Statistical Machine Learning Methods for Bioinformatics

III. Neural Network Theory

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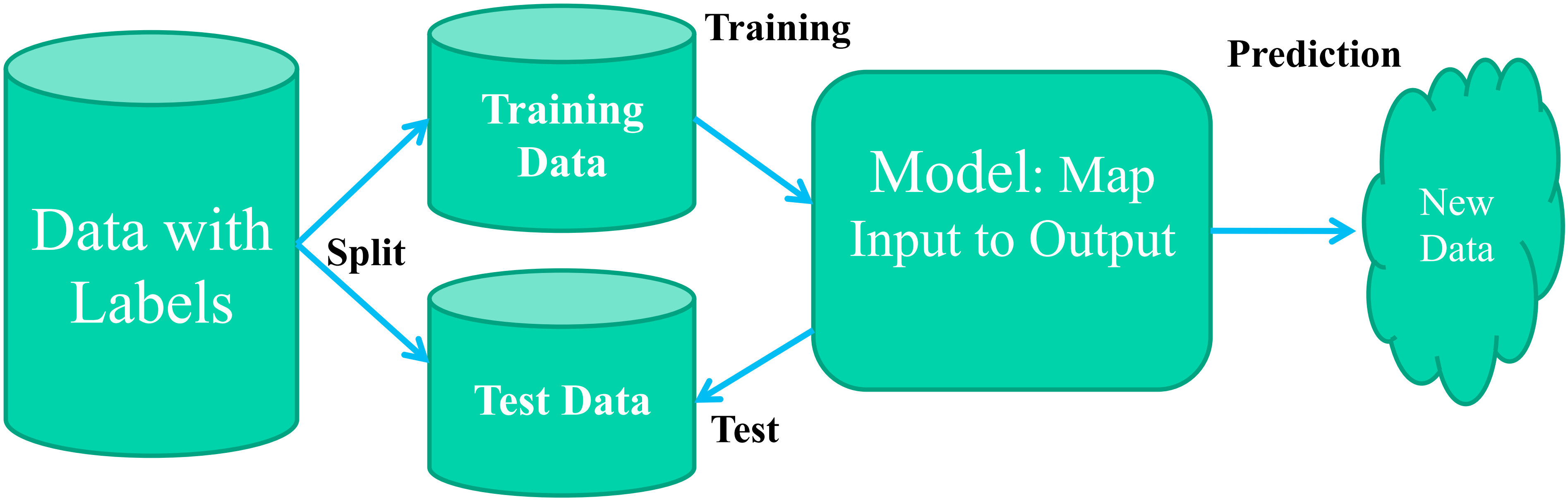
Classification Problem

Input								Output
Legs	weight	size	….				Feature m	Category / Label
4	100							Mammal
80	0.1							Bug

Question: How to automatically predict output given input?
Idea: Learn from known examples and generalize to unknown ones.

Data Driven Machine Learning Approach



Input: words of news
Output: politics, sports, entertainment, …

Training: Build a model (classifier)
Test: Test the model

Key idea: Learn from known data and Generalize to unseen data

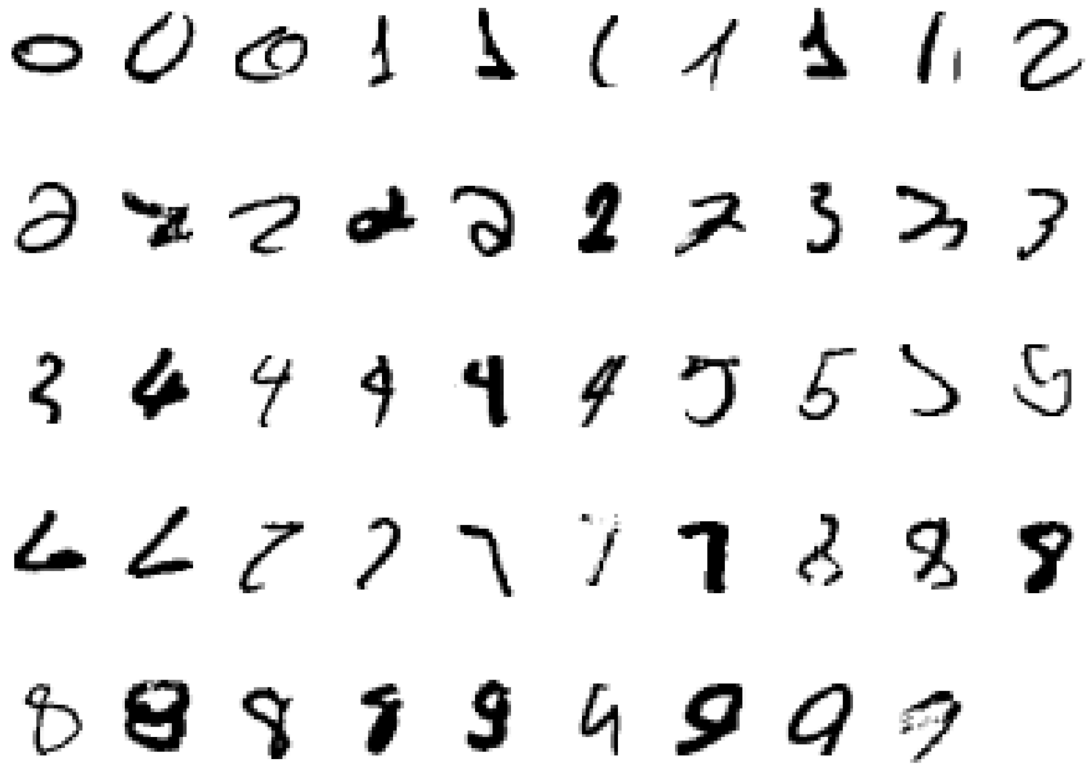
Outline

- Introduction
- Linear regression
- Linear Discriminant function (classification)
- One layer neural network / perceptron
- Multi-layer network
- Recurrent neural network
- Prevent overfitting
- Speedup learning

Machine Learning

- **Supervised learning** (training with labeled data), **un-supervised learning** (clustering un-labeled data), and **semi-supervised learning** (use both labeled and unlabeled data)
- Supervised learning: **classification** and **regression**
- **Classification**: output is discrete value
- **Regression**: output is real value

Learning Example: Recognize Handwriting



Classification: recognize each number
Clustering: cluster the same numbers together
Regression: predict the index of Dow-Jones

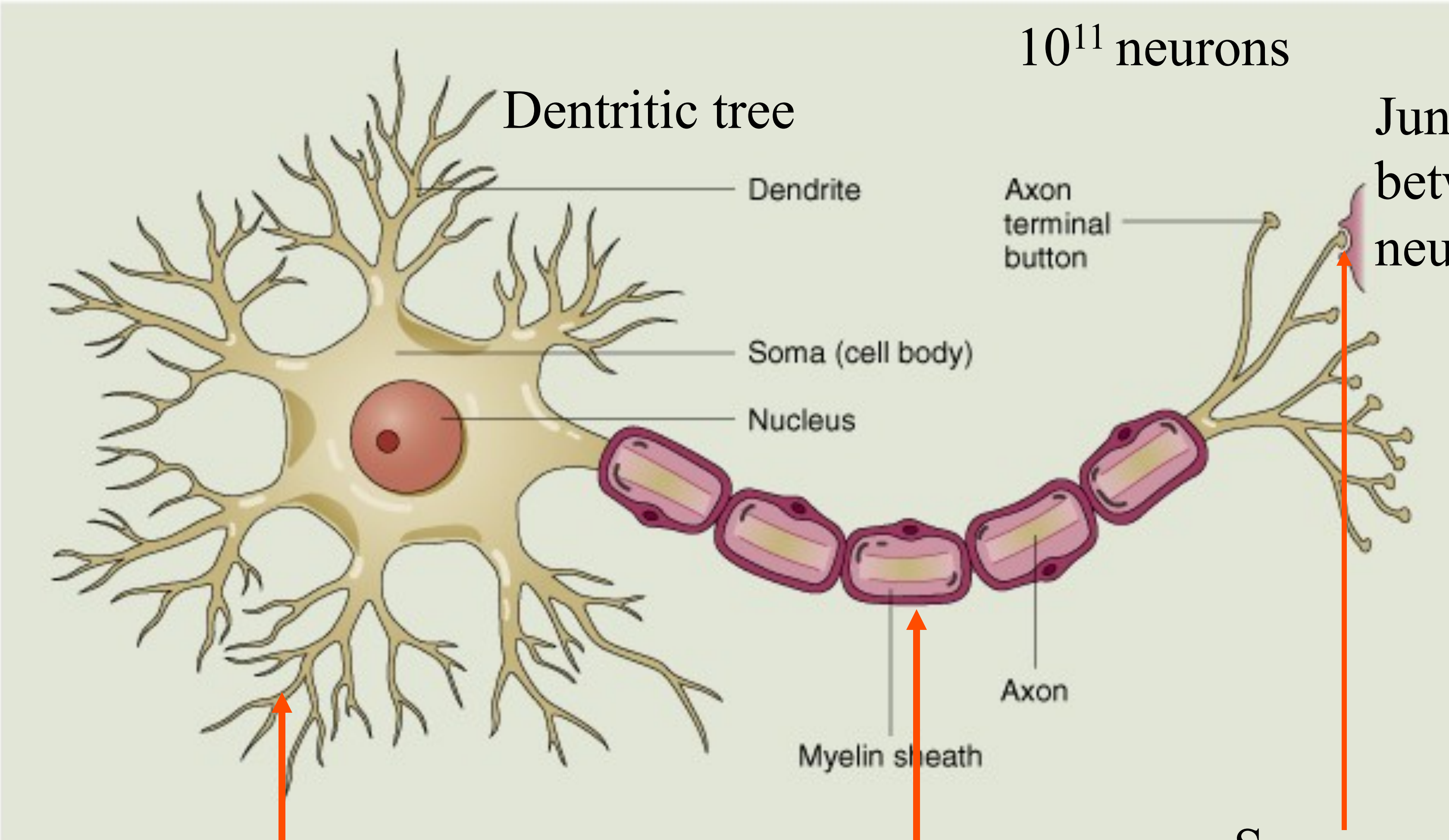
Neural Network

- Neural Network can do both supervised learning and un-supervised learning
- Neural Network can do both regression and classification
- Neural Network has both statistical and artificial intelligence roots

Roots of Neural Network

- Artificial intelligence root (neuron science)
- **Statistical root** (linear regression, generalized linear regression, discriminant analysis. This is our focus.)

