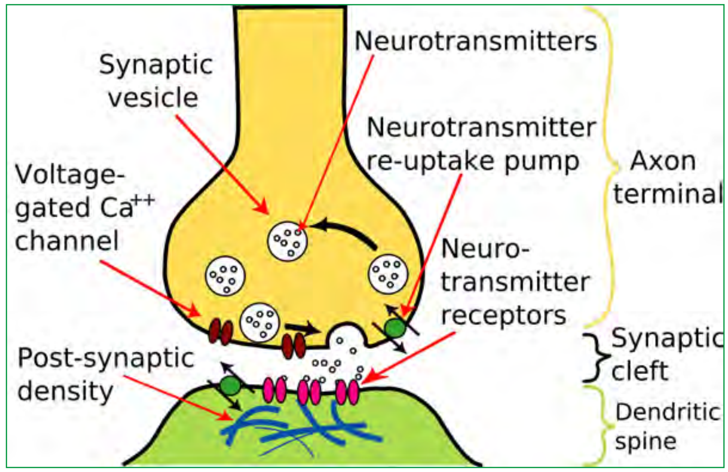
Some Recorded Action Potential Pulse Trains





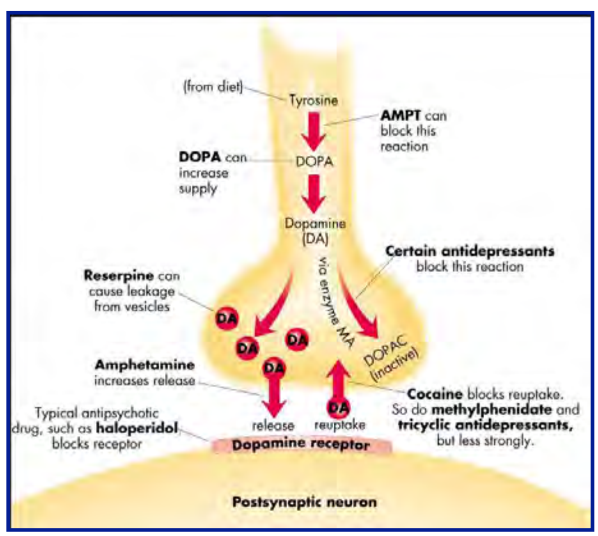
Electrochemical Signaling at Axon Hillock and Synapse



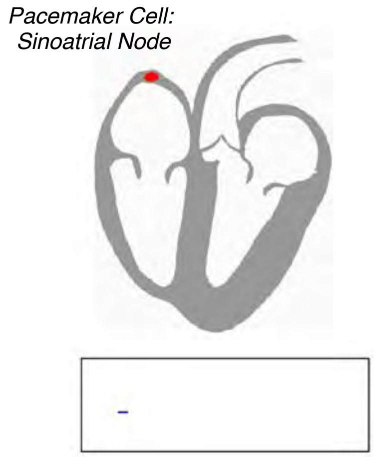


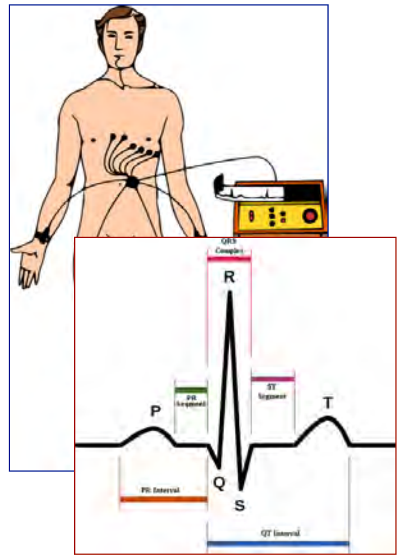
Synaptic Strength Can Be Increased or Decreased by Externalities

- **Synapses: learning elements of the nervous system**
  - **Action potentials enhanced or inhibited**
  - **Chemicals can modify signal transfer**
  - **Potentiation of pre- and post-synaptic cells**
- **Adaptation/Learning (potentiation)**
  - **Short-term**
  - **Long-term**

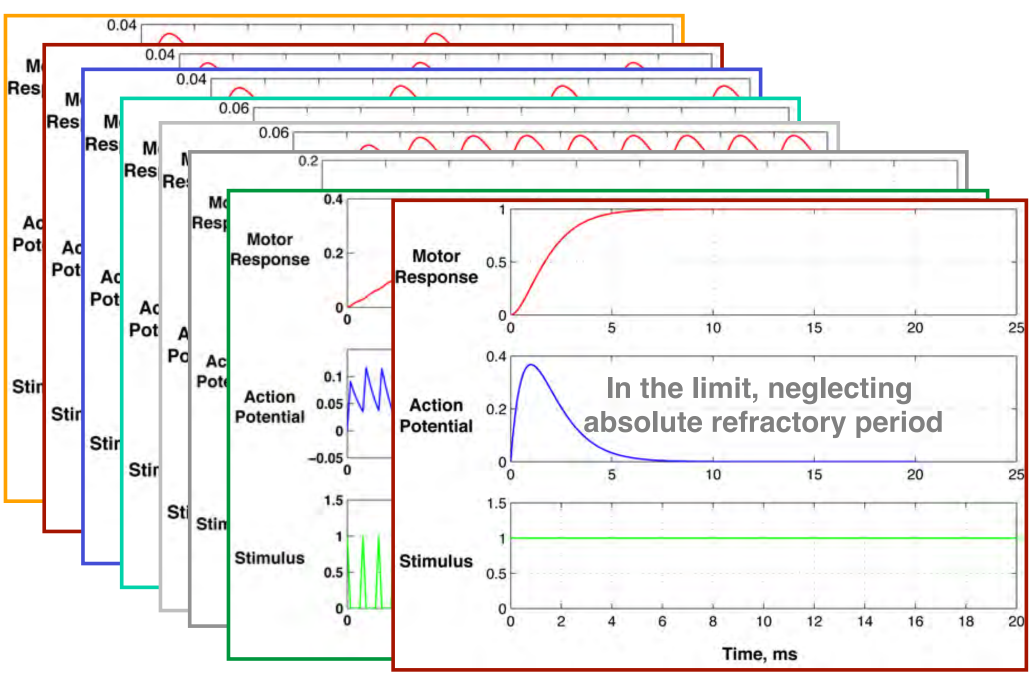


Cardiac Pacemaker and EKG Signals

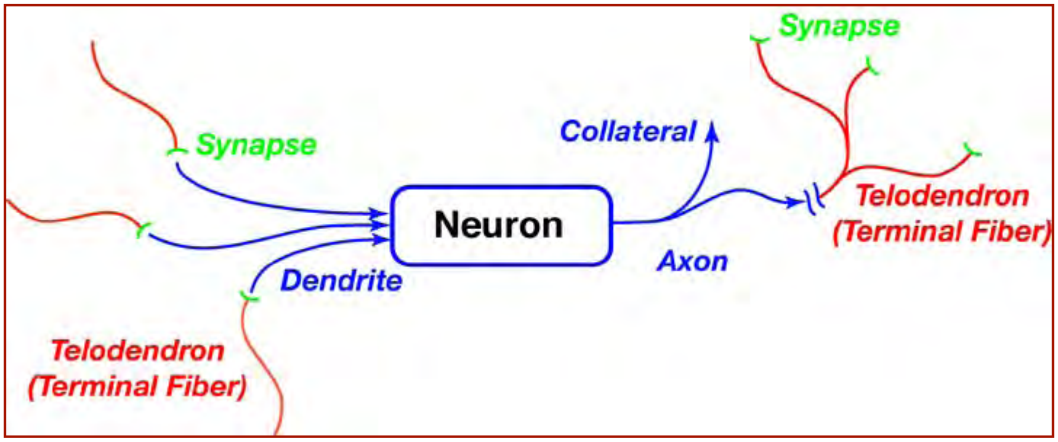




Impulse, Pulse-Train, and Step Response of a LTI 2nd-Order Neural Model



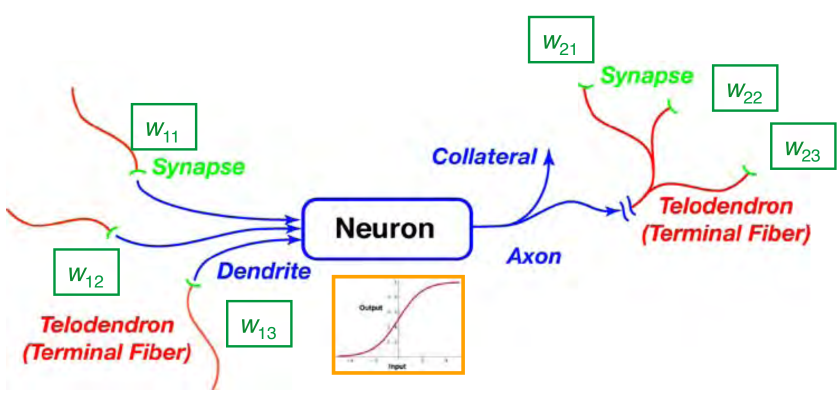
Multipolar Neuron



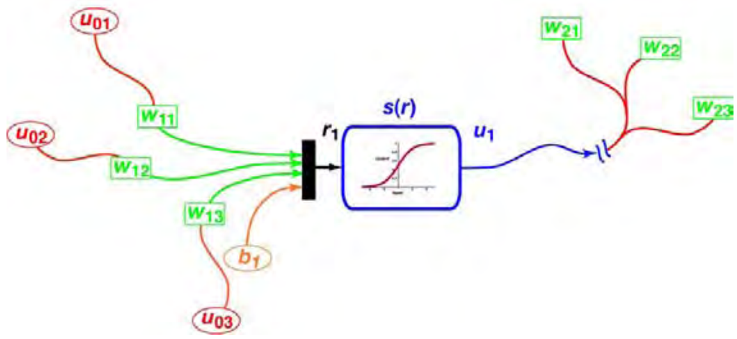
Mathematical Model of Neuron Components

Synapse effects represented by weights (gains or multipliers)