A Typical Cortical Neuron

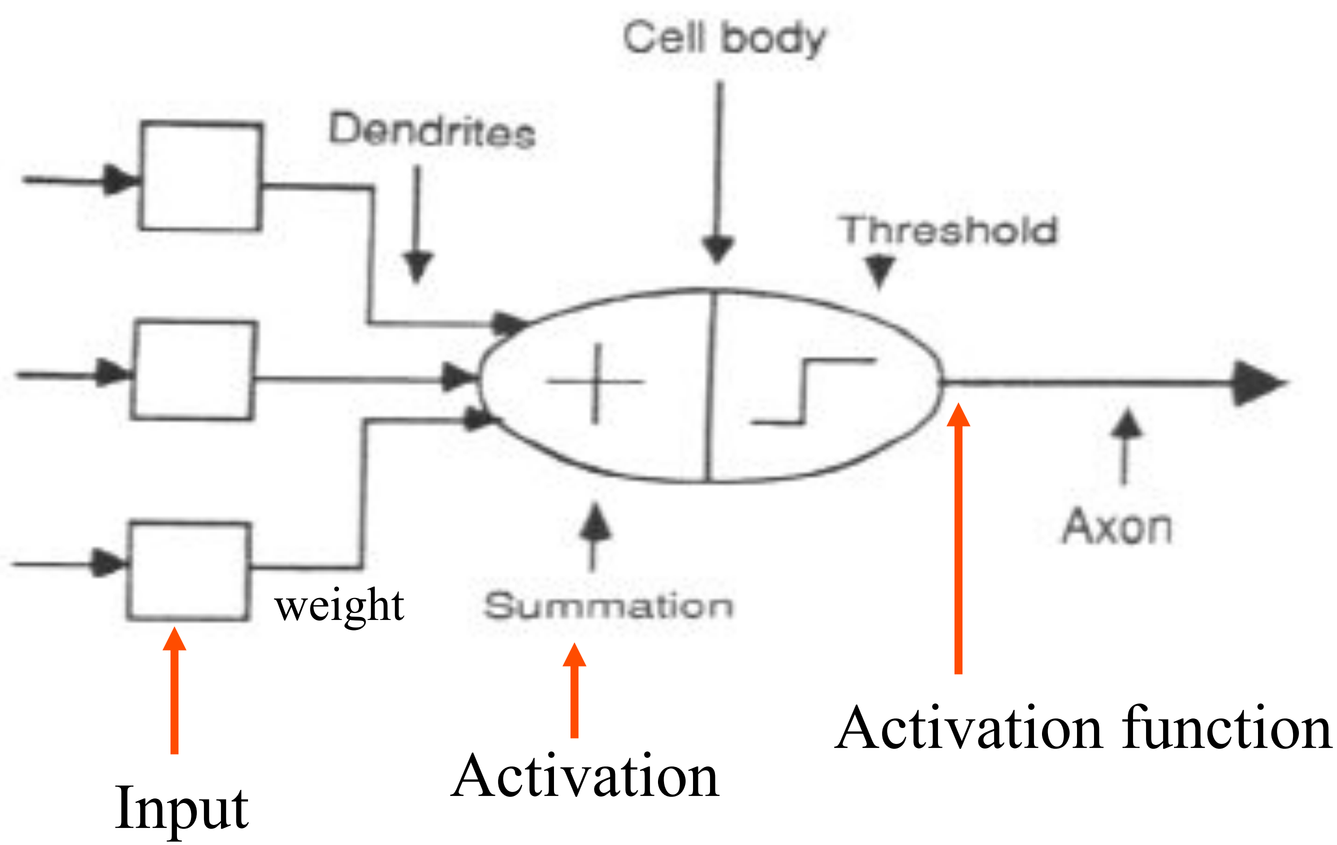


Synapse: control release chemical transmitters.

Axon: generate Potentials (Fire/not Fire)

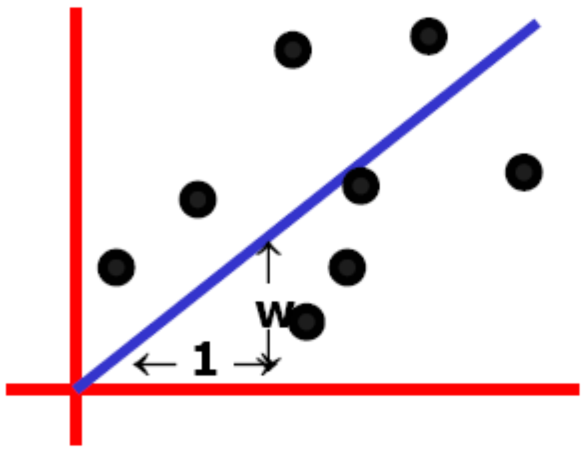
Collect chemical signals

A Neural Model



Adapted from http://www.doc.ic.ac.uk/~nd/surprise_96/journal/vol4/cs11/report.html

Statistics Root: Linear Regression Example



DATASET

inputs	outputs
$x_1 = 1$	$y_1 = 1$
$x_2 = 3$	$y_2 = 2.2$
$x_3 = 2$	$y_3 = 2$
$x_4 = 1.5$	$y_4 = 1.9$
$x_5 = 4$	$y_5 = 3.1$

Fish length vs. weight?

X: input or predictor
Y: output or response
Goal: learn a linear function E[y|x] = wx + b.

Adapted from A. Moore, 2003

Linear Regression

Definition of a linear model:

- $y = wx + b + noise$.
- noise ~ N $(0, \sigma^2)$, assume σ is a constant.
- $y \sim N(wx + b, \sigma^2)$
- Estimate expected value of y given x ($E[y|x] = wx + b$) .
- Given a set of data $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, to find the optimal parameters w and b.

Objective Function

- Least square error: $\sum_{i=1}^{N}(y_i - wx_i - b)^2$
- Maximum Likelihood: $\prod_{i=1}^{N} P(y_i \mid x_i, w, b)$
- Minimizing square error is equivalent to maximizing likelihood

Maximize Likelihood

$$\prod_{i=1}^{N} P(y_i \mid x_i, w, b) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - wx_i - b)^2}{2\sigma^2}}$$

Minimize negative log-likelihood:

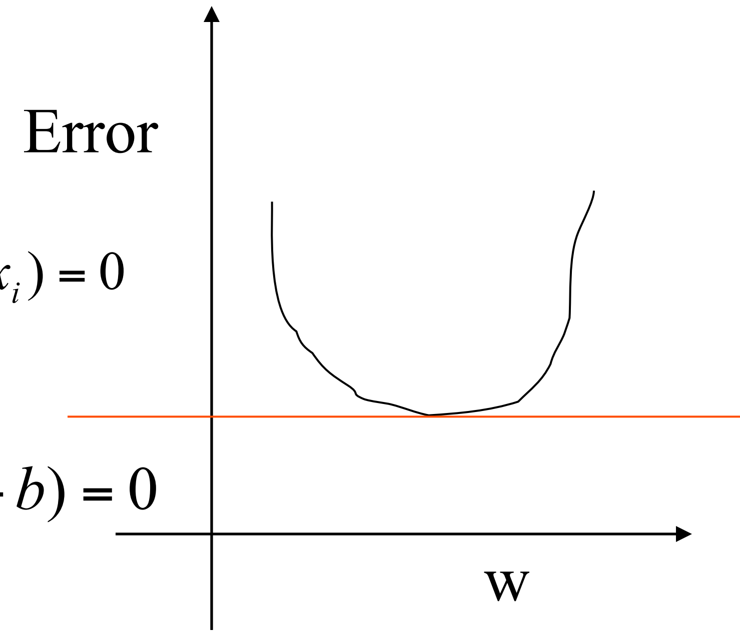
$$-\log\left(\prod_{i=1}^{N} P(y_i \mid x_i, w, b)\right) = -\log\left(\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - wx_i - b)^2}{2\sigma^2}}\right) = -\sum_{i=1}^{N}\left(-\log(\sqrt{2\pi\sigma^2}) - \frac{(y_i - wx_i - b)^2}{2\sigma^2}\right)$$

$$= \sum_{i=1}^{N}\left(\log(\sqrt{2\pi\sigma^2}) + \frac{(y_i - wx_i - b)^2}{2\sigma^2}\right)$$

Note: σ is a constant.

1-Variable Linear Regression

Minimize E $= \displaystyle\sum_{i=1}^{N} (y_i - wx_i - b)^2$



$$\frac{\partial E}{\partial W} = \sum_{i=1}^{N} 2(y_i - wx_i - b) * (-x_i) = \sum_{i=1}^{N} 2(-y_i x_i + wx_i^2 + bx_i) = 0$$

$$\frac{\partial E}{\partial b} = \sum_{i=1}^{N} 2(y_i - wx_i - b) * (-1) = \sum_{i=1}^{N} 2(-y_i + wx_i + b) = 0$$

$$w = \frac{\sum_{i=1}^{N} x_i y_i - N\overline{x}\overline{y}}{\sum_{i=1}^{N} x_i^2 - N\overline{x}\overline{x}} \qquad b = \frac{\sum_{i=1}^{N} (y_i - wx_i)}{N}$$

Linear Regression Demo

http://www.calpoly.edu/~srein/StatDemo/All.html

Multivariate Linear Regression

- How about multiple predictors: (x_1, x_2, …, x_d).
- $y = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_d x_d + \varepsilon$
- For multiple data points, each data point is represented as (y_i, x_i), x_i consists of d predictors (x_{i1}, x_{i2}, …, x_{id}).
- $y_i = w_0 + w_1 x_{i1} + w_2 x_{i2} + \ldots + w_d x_{id} + \varepsilon$

A Motivating Example

- Each day you get lunch at the cafeteria.
  - Your diet consists of fish, chips, and beer.
  - You get several portions of each
- The cashier only tells you the total price of the meal
  - After several days, you should be able to figure out the price of each portion.
- Each meal price gives a linear constraint on the prices of the portions:

$$price = x_{fish} w_{fish} + x_{chips} w_{chips} + x_{beer} w_{beer}$$

G. Hinton, 2006

Matrix Representation

***n* data points, *d* dimension**

$$\begin{pmatrix} y_1 \\ y_2 \\ \cdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1d} \\ 1 & x_{21} & \cdots & x_{2d} \\ \cdots & . & \cdots & . \\ 1 & x_{n1} & \cdots & x_{nd} \end{pmatrix} \times \begin{pmatrix} w_0 \\ w_1 \\ \cdots \\ w_d \end{pmatrix} + \varepsilon$$