Neuron firing frequency is modeled by linear gain or nonlinear element



The Neuron Function

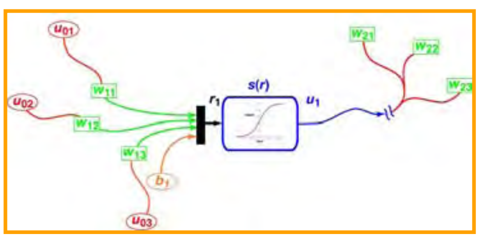


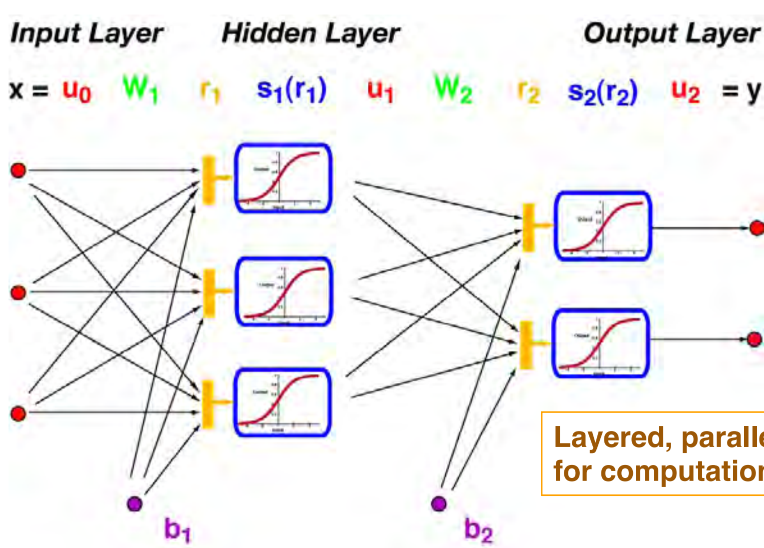
- Vector input, **u**, to a single neuron
  - Sensory input or output from upstream neurons
  - Linear operation produces scalar, r
  - Add bias, b, for zero adjustment
- Scalar output, u, of a single neuron (or node)
  - Scalar linear or nonlinear operation, $s(r)$

$$r = \mathbf{w}^T\mathbf{u} + b$$

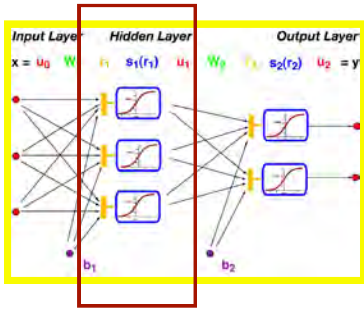
$$u = s(r)$$

Layout of a Neural Network





Layered, parallel structure for computation

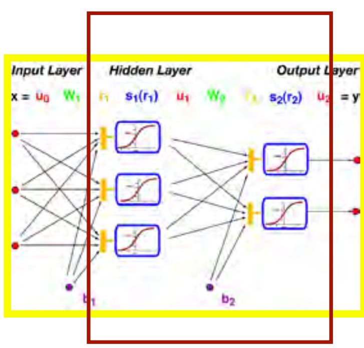


Input-Output Characteristics of a Neural Network Layer

- **Single layer**
  - Number of inputs = *n*
    - dim(u) = (*n* x 1)
  - Number of nodes = *m*
    - dim(r) = dim(b) = dim(s) = (*m* x 1)

$$\mathbf{r} = \mathbf{W}\mathbf{u} + \mathbf{b}$$
$$\mathbf{u} = \mathbf{s}(\mathbf{r})$$

$$\mathbf{W} = \begin{bmatrix} \mathbf{w}_1^T \\ \mathbf{w}_2^T \\ \\ \mathbf{w}_n^T \end{bmatrix}$$



Two-Layer Network

- **Two layers**
  - Number of nodes in each layer need not be the same
  - Node functions may be different, e.g.,
    - Sigmoid hidden layer
    - Linear output layer

$$\begin{aligned}
\mathbf{y} &= \mathbf{u}_2 \\
&= \mathbf{s}_2(\mathbf{r}_2) = \mathbf{s}_2(\mathbf{W}_2\mathbf{u}_1 + \mathbf{b}_2) \\
&= \mathbf{s}_2\left[\mathbf{W}_2\ \mathbf{s}_1(\mathbf{r}_1) + \mathbf{b}_2\right] \\
&= \mathbf{s}_2\left[\mathbf{W}_2\ \mathbf{s}_1(\mathbf{W}_1\mathbf{u}_0 + \mathbf{b}_1) + \mathbf{b}_2\right] \\
&= \mathbf{s}_2\left[\mathbf{W}_2\ \mathbf{s}_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2\right]
\end{aligned}$$

Is a Neural Network Serial or Parallel?

3^{rd}-degree power series

4 coefficients

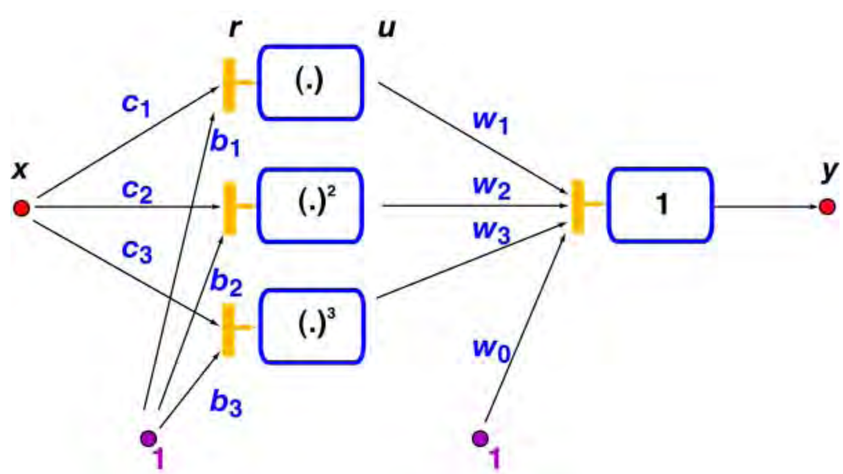
Express as a neural network?

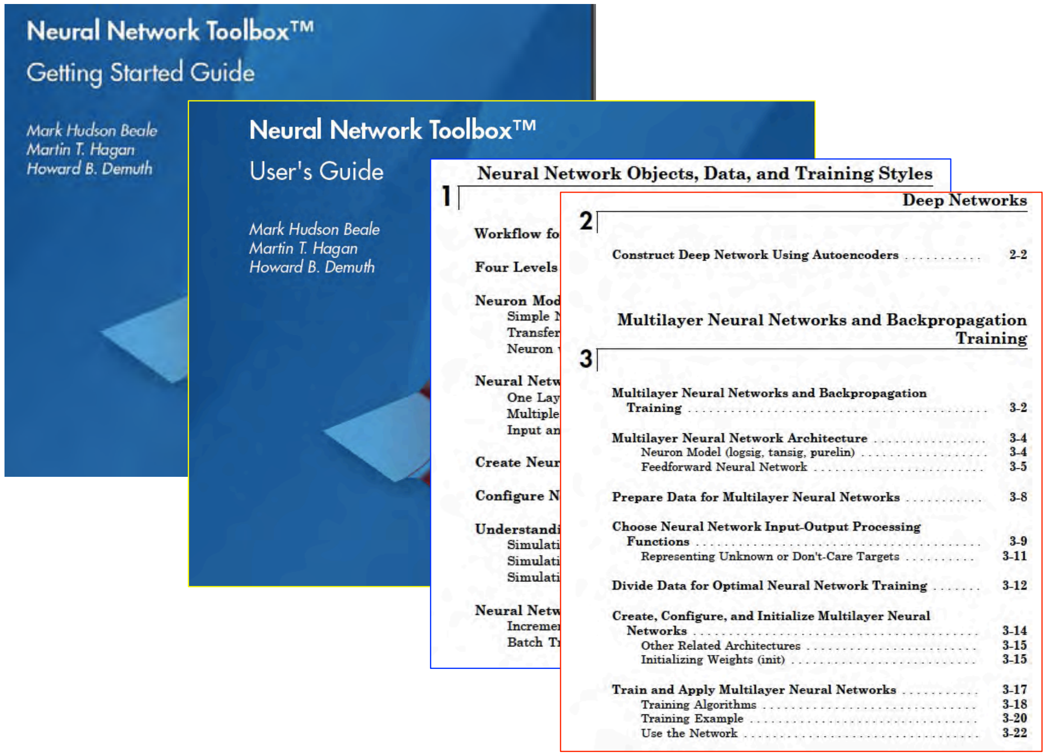
$$
\begin{aligned}
y &= a_0 + a_1 x + a_2 x^2 + a_3 x^3 \\
&= a_0' + a_1' r + a_2' r^2 + a_3' r^3 \\
&= a_0' + a_1'\left(c_1 x + b_1\right) + a_2'\left(c_1 x + b_2\right)^2 + a_3'\left(c_1 x + b_3\right)^3
\end{aligned}
$$

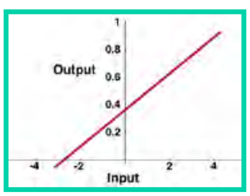
$$= w_0 + w_1 s_1(u) + w_2 s_2(u) + w_3 s_3(u)$$

Is a Neural Network Serial or Parallel?

Power series is serial, but it can be expressed as a parallel neural network (with dissimilar nodes)

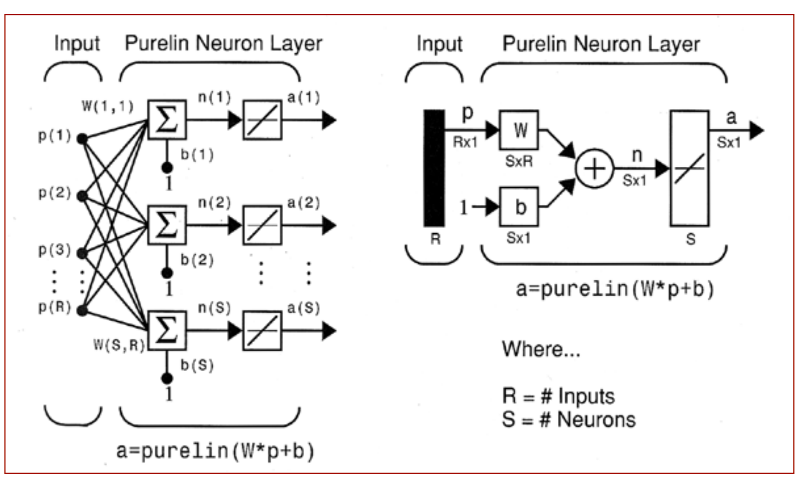






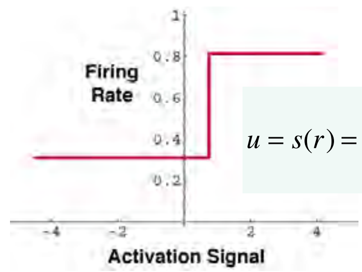
Linear Neural Network

- Outputs provide linear scaling of inputs
- Equivalent to matrix transformation of a vector, y = Wx + b
- Therefore, linear network is easy to train (left pseudoinverse)
- MATLAB symbology



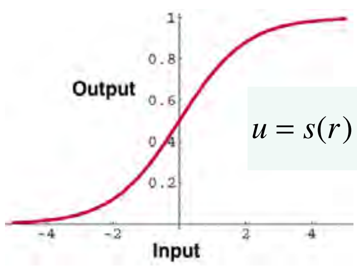
Idealizations of Nonlinear Neuron Input-Output Characteristic

Step function ("Perceptron")



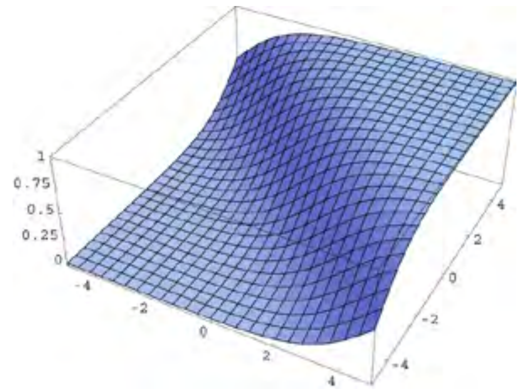
$$u = s(r) = \begin{cases} 1, & r > 0 \\ 0, & r \le 0 \end{cases}$$

Logistic sigmoid function



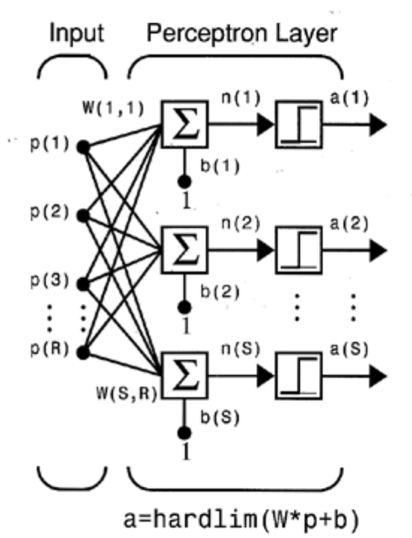
$$u = s(r) = \frac{1}{1 + e^{-r}}$$

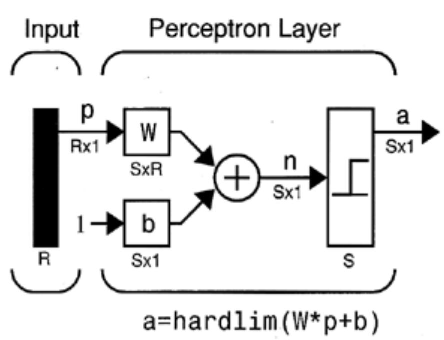
Sigmoid with two inputs, one output



$$u = s(r) = \frac{1}{1 + e^{-(w_1 r_1 + w_2 r_2 + b)}}$$

Perceptron Neural Network





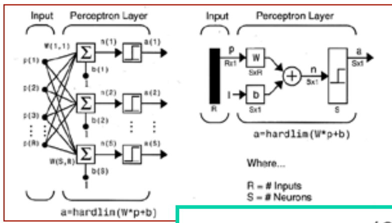
Where...

R = # Inputs
S = # Neurons

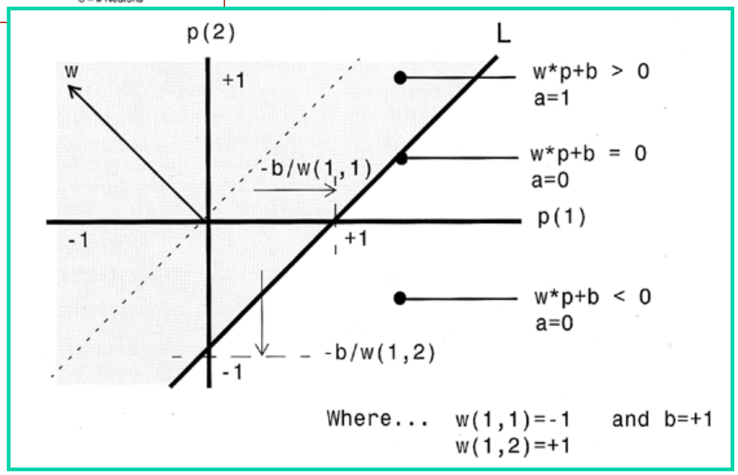
Each node is a step function

Weighted sum of features is fed to each node

Each node produces a linear classification of the input space



Perceptron Neural Network



Weights adjust slopes

Biases adjust zero crossing points

Single-Layer, Single-Node Perceptron Discriminants

$$u = s(\mathbf{w}^T\mathbf{x} + b) = \begin{cases} 1, & (\mathbf{w}^T\mathbf{x} + b) > 0 \\ 0, & (\mathbf{w}^T\mathbf{x} + b) \le 0 \end{cases}$$

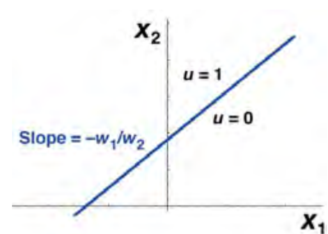
Two inputs, single step function

Discriminant

$$w_1x_1 + w_2x_2 + b = 0$$

$$or \quad x_2 = \frac{-1}{w_2}(w_1x_1 + b)$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



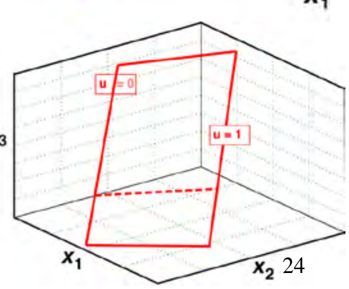
Three inputs, single step function

Discriminant

$$w_1x_1 + w_2x_2 + w_3x_3 + b = 0$$

$$or \quad x_3 = \frac{-1}{w_3}(w_1x_1 + w_2x_2 + b)$$

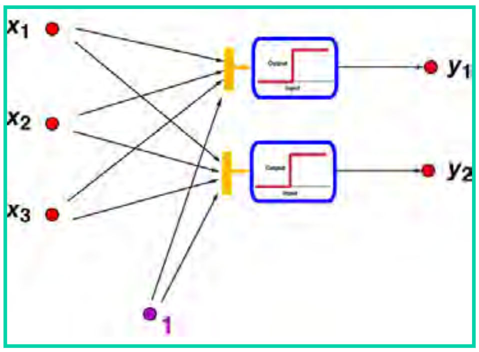
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

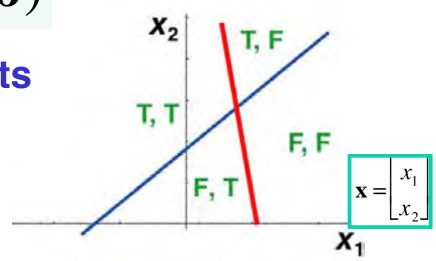


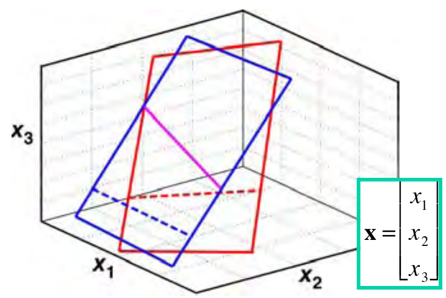
Single-Layer, Multi-Node Perceptron Discriminants

$$\mathbf{u} = \mathbf{s}(\mathbf{W}\mathbf{x} + \mathbf{b})$$

- Multiple inputs, nodes, and outputs
  - More inputs lead to more dimensions in discriminants
  - More outputs lead to more discriminants