n*1 n*(d+1) (d+1)*1

Matrix Representation: $\mathbf{Y} = \mathbf{XW} + \boldsymbol{\varepsilon}$

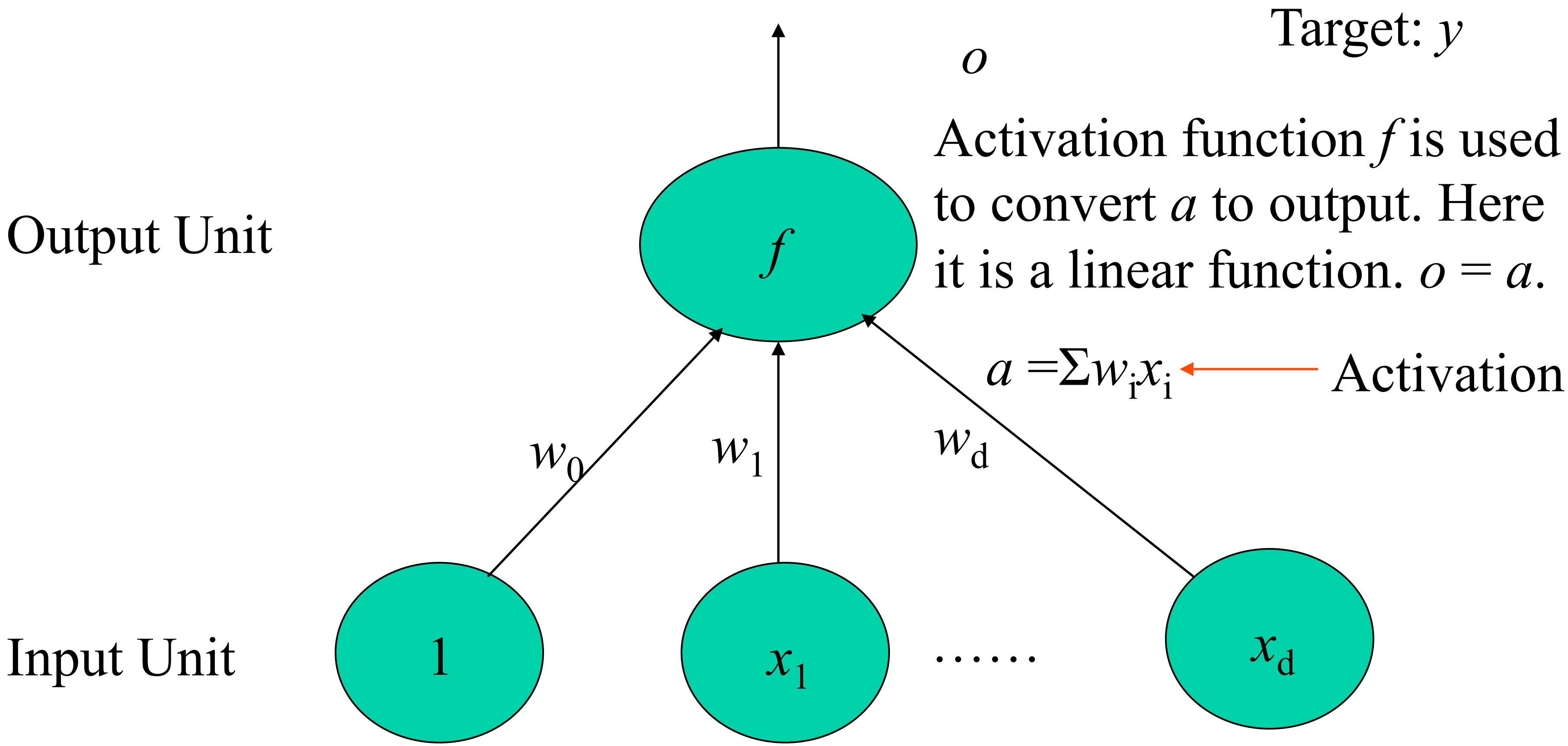
Multivariate Linear Regression

- Goal: minimize square error = $(Y-XW)^T(Y-XW) = Y^TY - 2X^TWY + W^TX^TXW$
- Derivative: $-2X^TY + 2X^TXW = 0$
- $W = (X^TX)^{-1}X^TY$
- Thus, we can solve linear regression using matrix inversion, transpose, and multiplication.

Difficulty and Generalization

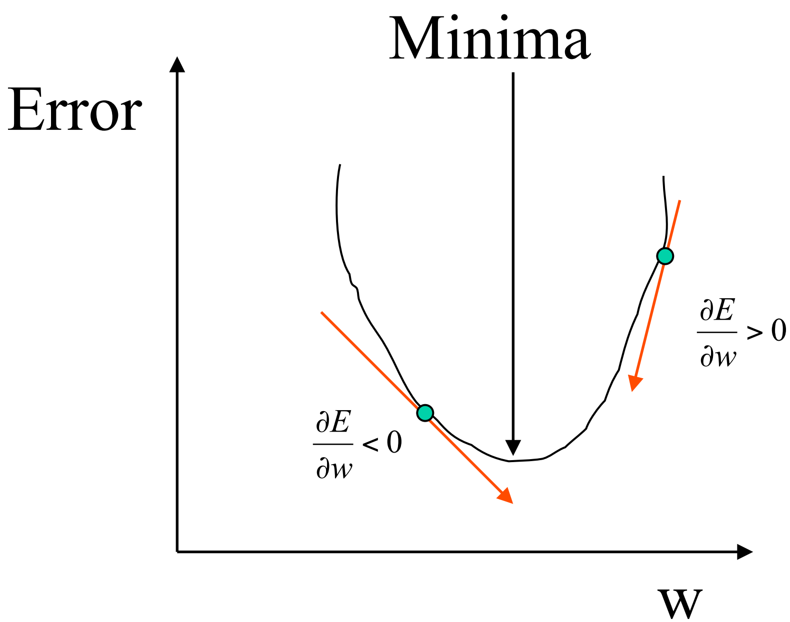
- Numerical computation issue. (a lot data points. Matrix inversion is impossible.)
- Singular matrix (determinant is zero) : no inversion
- How to handle non-linear data?
- Turns out neural network and its iterative learning algorithm can address this problem.

Graphical Representation: One Layer Neural Network for Regression



Gradient Descent Algorithm

- For a data $x = (x_1, x_2, \ldots x_d)$, error $E = (y - o)^2 = (y - w_0 x_0 - w_1 x_1 - \ldots - w_d x_d)^2$
- Partial derivative: $\nabla E|_{w_i} = \frac{\partial E}{\partial w_i} = 2(y-o)\frac{\partial o}{\partial w_i} = 2(y-o)(-x_i) = -2(y-o)x_i$



Update rule:

$$w_i^{(t+1)} = w_i^{(t)} + \eta(y - o)x_i$$

Famous Delta Rule

Algorithm of One-Layer Regression Neural Network

- Initialize weights w (small random numbers)
- **Repeat**

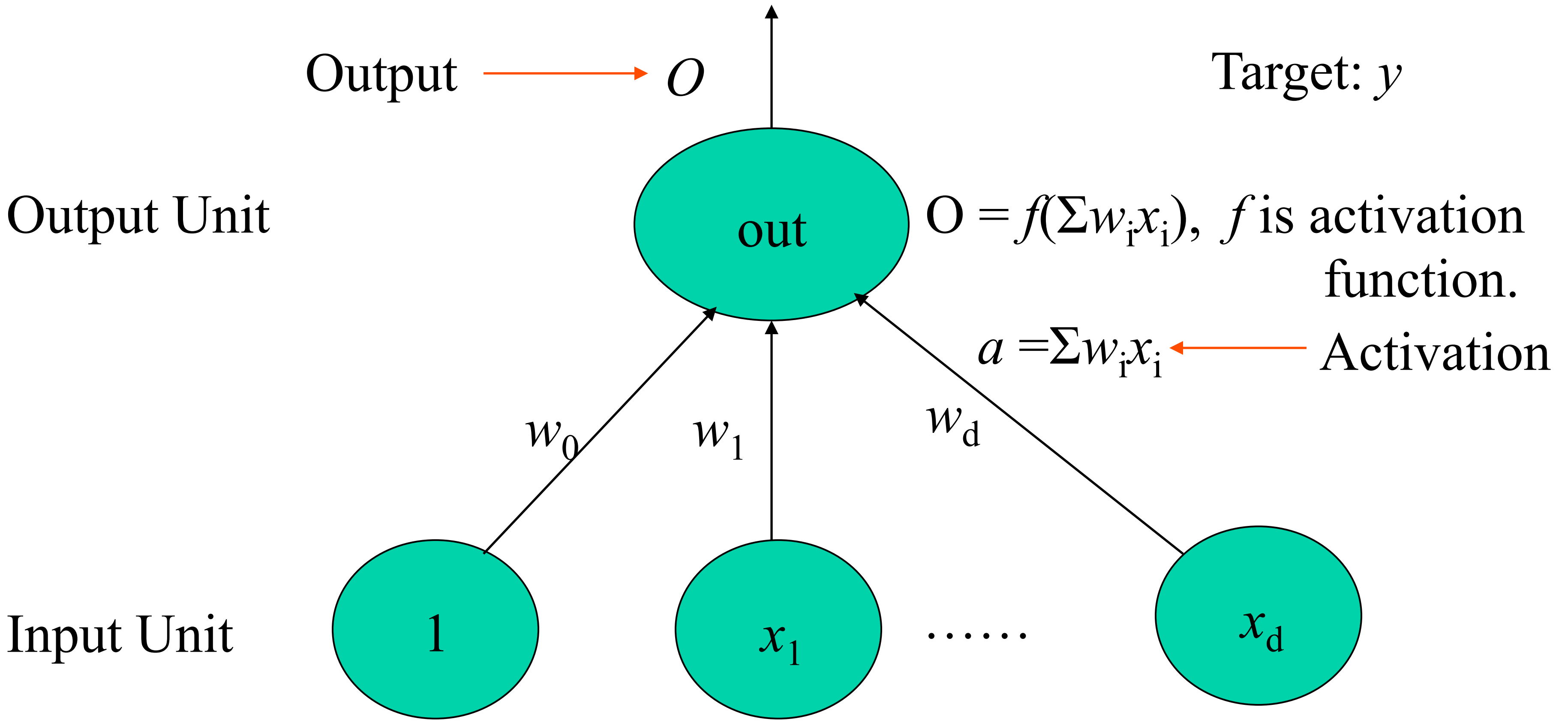
  Present a data point $x = (x_1, x_2, \ldots, x_d)$ to the network and compute output o.

  if $y > o$, add ηx_i to w_i.

  if $y < o$, add $-\eta x_i$ to w_i.
- **Until** $\Sigma(y_k - o_k)^2$ is zero or below a threshold or reaches the predefined number of iterations.

Comments: online learning: update weight for every x. batch learning: update weight every batch of x (i.e. $\Sigma \eta x_i$).

Graphical Representation: One Layer Neural Network for Regression

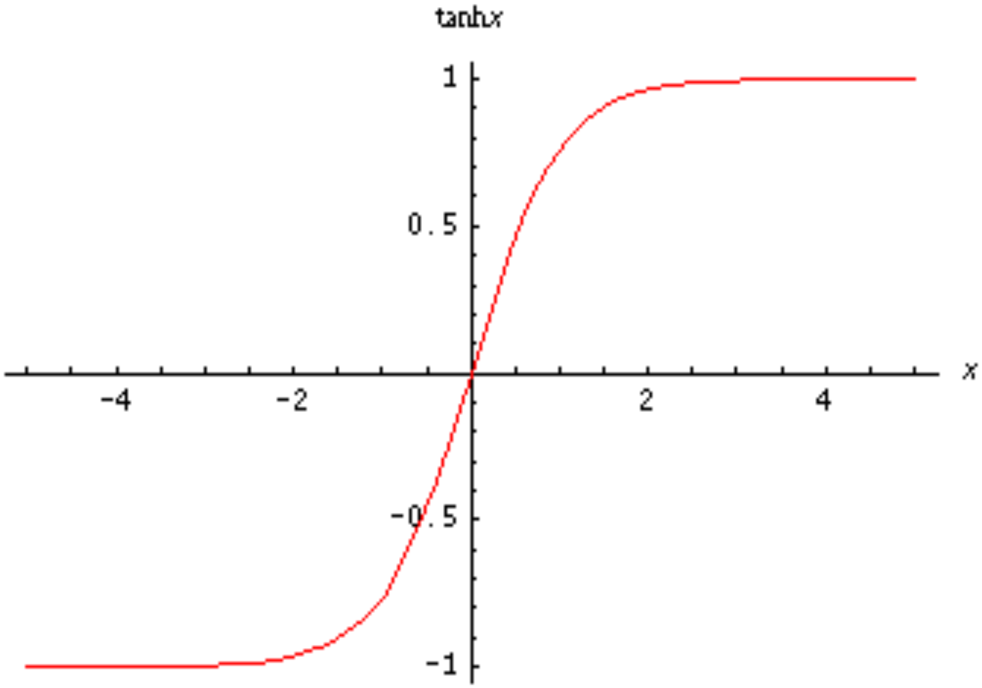


What about Hyperbolic Tanh Function for Output Unit

- Can we use activation function other than linear function?
- For instance, if we want to limit the output to be in [-1, +1], we can use hyperbolic Tanh function:

$$\frac{e^x - e^{-x}}{e^x + e^{-x}}$$

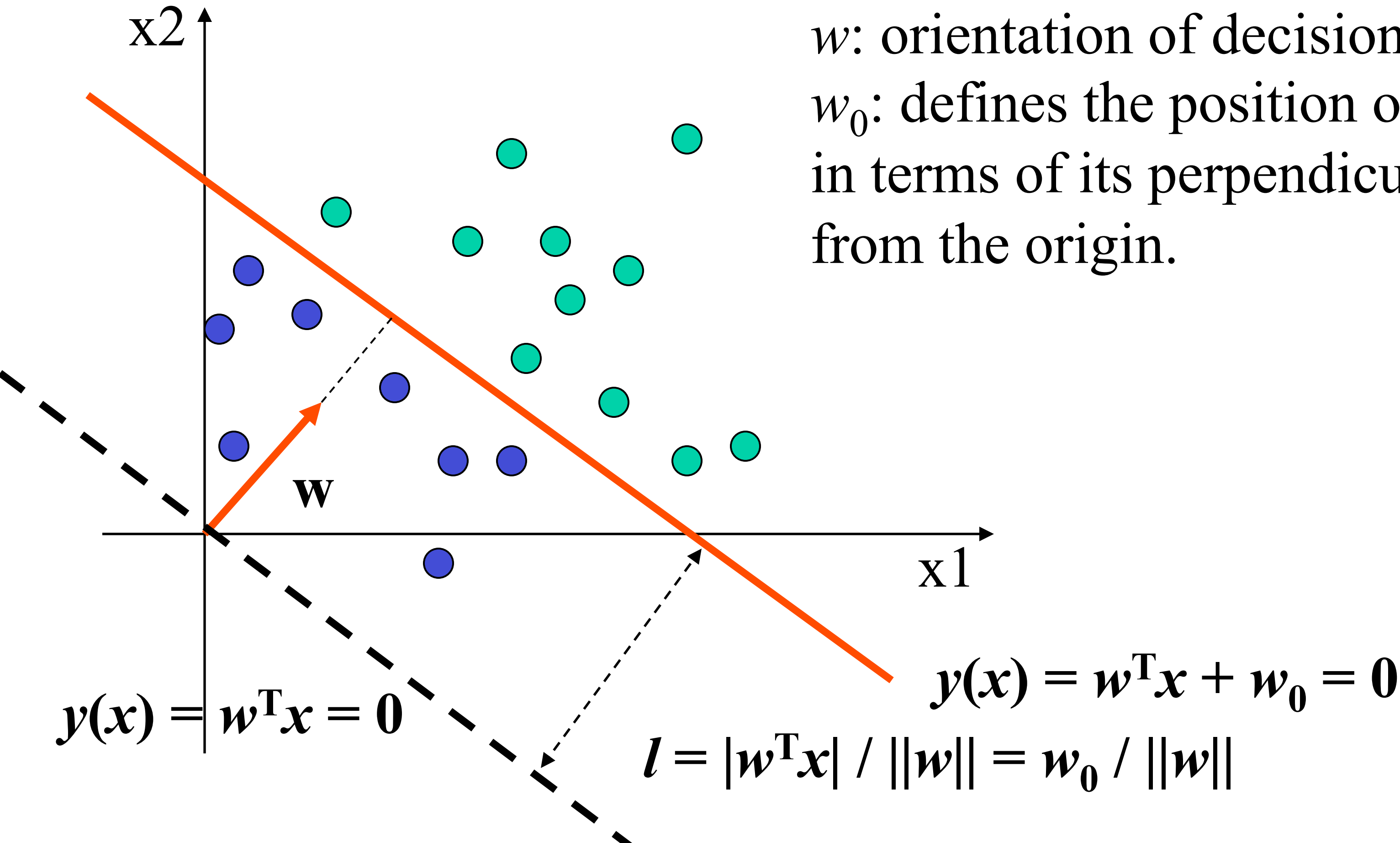
- The only thing to change is to use the new gradient.



Two-Category Classification

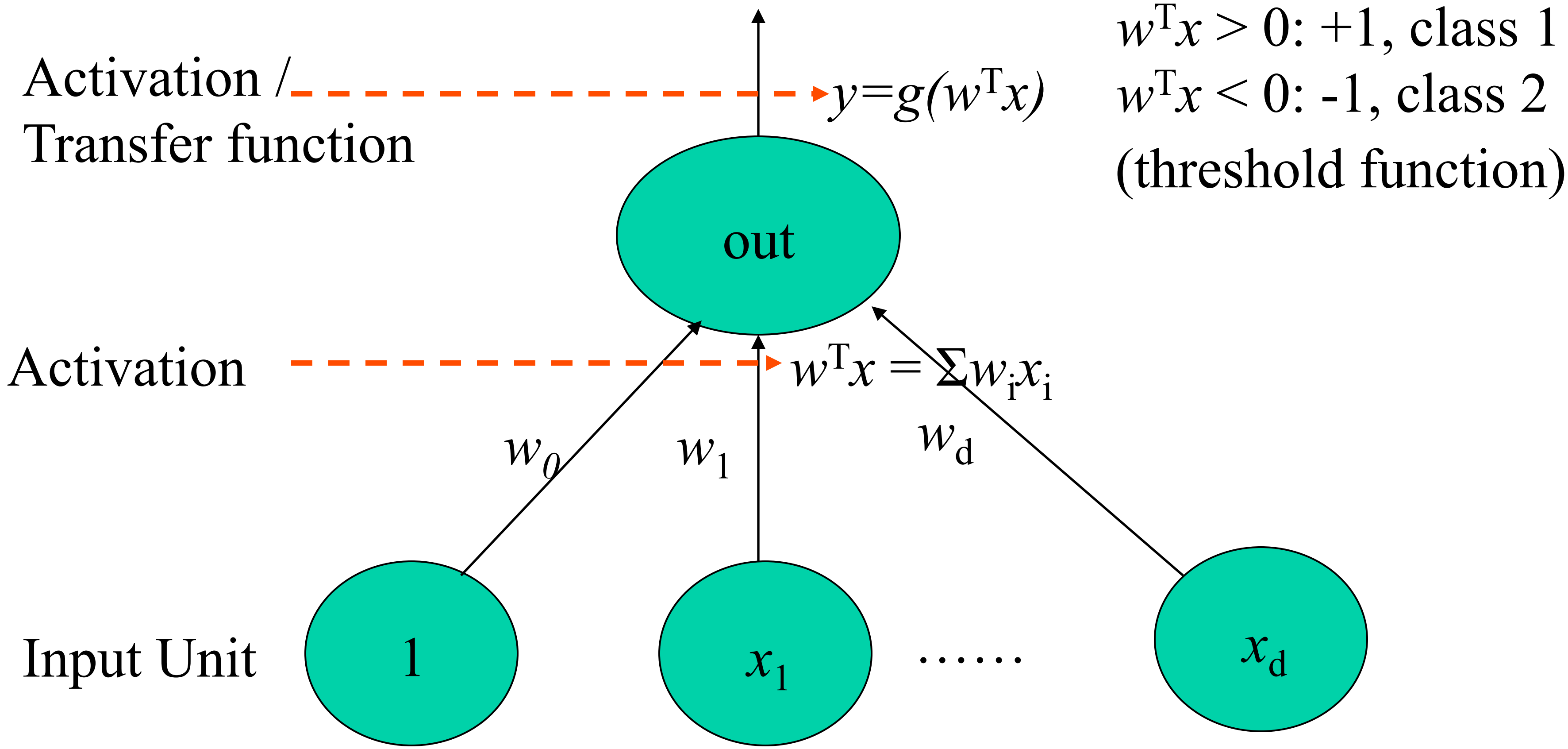
- Two classes: C_1 and C_2.
- Input feature vector: x.
- Define a discriminant function $y(x)$ such that x is assigned to C_1 if $y(x) > 0$ and to class C_2 if $y(x) < 0$.
- Linear discriminant function: $y(x) = w^T x + w_0 = \bar{w}^T \bar{x}$, where $\bar{x} = (1, x)$.
- w: weight vector, w_0: bias.

A Linear Decision Boundary in 2-D Input Space



w: orientation of decision boundary
w_0: defines the position of the plan in terms of its perpendicular distance from the origin.

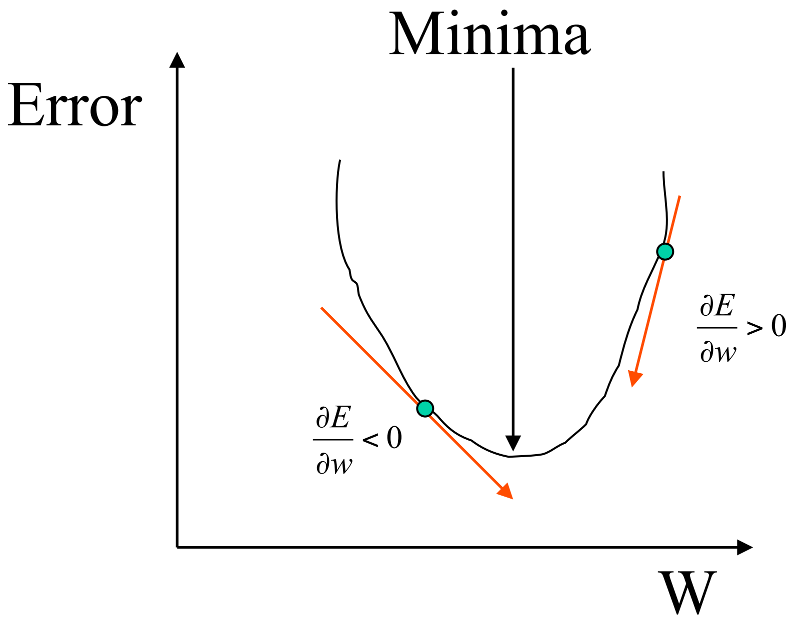
Graphical Representation: Perceptron, One-Layer Classification Neural Network



Perceptron Criterion

- Minimize classification error
- Input data (vector): $x^1, x^2, \ldots, x^N$ and corresponding target value $t^1, t^2, \ldots, t^N$.
- Goal: for all x in C_1 ($t = 1$), $w^T x > 0$, for all x in C_2 ($t = -1$), $w^T x < 0$. Or for all x: $w^T x t > 0$.
- Error: $E^{perc}(w) = -\sum_{x^n \in M} w^T x^n t^n$. M is the set of misclassified data points.

Gradient Descent



For each misclassified data point, adjust weight as follows:

$$w = w - \frac{\partial E}{\partial w} \times \eta = w + \eta\, x^n t^n$$

Perceptron Algorithm

- Initialize weight w
- **Repeat**

  For each data point (x^n, t^n)

  Classify each data point using current w.