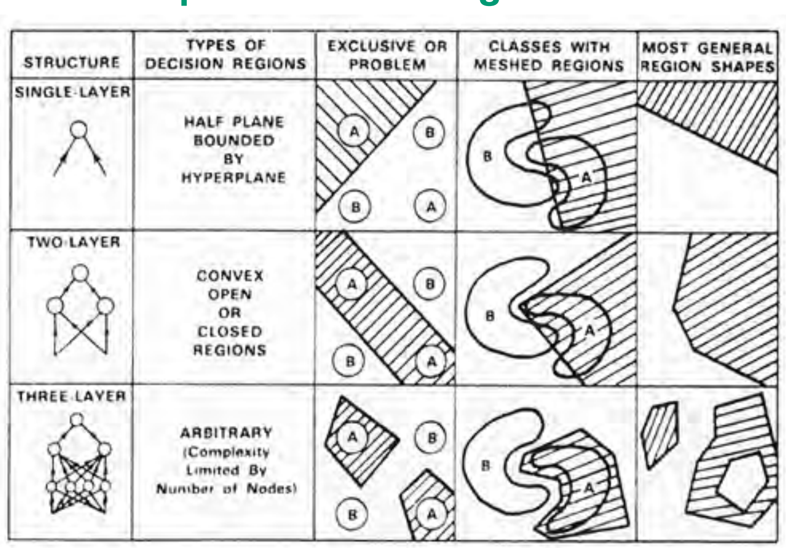


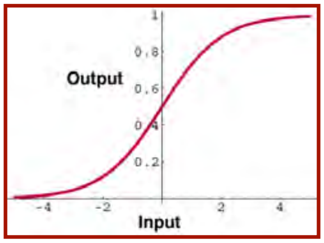
Multi-Layer Perceptrons Can Classify With Boundaries or Clusters

Classification capability of multi-layer perceptrons

Classifications of classifications

Open or closed regions





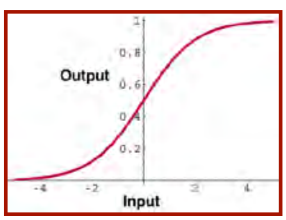
Sigmoid Activation Functions

- **Alternative sigmoid functions**
  - Logistic function: 0 to 1
  - Hyperbolic tangent: –1 to 1
  - Augmented ratio of squares: 0 to 1
- **Smooth nonlinear functions**

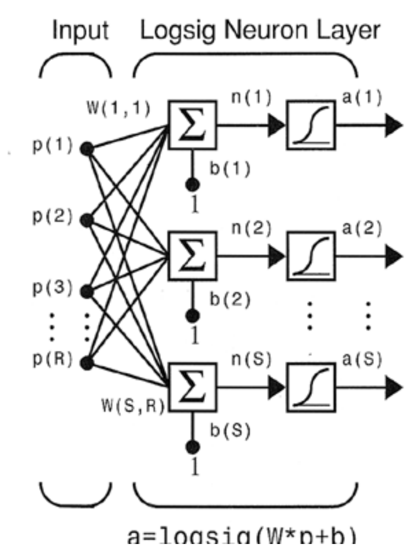
$$u = s(r) = \frac{1}{1+e^{-r}}$$

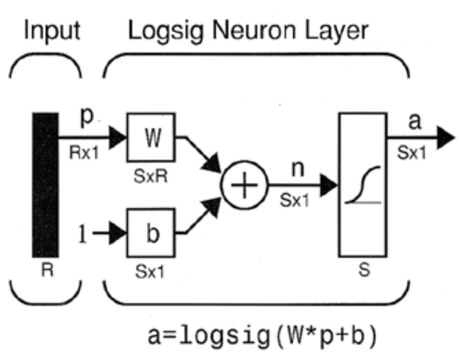
$$u = s(r) = \tanh r = \frac{1-e^{-2r}}{1+e^{-2r}}$$

$$u = s(r) = \frac{r^2}{1+r^2}$$



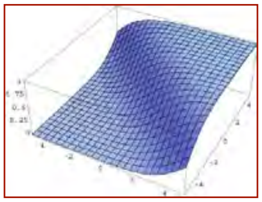
Sigmoid Neural Network





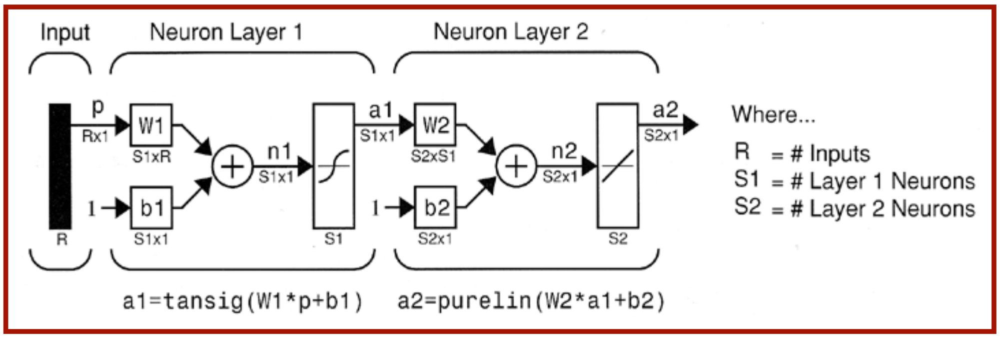
Where...

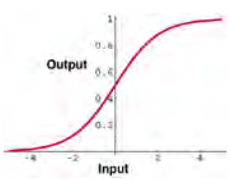
R = # Inputs
S = # Neurons



Single Sigmoid Layer is Sufficient …

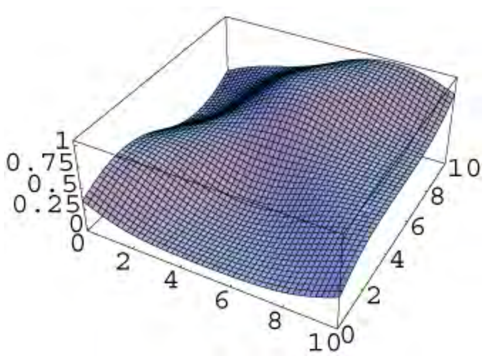
- **Sigmoid network with single hidden layer can approximate any continuous function**
- **Additional sigmoid layers not needed to characterize simple functions**
- **Typical sigmoid network contains**
  - **Single sigmoid hidden layer (nonlinear fit)**
  - **Single linear output layer (scaling)**

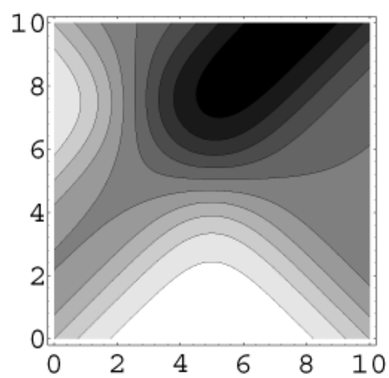




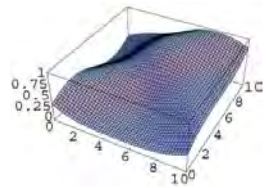
Typical Sigmoid Neural Network Output

Classification is not limited to linear discriminants



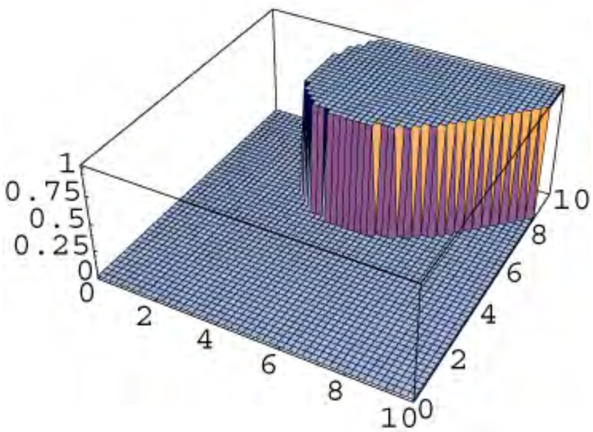


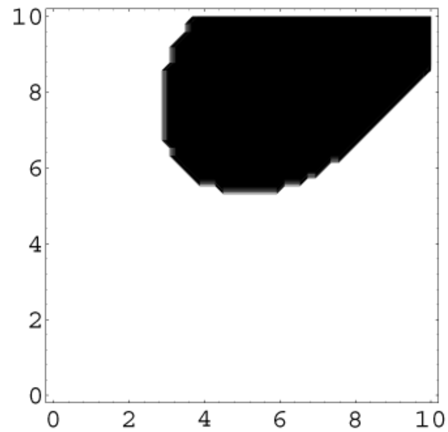
Sigmoid network can approximate a continuous nonlinear function to arbitrary accuracy with a single hidden layer



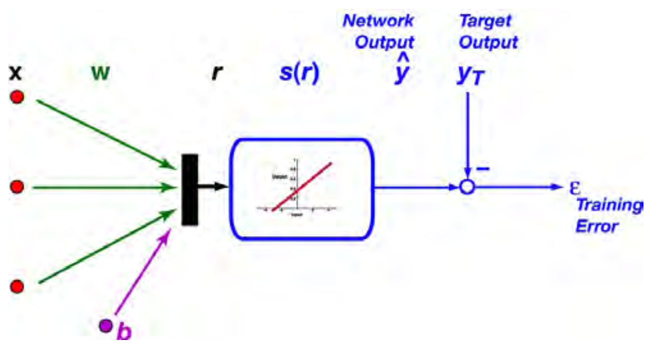
Thresholded Neural Network Output

Threshold gives "yes/no" output





Training Error and Cost for a Single Linear Neuron



$$\hat{y} = r = \hat{\mathbf{w}}^T \mathbf{x} + \hat{b}$$

- **Training error: difference between network output and target output**
- **Quadratic error cost**

$$\varepsilon = \hat{y} - y_T$$

$$J = \frac{1}{2}\varepsilon^2 = \frac{1}{2}\left(\hat{y} - y_T\right)^2 = \frac{1}{2}\left(\hat{y}^2 - 2\hat{y}\,y_T + y_T^{\,2}\right)$$

Linear Neuron Gradient

$$\hat{y} = r = \mathbf{w}^T \mathbf{x} + b$$
$$\frac{d\hat{y}}{dr} = 1$$

$$\varepsilon = \hat{y} - y_T$$
$$J = \frac{1}{2}\varepsilon^2 = \frac{1}{2}\left(\hat{y} - y_T\right)^2 = \frac{1}{2}\left(\hat{y}^2 - 2\hat{y}\,y_T + {y_T}^2\right)$$