  If $w^T x^n t^n > 0$ (correct), do nothing

  If $w^T x^n t^n < 0$ (wrong), $w^{new} = w + \eta x^n t^n$

  $w = w^{new}$
- **Until** w is not changed (all the data will be separated correctly, if data is linearly separable) or error is below a threshold.

Rosenblatt, 1962

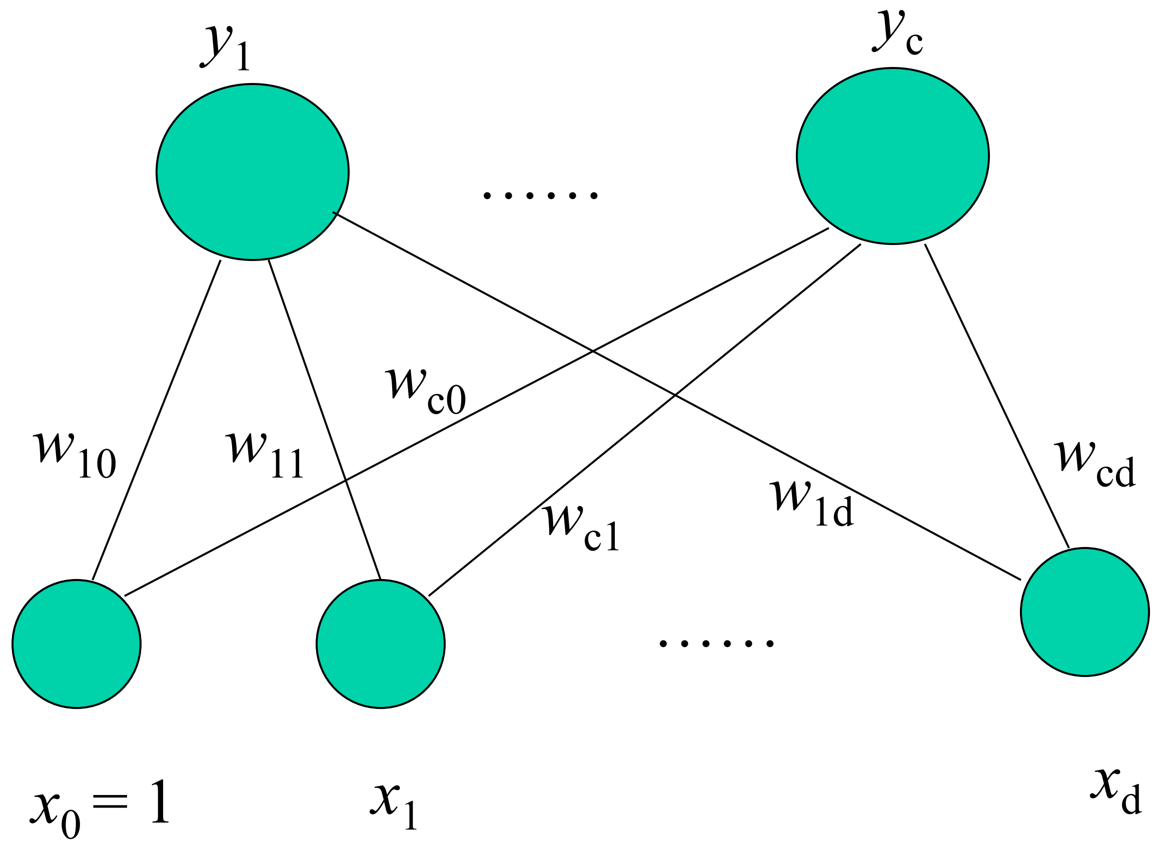
Perceptron Convergence Theorem

- For any data set which is linearly separable, the algorithm is guaranteed to find a solution in a finite number of steps (Rosenblatt, 1962; Block 1962; Nilsson, 1965; Minsky and Papert 1969; Duda and Hart, 1973; Hand, 1981; Arbib, 1987; Hertz et al., 1991)

Multi-Class Linear Discriminant Function

- c classes. Use one discriminant function $y_k(x) = w_k^T x + w_{k0}$ for each class C_k.
- A new data point x is assigned to class C_k if $y_k(x) > y_j(x)$ for all $j \neq k$.

One-Layer Multi-Class Perceptron



How to learn it?

Muti-Threshold Perceptron Algorithm

- Initialize weight w
- **Repeat**

  Present data point x to the network, if classification is correct, do nothing.

  if x is wrongly classified to C_i instead of true class C_j, adjust weights connected to C_i and C_j as follows.

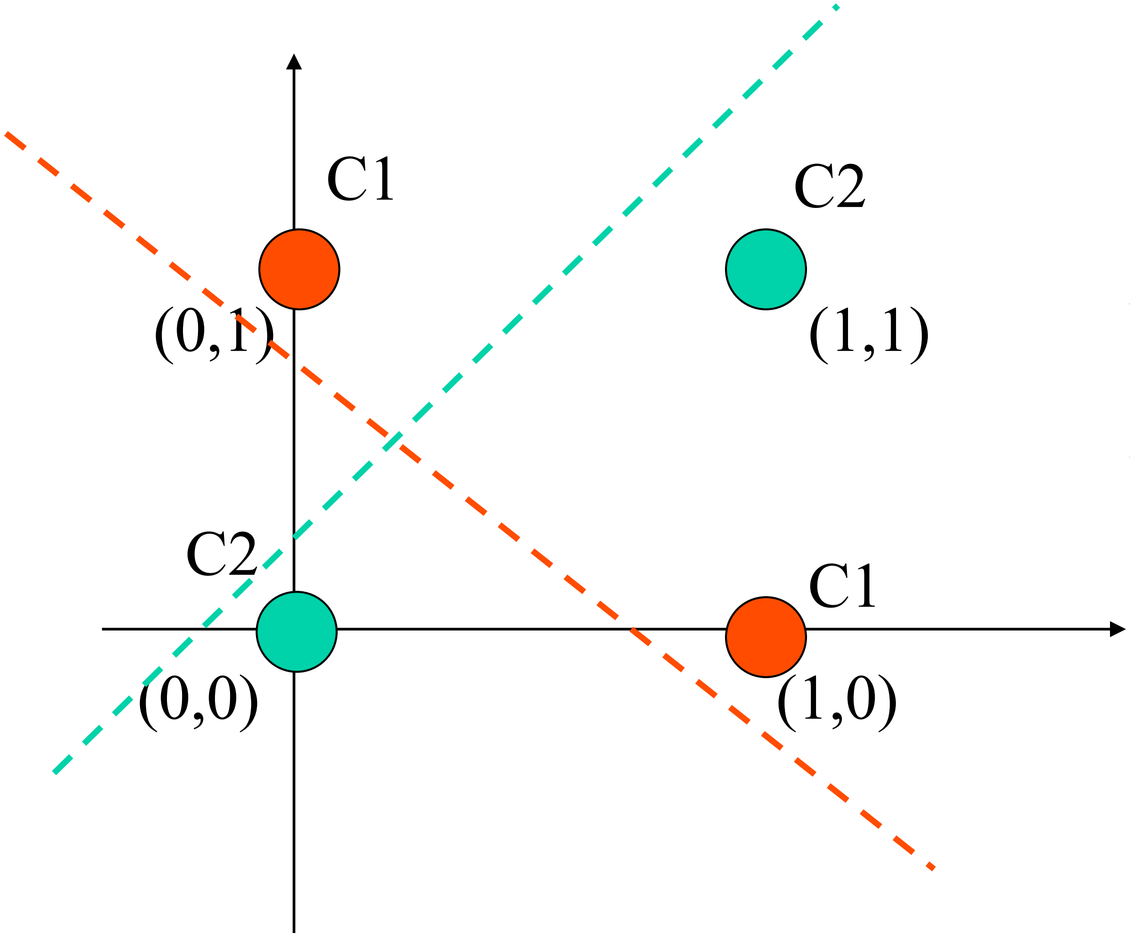
  Add $-\eta x_k$ to $w_{ik.}$ Add ηx_k to w_{jk}
- **Until** misclassification is zero or below a threshold.

Note: may also Add $-\eta x_k$ to w_{lk} for any l, $y_l > y_j$.

Limitation of the Perceptron

- Can’t not separate non-linear data completely.
- Or can’t not fit non-linear data well.
- Two directions to attack the problem: (1) extend to multi-layer neural network (2) map data into high dimension (SVM approach)

Exclusive OR Problem



Perceptron (or one-layer neural network) can not learn a function to separate the two classes perfectly.

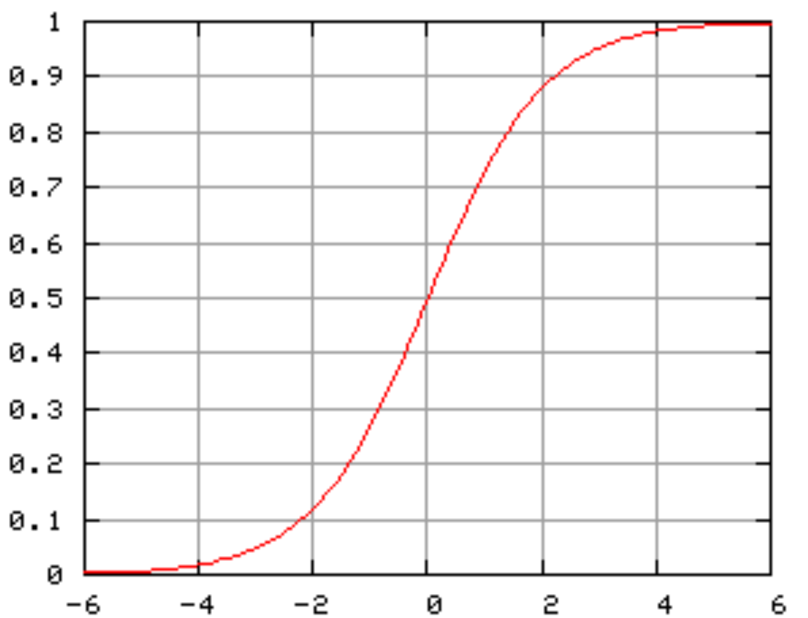
Logistic Regression

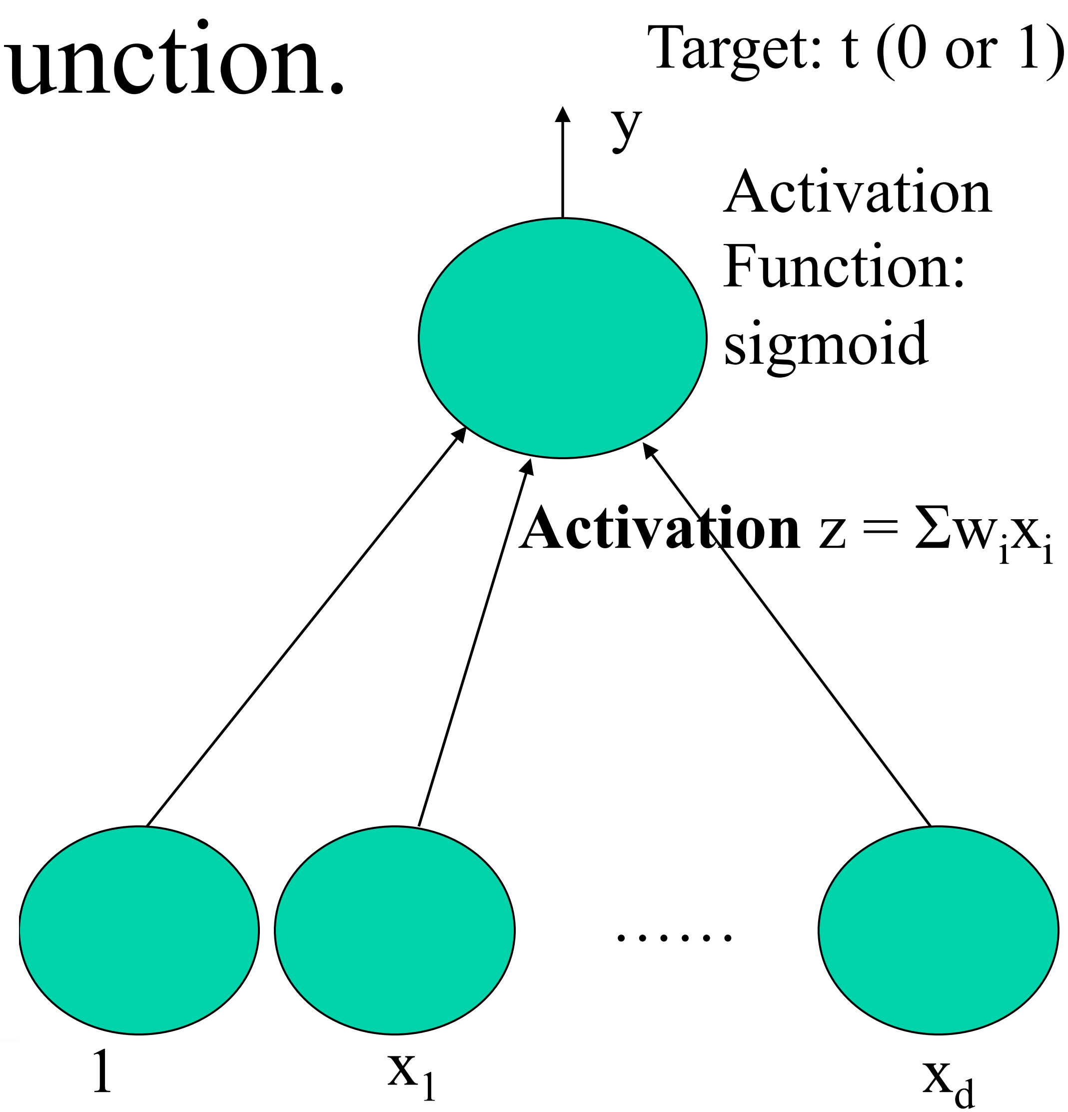
- Estimate posterior distribution: $P(C_1|x)$
- Dose – response estimation: in bioassay, the relation between dose level and death rate $P(\text{death} \mid x)$.
- We can not use 0/1 hard classification.
- We can not use unconstrained linear regression because $P(\text{death} \mid x)$ must be in $[0,1]$?

Logistic Regression and One Layer Neural Network With Sigmoid Function.

$$P(\text{death} \mid x) = \frac{1}{1 + e^{-wx}}$$

(Sigmoid function)





How to Adjust Weights?

- Minimize error E=(t-y)^2. For simplicity, we derive the formula for one data point. For multiple data points, just add the gradients together.

$$\frac{\partial E}{\partial w_i} = \frac{\partial E}{\partial y}\frac{\partial y}{\partial z}\frac{\partial z}{\partial w_i} = -2(t-y)y(1-y)x_i$$

Notice: $$\frac{\partial y}{\partial z} = \frac{\partial(\frac{1}{1+e^{-z}})}{\partial z} = \frac{1}{1+e^{-z}}(1-\frac{1}{1+e^{-z}}) = y(1-y)$$

Error Function and Learning

- Least Square
- Maximum likelihood: output y is the probability of being in C_1 (t=1). 1- y is the probability of being in C_2. So what is probability of $P(t|x) = y^t(1-y)^{1-t}$.
- Maximum likelihood is equivalent to minimize negative log likelihood:

  $E = -\log P(t|x) = -t\log y - (1-t)\log(1-y)$. (cross entropy)

How to Adjust Weights?

- Minimize error E= -tlog*y* - (1-*t*)log(1-*y*). For simplicity, we derive the formula for one data point. For multiple data points, just add the gradients together.

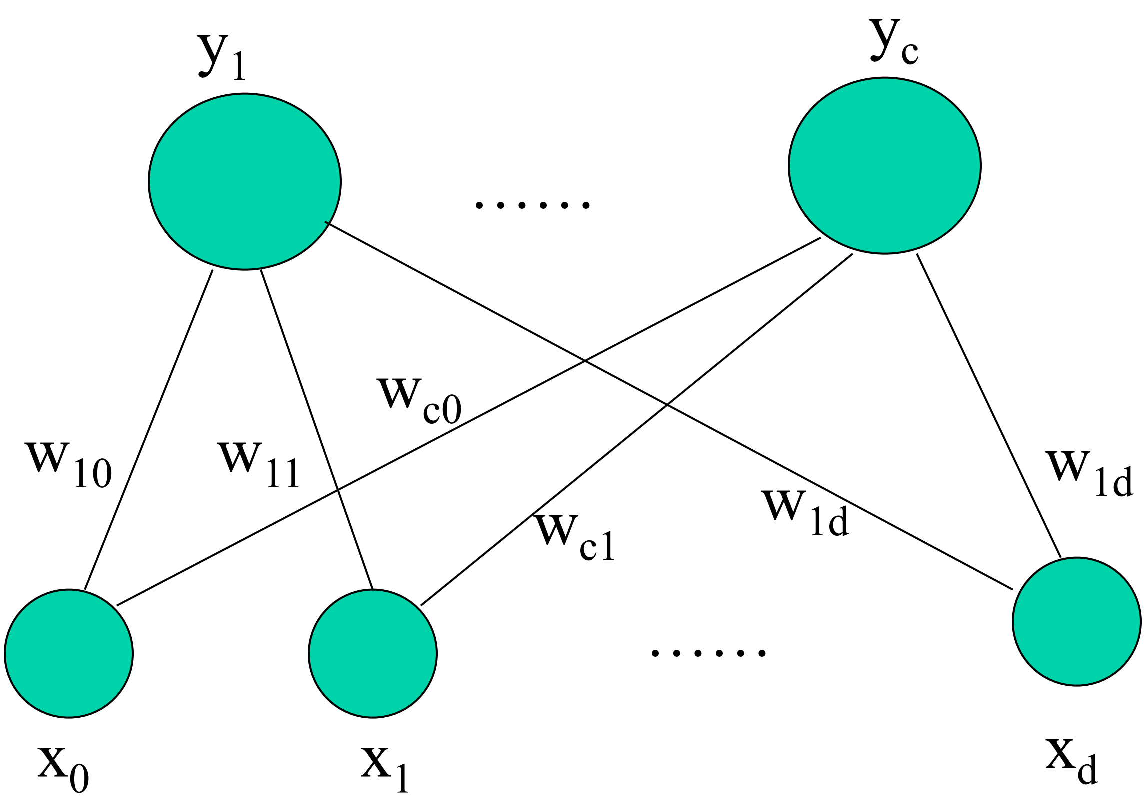
$$\frac{\partial E}{\partial y} = -\frac{t}{y} - \frac{1-t}{1-y}(-1) = -\frac{t}{y} - \frac{t-1}{1-y} = \frac{y-t}{y(1-y)}$$

$$\frac{\partial E}{\partial w_i} = \frac{\partial E}{\partial y}\frac{\partial y}{\partial z}\frac{\partial z}{\partial w_i} = \frac{y-t}{y(1-y)}y(1-y)x_i = (y-t)x_i$$

Update rule: $w_i^{(t+1)} = w_i^t + \eta(t-y)x_i$

Multi-Class Logistic Regression

- Transfer (or activation) function is normalized exponentials (or soft max)



$$y_i = \frac{e^{a_i}}{\sum_{j=1}^{c} e^{a_j}}$$

Activation Function

$$a_i = \sum_{j=0}^{d} w_{ij} x_j$$

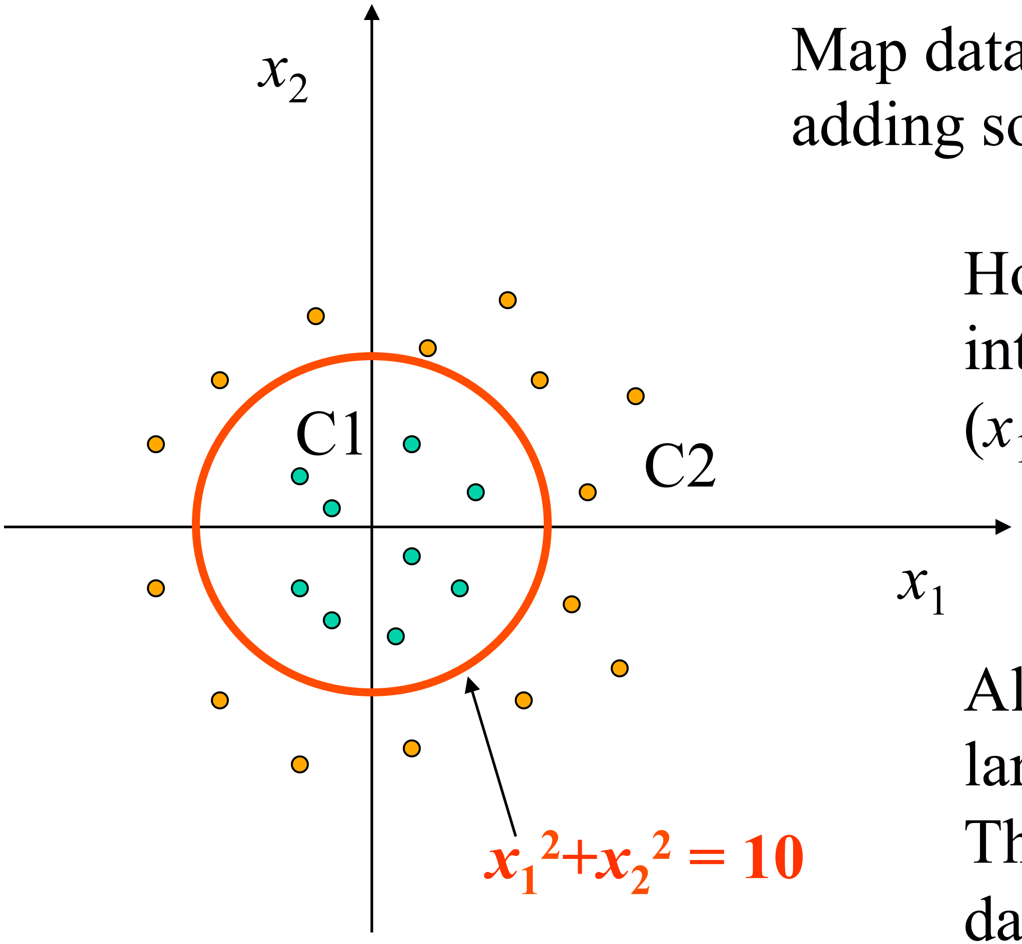
Activation to Node O_i

How to learn this network? Once again, gradient descent.

Questions?

- Is logistic regression a linear regression?
- Can logistic regression handle non-linearly separable data?
- How to introduce non-linearity?