- **Training (control) parameter, p**
  - **Input weights, w (n x 1)**
  - **Bias, b (1 x 1)**

$$\mathbf{p} = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix} = \begin{bmatrix} p_1 \\ p_2 \\ \ldots \\ p_{n+1} \end{bmatrix}$$

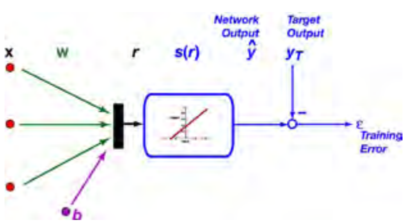
- **Optimality condition** $\dfrac{\partial J}{\partial \mathbf{p}} = \mathbf{0}$

- **Gradient**

$$\frac{\partial J}{\partial \mathbf{p}} = \left(\hat{y} - y_T\right)\frac{\partial y}{\partial \mathbf{p}} = \left(\hat{y} - y_T\right)\frac{\partial y}{\partial r}\frac{\partial r}{\partial \mathbf{p}}$$

$$\text{where}$$

$$\frac{\partial r}{\partial \mathbf{p}} = \begin{bmatrix} \dfrac{\partial r}{\partial p_1} & \dfrac{\partial r}{\partial p_2} & \ldots & \dfrac{\partial r}{\partial p_{n+1}} \end{bmatrix} = \frac{\partial\left(\mathbf{w}^T\mathbf{x} + b\right)}{\partial \mathbf{p}} = \begin{bmatrix} \mathbf{x}^T & 1 \end{bmatrix}$$



Steepest-Descent Learning for a Single Linear Neuron

Gradient

$$\frac{\partial J}{\partial \mathbf{p}} = \left(\hat{y} - y_T\right)\begin{bmatrix} \mathbf{x}^T & 1 \end{bmatrix} = \left[\left(\mathbf{w}^T\mathbf{x} + b\right) - y_T\right]\begin{bmatrix} \mathbf{x}^T & 1 \end{bmatrix}$$

Steepest-descent algorithm

$\eta =$ learning rate
$k =$ iteration index(epoch)

$$\mathbf{p}_{k+1} = \mathbf{p}_k - \eta\left(\frac{\partial J}{\partial \mathbf{p}}\right)_k^T = \mathbf{p}_k - \eta\left(\hat{y}_k - y_{T_k}\right)\begin{bmatrix} \mathbf{x}_k \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_k - \eta\left[\left(\mathbf{w}_k^T\mathbf{x}_k + b_k\right) - y_{T_k}\right]\begin{bmatrix} \mathbf{x}_k \\ 1 \end{bmatrix}$$

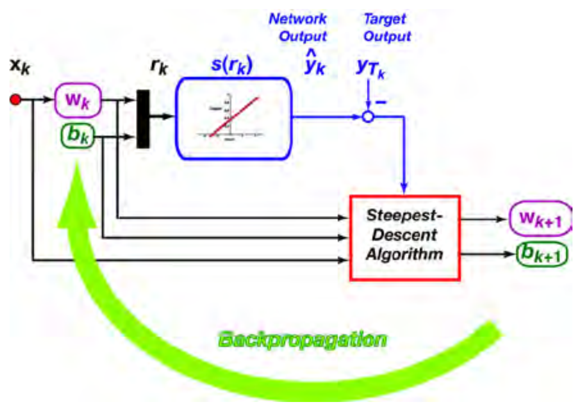
Backpropagation for a Single Linear Neuron

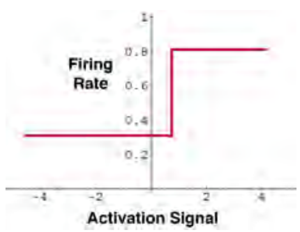
- **Training set** (n members)
  - Target outputs, $\mathbf{y}_T$ (1 x n)
  - Feature set, **X** (m x n)

$$\begin{bmatrix} \mathbf{y}_T \\ \mathbf{X} \end{bmatrix} = \begin{bmatrix} \mathbf{y}_{T_1} & \mathbf{y}_{T_2} & \cdots & \mathbf{y}_{T_n} \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \end{bmatrix}$$

- **Initialize w and *b***
  - Random set
  - Prior training result
- **Estimate w and *b* recursively**
  - Off line (random or repetitive sequence)
  - On line (measured training features and target)
- … until $\partial J/\partial \mathbf{p} \sim 0$

$$\begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_k - \eta\left[\left(\mathbf{w}_k^T\mathbf{x}_k + b_k\right) - y_{T_k}\right]\begin{bmatrix} \mathbf{x}_k \\ 1 \end{bmatrix}$$





Steepest-Descent Algorithm for a Single-Step Perceptron

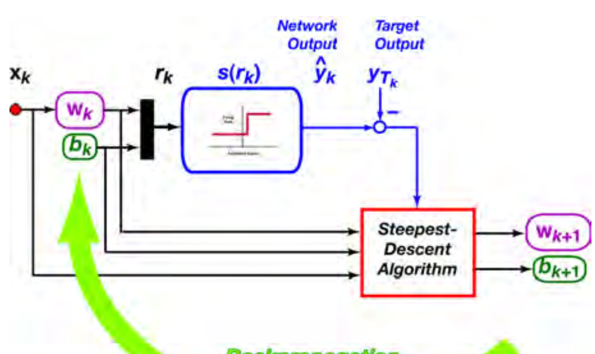
- **Neuron output is discontinuous**

$$y = s(r) = \begin{cases} 1, & r > 0 \\ 0, & r \le 0 \end{cases}$$

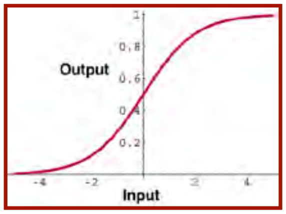
- **Binary target output**
  - y_T = 0 or 1, for classification

$$\left(\hat{y}_k - y_{T_k}\right) = \begin{cases} 1, & y_k = 1,\ \ y_{T_k} = 0 \\ 0, & y_k = y_{T_k} \\ -1, & y_k = 0,\ \ y_{T_k} = 1 \end{cases}$$

$$\begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_k - \eta\left[\hat{y}_k - y_{T_k}\right]\begin{bmatrix} \mathbf{x}_k \\ 1 \end{bmatrix}$$



$$\begin{bmatrix} \mathbf{y}_T \\ \mathbf{X} \end{bmatrix} = \begin{bmatrix} \mathbf{y}_{T_1} & \mathbf{y}_{T_2} & \cdots & \mathbf{y}_{T_n} \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \end{bmatrix}$$



Training Variables for a Single Sigmoid Neuron

Input-output characteristic and 1st derivative

$$y = s(r) = \frac{1}{1+e^{-r}}$$

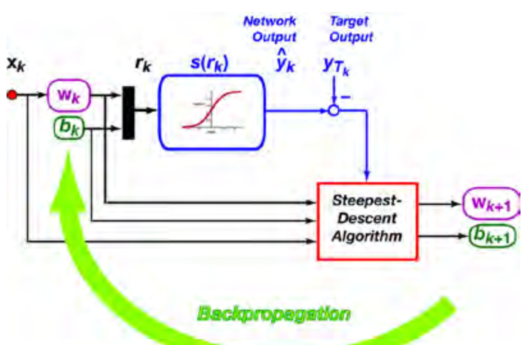
$$\frac{dy}{dr} = \frac{ds(r)}{dr} = \frac{e^{-r}}{\left(1+e^{-r}\right)^2} = e^{-r}s^2(r)$$
$$= \left[\left(1+e^{-r}\right)-1\right]s^2(r) = \left(\frac{1}{s(r)}-1\right)s^2(r)$$
$$= \left[\frac{1-s(r)}{s(r)}\right]s^2(r) = \left[1-s(r)\right]s(r) = (1-y)y$$

Training error and quadratic error cost

$$\varepsilon = \hat{y} - y_T$$
$$J = \frac{1}{2}\varepsilon^2 = \frac{1}{2}\left(\hat{y}-y_T\right)^2 = \frac{1}{2}\left(\hat{y}^2 - 2\hat{y}y_T + y_T{}^2\right)$$

Control parameter

$$\mathbf{p} = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix} = \begin{bmatrix} p_1 \\ p_2 \\ \dots \\ p_{n+1} \end{bmatrix}$$



Training a Single Sigmoid Neuron

$$\frac{\partial J}{\partial \mathbf{p}} = \left(\hat{y}-y_T\right)\frac{\partial y}{\partial \mathbf{p}} = \left(\hat{y}-y_T\right)\frac{\partial \hat{y}}{\partial r}\frac{\partial r}{\partial \mathbf{p}}$$

where

$$r = \mathbf{w}^T\mathbf{x} + b$$
$$\frac{d\hat{y}}{dr} = (1-\hat{y})\hat{y}$$
$$\frac{\partial r}{\partial \mathbf{p}} = \begin{bmatrix} \mathbf{x}^T & 1 \end{bmatrix}$$

$$\frac{\partial J}{\partial \mathbf{p}} = \left(\hat{y}-y_T\right)\left(1-\hat{y}\right)\hat{y}\begin{bmatrix} \mathbf{x}^T & 1 \end{bmatrix}$$

$$\mathbf{p}_{k+1} = \mathbf{p}_k - \eta\left(\frac{\partial J}{\partial \mathbf{p}}\right)_k^T$$

or

$$\begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_k - \eta\left(\hat{y}_k - y_T\right)\left(1-\hat{y}\right)\hat{y}_k\begin{bmatrix} \mathbf{x}_k \\ 1 \end{bmatrix}$$

See Supplemental Material for training multiple sigmoids

MATLAB Network Training Algorithms

```
Backpropagation training functions that use Jacobian derivatives

  These algorithms can be faster but require more memory than gradient
  backpropation.  They are also not supported on GPU hardware.

  trainlm    - Levenberg-Marquardt backpropagation.
  trainbr    - Bayesian Regulation backpropagation.

Backpropagation training functions that use gradient derivatives

  These algorithms may not be as fast as Jacobian backpropagation.
  They are supported on GPU hardware with the Parallel Computing Toolbox.

  trainbfg   - BFGS quasi-Newton backpropagation.
  traincgb   - Conjugate gradient backpropagation with Powell-Beale restarts.
  traincgf   - Conjugate gradient backpropagation with Fletcher-Reeves updates.
  traincgp   - Conjugate gradient backpropagation with Polak-Ribiere updates.
  traingd    - Gradient descent backpropagation.
  traingda   - Gradient descent with adaptive lr backpropagation.
  traingdm   - Gradient descent with momentum.
  traingdx   - Gradient descent w/momentum & adaptive lr backpropagation.
  trainoss   - One step secant backpropagation.
  trainrp    - RPROP backpropagation.
  trainscg   - Scaled conjugate gradient backpropagation.

Supervised weight/bias training functions

  trainb     - Batch training with weight & bias learning rules.
  trainc     - Cyclical order weight/bias training.
  trainr     - Random order weight/bias training.
  trains     - Sequential order weight/bias training.

Unsupervised weight/bias training functions

  trainbu    - Unsupervised batch training with weight & bias learning rules.
  trainru    - Unsupervised random order weight/bias training.
```

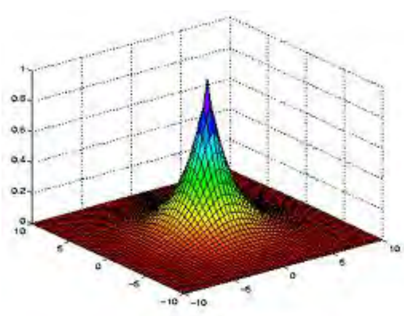

Radial Basis Function

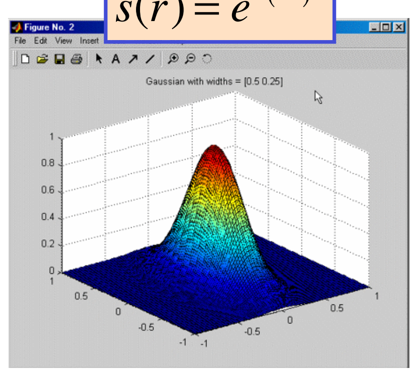
Unimodal, axially symmetric function, e.g., exponential

$$s(r) = e^{-|ar|^n}, \quad r = \sqrt{\left(\mathbf{x} - \mathbf{x}_{center}\right)^T \left(\mathbf{x} - \mathbf{x}_{center}\right)}$$

$$s(r) = e^{-|ar|}$$

$$s(r) = e^{-(ar)^2}$$

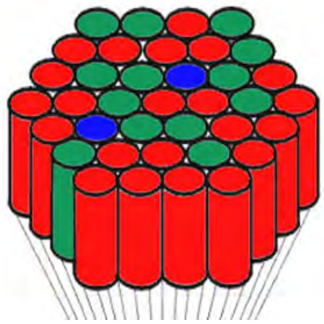


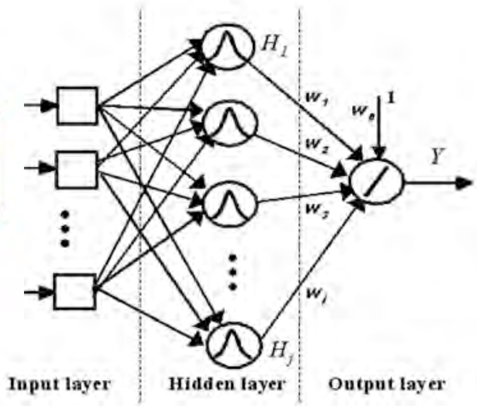


Mimics stimulus field of a neuron receptor

Radial Basis Function Network

Array of RBFs typically centered on a fixed grid





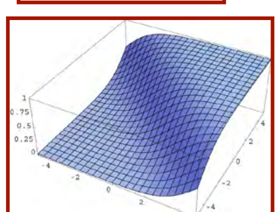
http://en.wikipedia.org/wiki/Radial_basis_function_network

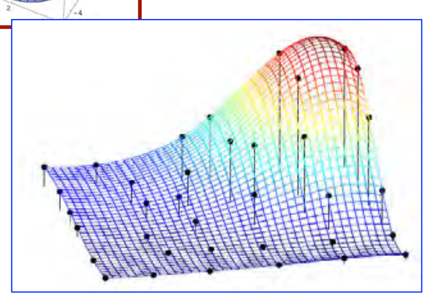
Sigmoid vs. Radial Basis Function Node

Sigmoid function | *Radial basis functions*

- **Considerations for selecting the basis function**
  - **Prior knowledge of surface to be approximated**
  - **Global vs. compact support**
  - **Number of neurons required**
  - **Training and untraining issues**

$$s(r) = \frac{1}{1+e^{-r}}$$

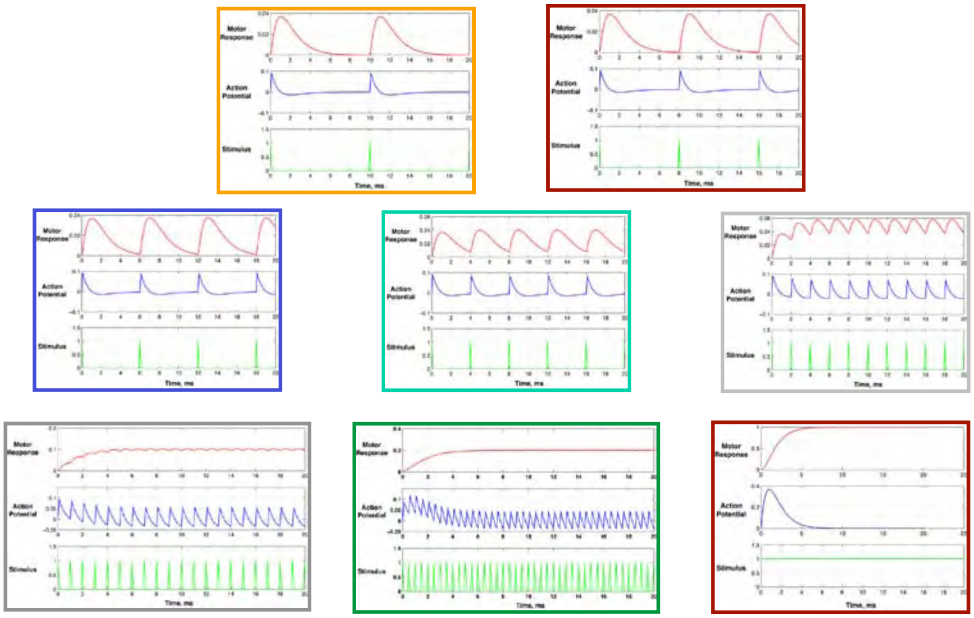




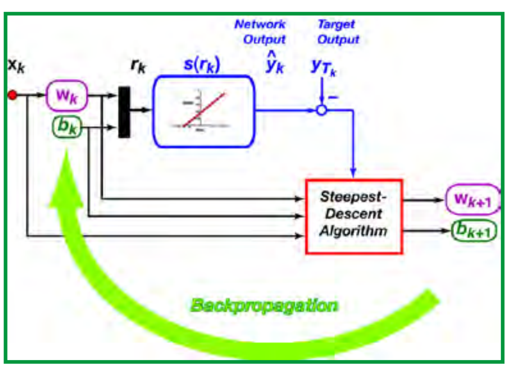
Next Time: Neural Networks

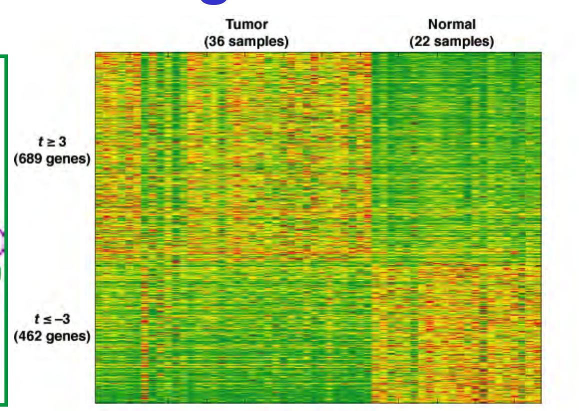
Supplementary Material

Impulse, Pulse-Train, and Step Response of a LTI 2nd-Order Neural Model



Microarray Training Set



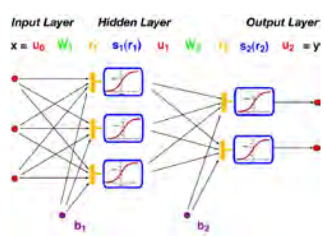


$$\begin{bmatrix} \textit{Identifier} \\ \mathbf{y}_T \\ \mathbf{X} \end{bmatrix} = \begin{bmatrix} \textit{Sample } 1 & \textit{Sample } 2 & \textit{Sample } 3 & \ldots & \textit{Sample } n-1 & \textit{Sample } n \\ \textit{Tumor} & \textit{Tumor} & \textit{Tumor} & \ldots & \textit{Normal} & \textit{Normal} \\ \textit{Gene A Level} & \textit{Gene A Level} & \textit{Gene A Level} & \ldots & \textit{Gene A Level} & \textit{Gene A Level} \\ \textit{Gene B Level} & \textit{Gene B Level} & \textit{Gene B Level} & \ldots & \textit{Gene B Level} & \textit{Gene B Level} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \textit{Gene m Level} & \textit{Gene m Level} & \textit{Gene m Level} & \ldots & \textit{Gene m Level} & \textit{Gene m Level} \end{bmatrix}$$