Support Vector Machine Approach



Map data point into high dimension, e.g. adding some non-linear features.

How about we augument feature into three dimension (x_1, x_2, $x_1^2+x_2^2$).

All data points in class C2 have a larger value for the third feature Than data points in C1. Now data is linearly separable.

Neural Network Approach

- Multi-Layer Perceptrons
- In addition to input nodes and output nodes, some hidden nodes between input / output nodes are introduced.
- Use hidden units to learn internal features to represent data. Hidden nodes can learn internal representation of data that are not explicit in the input features.
- Transfer function of hidden units are non-linear function

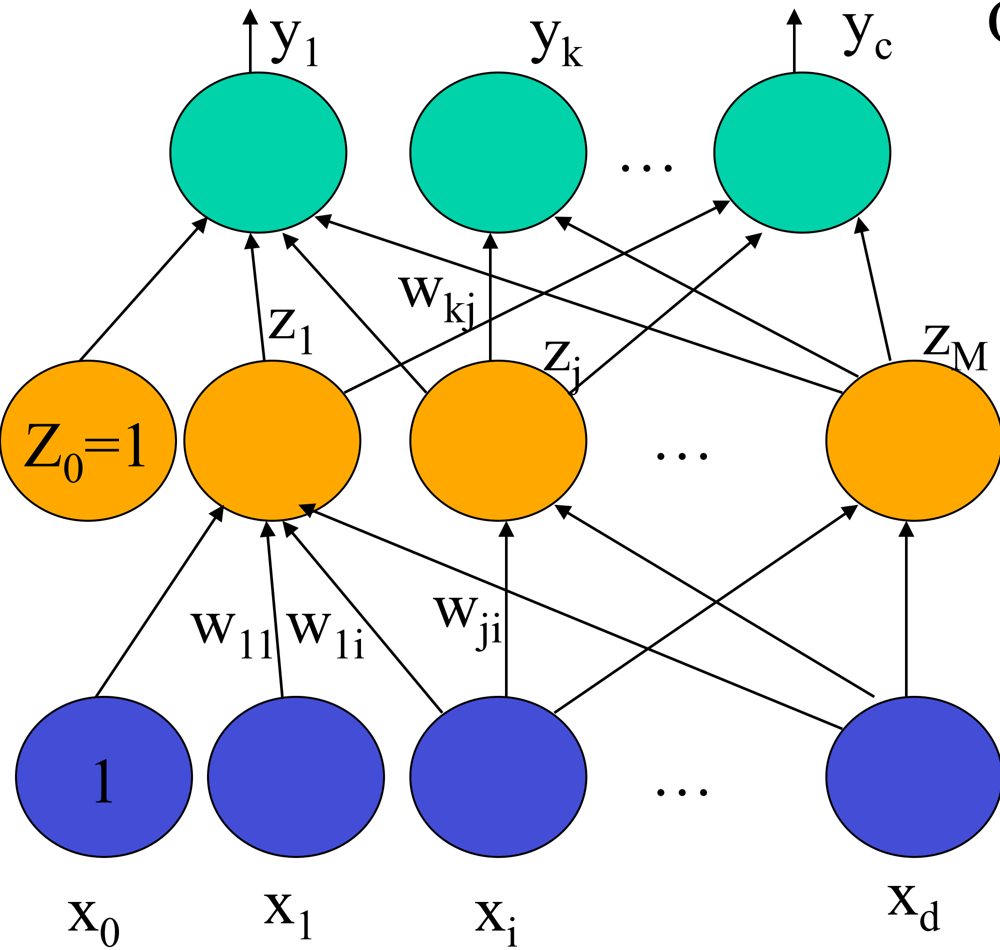
Multi-Layer Perceptron

- Connections go from lower layer to higher layer. (usually from input layer to hidden layer, to output layer)
- Connection between input/hidden nodes, input/output nodes, hidden/hidden nodes, hidden/output nodes are arbitrary as long as there is no loop (must be feed-forward).
- However, for simplicity, we usually only allow connection from input nodes to hidden nodes and from hidden nodes to output nodes. The connections with a layer are disallowed.

Multi-Layer Perceptron

- Two-layer neural network (one hidden and one output) with non-linear activation function is a **universal function approximator** (see Baldi and Brunak 2001 or Bishop 96 for the proof), i.e. it can approximate any numeric function with arbitrary precision given a set of appropriate weights and hidden units.
- Thus, we usually use two-layer (or three-layer if you count the input as one layer) neural network. Increasing the number of layers is occasionally helpful.

Two-Layer Neural Network



Output

Activation function: f (linear,sigmoid, softmax)

Activation of unit a_k: $\sum_{j=0}^{M} w_{kj} z_j$

Activation function: g (linear, tanh, sigmoid)

Activation of unit a_j: $\sum_{i=0}^{d} w_{ji} x_i$

$$y_k = f\left(\sum_{j=0}^{M} w_{kj} \times g\left(\sum_{i=0}^{d} w_{ji} x_i\right)\right)$$

Adjust Weights by Training

- How to adjust weights?
- Adjust weights using known examples (training data) (x_1,x_2,x_3,…,x_d,t).
- Try to adjust weights so that the difference between the output of the neural network y and t (target) becomes smaller and smaller.
- Goal is to minimize Error (difference) as we did for one layer neural network

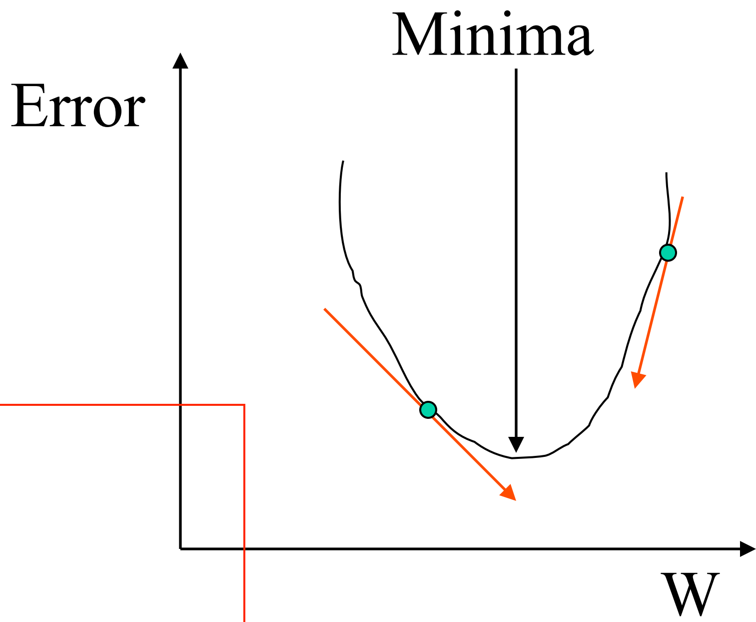
Adjust Weights using Gradient Descent (Back-Propagation)

Known:

Data: $(x_1,x_2,x_3,\ldots,x_n)$ target t.

Unknown weights w:

$w_{11}, w_{12}, \ldots$



Randomly initialize weights

Repeat

for each example, compute output y

calculate error $E = (y-t)^2$

compute the derivative of E over w: $dw = \frac{\partial E}{\partial w}$

$w_{\text{new}} = w_{\text{prev}} - \eta * dw$

Until error doesn't decrease or max num of iterations

Note: η is learning rate or step size.

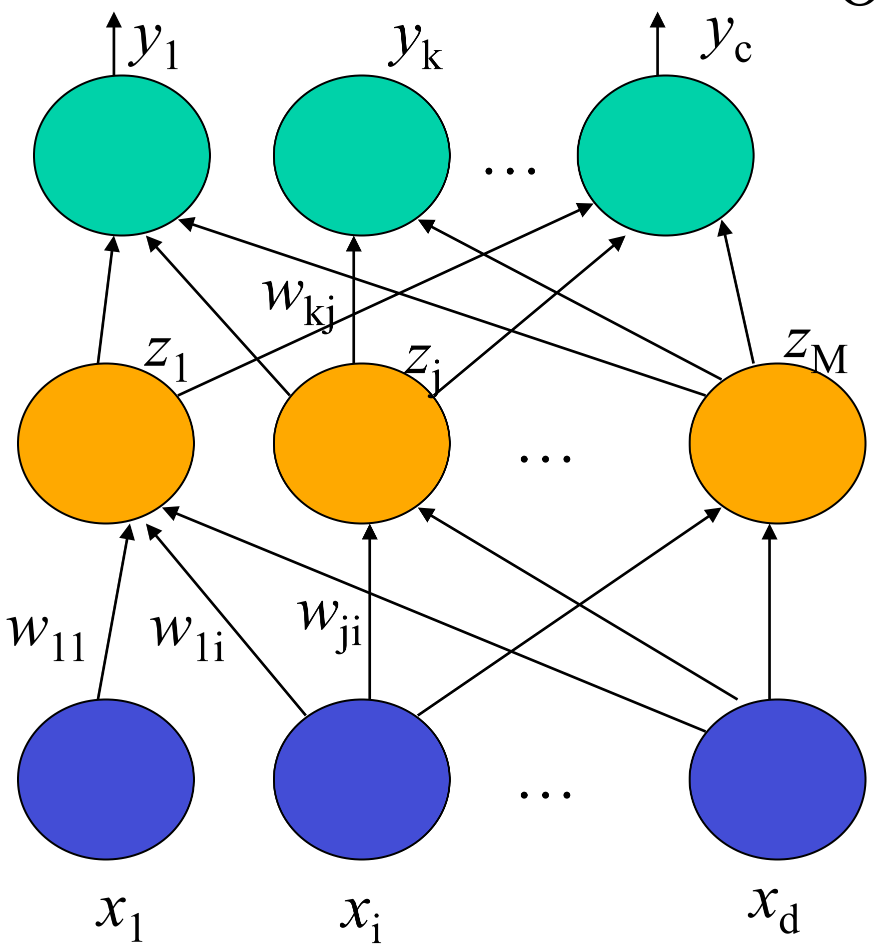
Insights

- We know how to compute the derivative of one layer neural network? How to change weights between input layer and hidden layer?
- Should we compute the derivative of each w separately or we can reuse intermediate results? We will have an efficient back-propagation algorithm.
- We will derive learning for one data example. For multiple examples, we can simply add the derivatives from them for a weight parameter together.

Neural Network Learning: Two Processes

- Forward propagation: present an example (data) into neural network. Compute activation into units and output from units.
- Backward propagation: propagate error back from output layer to the input layer and compute derivatives (or gradients).