Microarray Training Data

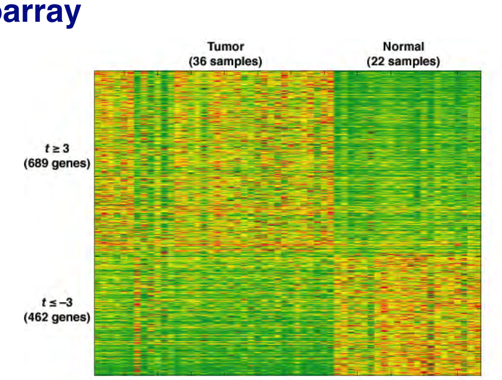
- **First row: Target classification**
- **2^{nd}-5^{th} rows: Up-regulated genes**
- **6^{th}-10^{th} rows: Down-regulated genes**

```
Lab Analysis of Tissue Samples
   Tumor    =[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 ...
              1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ...
              0 0 0 0 0 0 0 0];

Normalized Data: Up-Regulated in Tumor
   U22055  =   [138   68    93    62    30    81    121   7     82    24    -2    -48   38    ...
                82    118   55    103   102   87    62    69    14    101   25    47    48    75    ...
                59    62    116   54    96    90    130   70    75    74    35    149   97    21    ...
                14    -51   -3    -81   57    -4    16    28    -73   -4    45    -28   -9    -13   ...
                25    25    19    -21   3     19    34];
.........
Normalized Data: Up-Regulated in Normal
   M96839  =   [3     -23   3     12    -22   0     4     29    -73   32    5     -13   -16   14    ...
                2     24    18    19    9     -13   -20   -3    -22   6     -5    -12   9     28    ...
                20    -9    30    -15   18    1     -16   12    -9    3     -35   23    3     5     ...
                33    29    47    19    32    34    20    55    49    20    10    36    70    50    ...
                15    45    56    41    31    40];
```

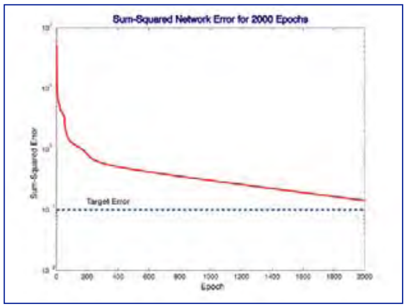
Neural Network Classification Example

- **~7000 genes expressed in 62 microarray samples**
  - **Tumor = 1**
  - **Normal = 0**
- **8 genes in strong feature set**
  - **4 with Mean Tumor/Normal > 20:1**
  - **4 with Mean Normal/Tumor > 20:1**
  - **and minimum variance within up-regulated set**



Dukes Stages: A -> B -> C -> D

Neural Network Training Results:
Tumor/Normal Classification, 8 Genes, 4 Nodes



- Training begins with a random set of weights
- Adjustable parameters
  - Learning rate
  - Target error
  - Maximum # of epochs
- Non-unique sets of trained weights

Binary network output (0,1) after rounding

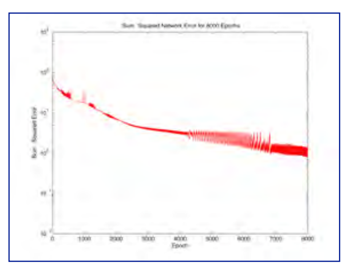
Zero classification errors

Classification =
Columns 1 through 13
1 1 1 1 1 1 1 1 1 1 1 1 1
Columns 14 through 26
1 1 1 1 1 1 1 1 1 1 1 1 1
Columns 27 through 39
1 1 1 1 1 1 1 1 1 1 1 1 1
Columns 40 through 52
1 0 0 0 0 0 0 0 0 0 0 0 0
Columns 53 through 62
0 0 0 0 0 0 0 0 0 0

Neural Network Training Results:
Tumor Stage/Normal Classification
8 Genes, 16 Nodes

- Colon cancer classification
  - 0 = Normal
  - 1 = Adenoma
  - 2 = A Tumor
  - 3 = B Tumor
  - 4 = C Tumor
  - 5 = D Tumor

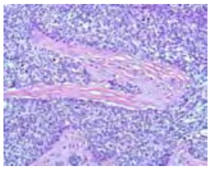
Scalar network output with varying magnitude



Target =
[2 1 3 3 3 3 3 3 3 3
3 3 3 3 3 3 3 3 3 3 4
4 4 4 4 4 4 4 4 5 5 5
5 5 5 5 5 1 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0]

One classification error

Classification =
Columns 1 through 13
2 1 3 3 3 3 3 3 3 3 3 3 3
Columns 14 through 26
3 3 3 3 3 3 3 4 4 $\boxed{5}$ 4 4 4
Columns 27 through 39
4 4 4 5 5 5 5 5 5 5 5 1 0
Columns 40 through 52
0 0 0 0 0 0 0 0 0 0 0 0 0
Columns 53 through 60
0 0 0 0 0 0 0 0



Ranking by EWS *t* Values (Top and Bottom 12)

- 24 transcripts selected from 12 highest and lowest *t* values for EWS vs. remainder

Image ID	Sort by EWS t Value Transcript Description	EWS t Value	BL t Value	NB t Value	RMS t Value
770394	Fc fragment of IgG, receptor, transporter, alpha	12.04	-6.67	-6.17	-4.79
1435862	antigen identified by monoclonal antibodies 12E7, F21 and O13	9.09	-6.75	-5.01	-4.03
377461	caveolin 1, caveolae protein, 22kD	8.82	-5.97	-4.91	-4.78
814260	follicular lymphoma variant translocation 1	8.17	-4.31	-4.70	-5.48
491565	Cbp/p300-interacting transactivator, with Glu/Asp-rich carboxy-terminal domain	7.60	-5.82	-2.62	-3.68
841641	cyclin D1 (PRAD1: parathyroid adenomatosis 1)	6.84	-9.93	0.56	-4.30
1471841	ATPase, Na+/K+ transporting, alpha 1 polypeptide	6.65	-3.56	-2.72	-4.69
866702	protein tyrosine phosphatase, non-receptor type 13	6.54	-4.99	-4.07	-4.84
713922	glutathione S-transferase M1	6.17	-5.61	-5.16	-1.97
308497	KIAA0467 protein	5.99	-6.69	-6.63	-1.11
770868	NGFI-A binding protein 2 (ERG1 binding protein 2)	5.93	-6.74	-3.88	-1.21
345232	lymphotoxin alpha (TNF superfamily, member 1)	5.61	-8.05	-2.49	-1.19
786084	chromobox homolog 1 (Drosophila HP1 beta)	-5.04	-1.05	9.65	-0.62
796258	sarcoglycan, alpha (50kD dystrophin-associated glycoprotein)	-5.04	-3.31	-3.86	6.83
431397		-5.04	2.64	2.19	0.64
825411	N-acetylglucosamine receptor 1 (thyroid)	-5.06	-1.45	5.79	0.76
859359	quinone oxidoreductase homolog	-5.23	-7.27	0.78	5.40
75254	cysteine and glycine-rich protein 2 (LIM domain only, smooth muscle)	-5.30	-4.11	2.20	3.68
448386		-5.38	-0.42	3.76	0.14
68950	cyclin E1	-5.80	0.03	-1.58	5.10
774502	protein tyrosine phosphatase, non-receptor type 12	-5.80	-5.56	3.76	3.66
842820	inducible poly(A)-binding protein	-6.14	0.60	0.66	3.80
214572	ESTs	-6.39	-0.08	-0.22	4.56
295985	ESTs	-9.26	-0.13	3.24	2.95

Repeated for BL vs. remainder, NB vs. remainder, and RMS vs. remainder

MATLAB Program for Neural Network Analysis with Leave-One-Out Validation - Initialization(1)

```
'Leave-One-Out Neural Network Analysis of Khan Data'

%   Neural Network with Vector Output
%   Based on 63 Samples of 8 Positive and Negative t-Value Metagenes

%   12/5/2007

    clear

    Target  =   [ones(1,23) zeros(1,40)
        zeros(1,23) ones(1,8) zeros(1,32)
        zeros(1,31) ones(1,12) zeros(1,20)
        zeros(1,43) ones(1,20)];

    TrainingData    =   [2.489          2.725     2.597     2.831   ...
        .....
        .....
        .....
        .....
        .....
        .....
        .....];
        .....
```

MATLAB Program for Neural Network Analysis with Leave-One-Out Validation - Initialization(2)

```
%   Validation Sample and Leave-One-Out Training Set

    MisClass    =   0;
    iSamLog     =   [];
    iRepLog     =   [];
    ErrorLog    =   [];
    OutputLog   =   [];
    SizeTarget  =   size(Target);
    SizeTD      =   size(TrainingData);

%   Preprocessing of Training Data

    [TrainingData,minp,maxp,tn,mint,maxt] =   premnmx(TrainingData,Target);
```

premnmx has been replaced by *mapminmax* in MATLAB

MATLAB Program for Neural Network Analysis with Leave-One-Out Validation - Initialization(3)

```
for iSam = 1:SizeTD(2)
        ValidSample             =   TrainingData(:,iSam);
        ReducedData             =   TrainingData;
        ReducedData(:,iSam)     =   [];
        ReducedTarget           =   Target;
        ReducedTarget(:,iSam)   =   [];
        Repeats                 =   2;
```

MATLAB Program for Neural Network Analysis with Leave-One-Out Validation - Training(1)

```
for i = 1:Repeats
            Range   =   minmax(ReducedData);
            Neurons =   [12,4];
            Nodes   =   {'logsig', 'purelin'};
            Beta    =   0.5;
            Epochs  =   200;
            Trainer =   'trainbr';

            Net     =   newff(Range,Neurons,Nodes,Trainer);

            Net.trainParam.show     =   100;
            Net.trainParam.lr       =   Beta;
            Net.trainParam.epochs   =   Epochs;
            Net.trainParam.goal     =   0.001;

            [Net,TrainingRecord]    =   train(Net,ReducedData,ReducedTarget);

            NetOutput   =   sim(Net, ReducedData);
            Rounded     =   round(NetOutput);
            Error       =   ReducedTarget - Rounded;ar
```

newff has been replaced by *netfit*

MATLAB Program for Neural Network Analysis with Leave-One-Out Validation - Training(2)

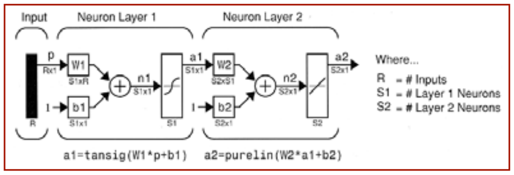
```
%           Validation with Single Sample

            NovelOutput     =   sim(Net,ValidSample);
            LengthNO        =   length(NovelOutput);
            NovelRounded    =   round(NovelOutput);
            NovelRounded    =   max(NovelRounded,zeros(LengthNO,1));
            NovelRounded    =   min(NovelRounded,ones(LengthNO,1));

%       If no actual output is greater than 0.5, choose the largest
%       for k = 1:SizeNO(2)

            if (isequal(NovelRounded,zeros(LengthNO,1)))
                [c,j]               =   max(NovelOutput);
                NovelRounded(j,1)   =   1;
            end

            AbsDiff         =   abs(NovelOutput - NovelRounded);-
```

MATLAB Program for Neural Network Analysis with Leave-One-Out Validation - Training(3)

```
%       If two rounded outputs are "1", choose the one whose actual output is
%       closest to "1"
            for j = 1:(LengthNO - 1)
                if NovelRounded(j) == 1
                    for k = (j + 1):LengthNO
                        if NovelRounded(k) == 1
                            if (AbsDiff(j) < AbsDiff(k))
                                NovelRounded(k) = 0;
                            else
                                NovelRounded(j) = 0;
                            end
                        end
                    end
                end
            end

            NovelError      =   Target(:,iSam) - NovelRounded;
```


MATLAB Program for Neural Network Analysis with Leave-One-Out Validation - Training(4)

```
            if (~isequal(NovelError,zeros(LengthNO,1)))
                MisClass    =   MisClass + 1;
                iSamLog     =   [iSamLog iSam];
                iRepLog     =   [iRepLog i];
                ErrorLog    =   [ErrorLog NovelError];
                OutputLog   =   [OutputLog NovelOutput];
            end
        end
    end

    MisClass
    iSamLog
    iRepLog
    ErrorLog
    OutputLog

    Trials      =   iSam * Repeats
```



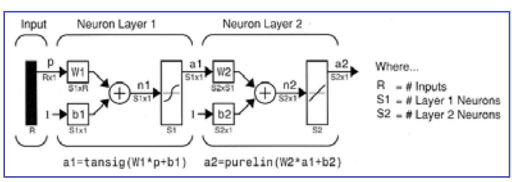
Training a Sigmoid Network

Two parameter vectors for 2-layer network

$$\mathbf{p}_{1,2} = \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}_{1,2} = \begin{bmatrix} p_1 \\ p_2 \\ \dots \\ p_{n+1} \end{bmatrix}_{1,2}$$

Output vector

$$\begin{aligned}
\hat{\mathbf{y}} &= \mathbf{u}_2 \\
&= \mathbf{s}_2(\mathbf{r}_2) = \mathbf{s}_2(\mathbf{W}_2\mathbf{u}_1 + \mathbf{b}_2) \\
&= \mathbf{s}_2\left[\mathbf{W}_2\ \mathbf{s}_1(\mathbf{r}_1) + \mathbf{b}_2\right] \\
&= \mathbf{s}_2\left[\mathbf{W}_2\ \mathbf{s}_1(\mathbf{W}_1\mathbf{u}_0 + \mathbf{b}_1) + \mathbf{b}_2\right] \\
&= \mathbf{s}_2\left[\mathbf{W}_2\ \mathbf{s}_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2\right]
\end{aligned}$$



Training a Sigmoid Network

$$\mathbf{p}_{1,2k} = \mathbf{p}_{1,2k} - \eta \left(\frac{\partial J}{\partial \mathbf{p}_{1,2}} \right)_k^T$$

where

$$\frac{\partial J}{\partial \mathbf{p}_{1,2}} = (\hat{\mathbf{y}} - \mathbf{y}_T)\frac{\partial \mathbf{y}}{\partial \mathbf{p}_{1,2}} = (\hat{\mathbf{y}} - \mathbf{y}_T)\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{r}_{1,2}}\frac{\partial \mathbf{r}_{1,2}}{\partial \mathbf{p}_{1,2}}$$

where

$$\mathbf{r}_{1,2} = \mathbf{W}_{1,2}\mathbf{u}_{0,1} + \mathbf{b}_{1,2}$$

$$\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{r}_2} = \mathbf{I}; \quad \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{r}_1} = \begin{bmatrix} (1-\hat{y}_1)\hat{y}_1 & 0 & \dots & 0 \\ 0 & (1-\hat{y}_2)\hat{y}_2 & \dots & 0 \\ \dots & \dots & \dots & 0 \\ 0 & 0 & \dots & (1-\hat{y}_n)\hat{y}_n \end{bmatrix}$$

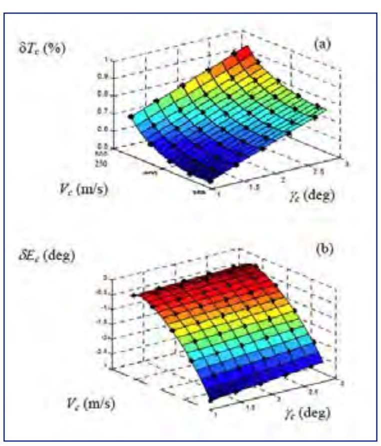
$$\frac{\partial \mathbf{r}_1}{\partial \mathbf{p}_1} = \begin{bmatrix} \mathbf{x}^T & 1 \end{bmatrix}; \quad \frac{\partial \mathbf{r}_2}{\partial \mathbf{p}_2} = \begin{bmatrix} \mathbf{u}_1^T & 1 \end{bmatrix}$$

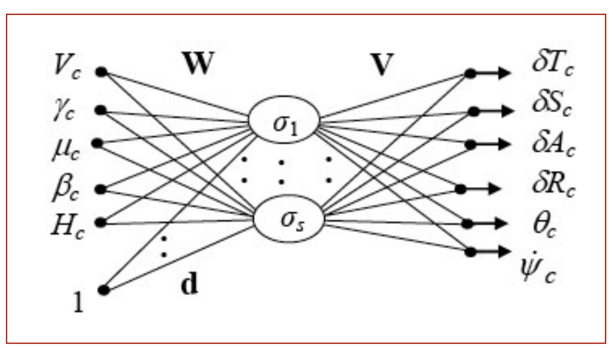
Algebraic Training of a Neural Network

Ferrari, S. and Stengel, R.,
Smooth Function Approximation Using Neural Networks (pdf), *IEEE Trans. Neural Networks*, Vol. 16, No. 1, Jan 2005, pp. 24-38 (with S. Ferrari).

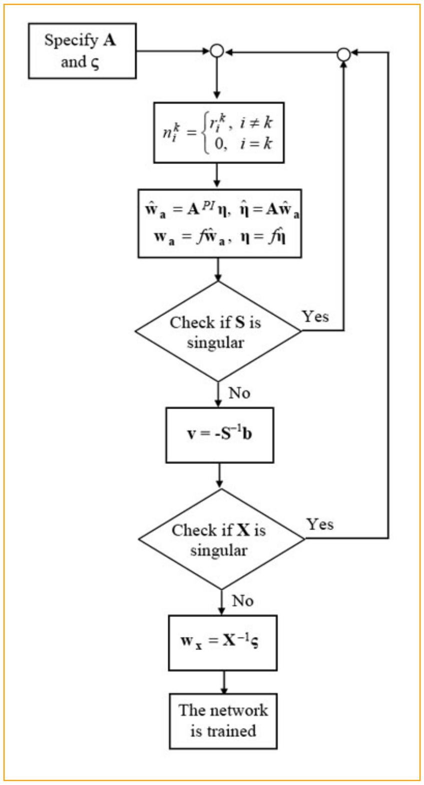
Algebraic Training for Exact Fit to a Smooth Function

- **Smooth functions define equilibrium control settings at many operating points**
- **Neural network required to fit the functions**

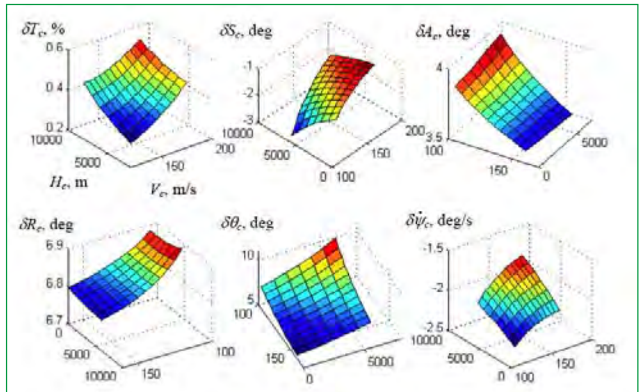




Ferrari and Stengel



Algorithm for Network Training



δT_c : Throttle command
δS_c : Spoiler command
δA_c : Aileron command
δR_c : Rudder command
$\delta \theta_c$: Pitch angle command
$\delta \dot{\psi}_c$: Yaw rate command

Results for Network Training

- **45-node example**
- **Algorithm is considerably faster than search methods**

Algorithm:	Time (Scaled):	Flops:	Lines of code (MATLAB®):	Epochs:	Final error:
Algebraic	1	2×10^5	8	1	0
Levenberg-Marquardt	50	5×10^7	150	6	10^{-26}
Resilient Backprop.	150	1×10^7	100	150	0.006