Forward Propagation



Output y_k

Activation function: f (linear,sigmoid, softmax)

Activation of unit a_k: $\sum_{j=1}^{M} w_{kj} z_j$

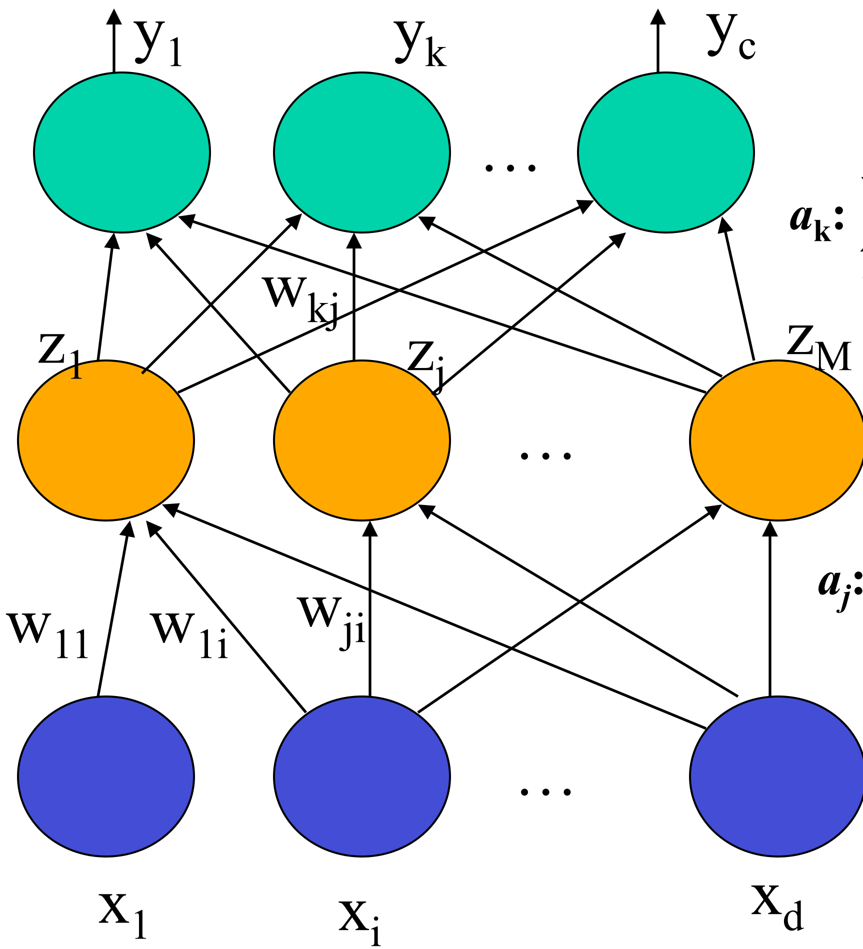
z_j

Activation function: g (linear, tanh, sigmoid)

Activation of unit a_j: $\sum_{i=1}^{d} w_{ji} x_i$

Time complexity?
O(dM + MC) = O(W)

Backward Propagation



f

a_k: $\sum_{j=1}^{M} w_{kj} z_j$

g

a_j: $\sum_{i=1}^{d} w_{ji} x_i$

$$E = \frac{1}{2}\sum_{k=1}^{C}(y_k - t_k)^2$$

$$\frac{\partial E}{\partial y_k} = y_k - t_k$$

$$\frac{\partial E}{\partial a_k} = \frac{\partial E}{\partial y_k}\frac{\partial y_k}{\partial a_k} = (y_k - t_k) f'(a_k) = \delta_k$$

$$\frac{\partial E}{\partial w_{kj}} = \frac{\partial E}{\partial a_k}\frac{\partial a_k}{\partial w_{kj}} = \delta_k z_j$$

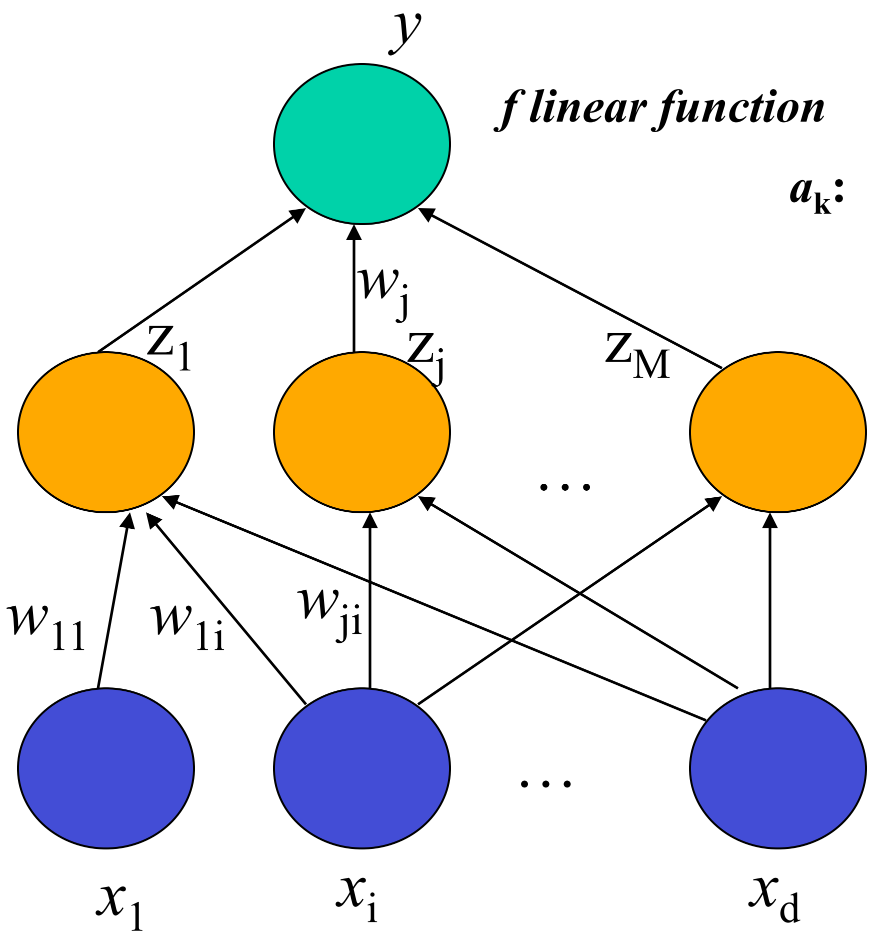
$$\frac{\partial E}{\partial a_j} = \sum_{k=1}^{c}\frac{\partial E}{\partial y_k}\frac{\partial y_k}{\partial a_k}\frac{\partial a_k}{\partial z_j}\frac{\partial z_j}{\partial a_j} = \sum_{k=1}^{C}\delta_k w_{kj} g'(a_j) = \delta_j$$

$$\frac{\partial E}{\partial w_{ji}} = \frac{\partial E}{\partial a_j}\frac{\partial a_j}{\partial wji} = \delta_j x_i$$

If no back-propagation, time complexity is: (MdC+CM)

Time complexity?
O(CM+Md) = O(W)

Example



f linear function

a_k:

g is sigmoid:

a_j: $\sum_{i=1}^{M} w_{ji} x_i$

$$E = \frac{1}{2}(y - t)^2$$

$$\delta = \frac{\partial E}{\partial a_k} = \frac{\partial E}{\partial y}\frac{\partial y}{\partial a_k} = (y - t)$$

$$\frac{\partial E}{\partial w_j} = \delta z_j$$

$$\delta_j = \delta w_j g'(a_j) = (y - t) w_j z_j (1 - z_j)$$

$$\frac{\partial E}{\partial w_{ji}} = \delta_j x_i = (y - t) w_j z_j (1 - z_j) x_i$$

Algorithm

- **Initialize** weights w
- **Repeat**

  For each data point x, do the following:

  Forward propagation: compute outputs and activations

  Backward propagation: compute errors for each output units and hidden units. Compute gradient for each weight.

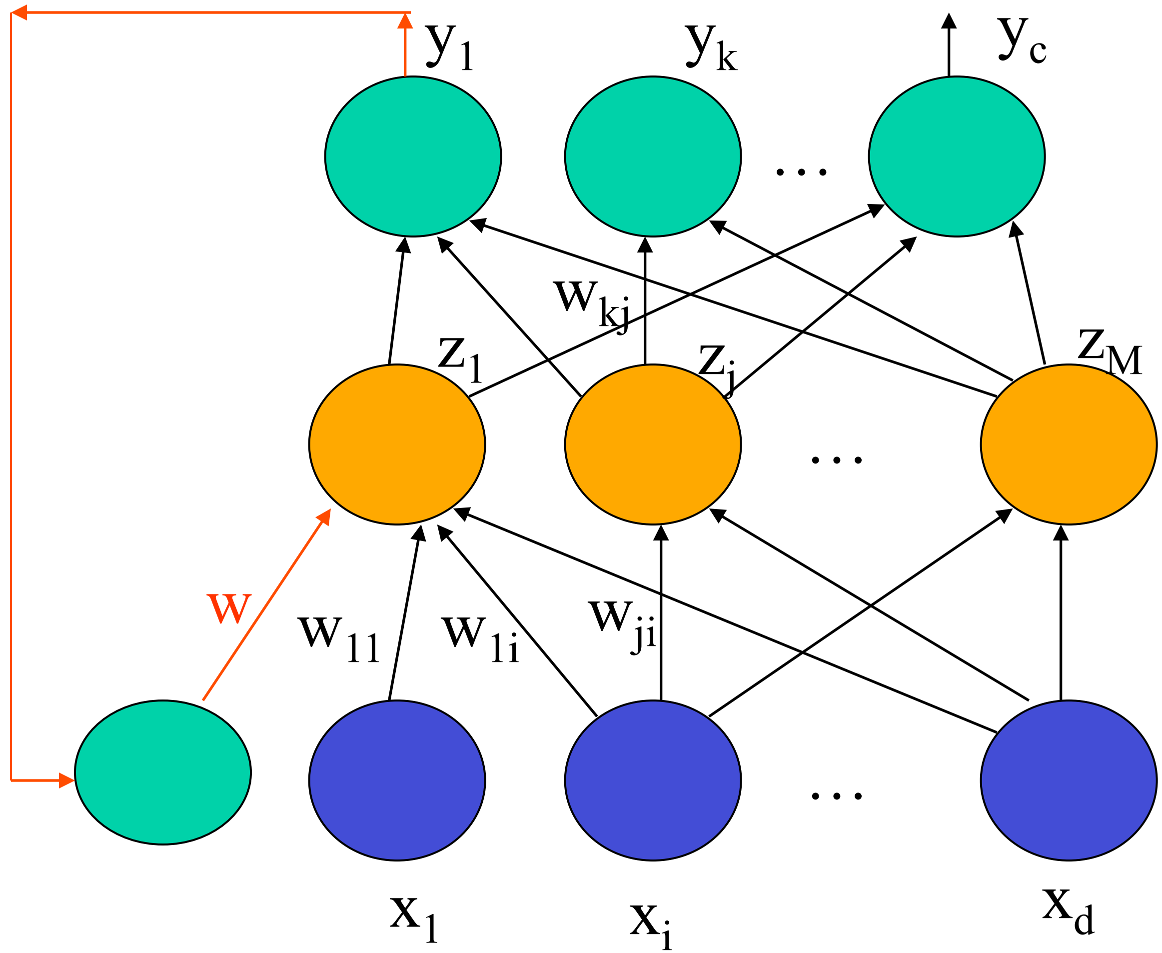
  Update weight $w = w - \eta \, (\partial E / \partial w)$

- **Until** a number of iterations or errors drops below a threshold.

Implementation Issue

- What should we store?
- An input vector x of *d* dimensions
- A M*d matrix $\{w_{ji}\}$ for weights between input and hidden units
- An activation vector of M dimensions for hidden units
- An output vector of M dimensions for hidden units
- A C*M matrix $\{w_{kj}\}$ for weights between hidden and output units
- An activation vector of C dimensions for output units
- An output vector of C dimensions for output units
- An error vector of C dimensions for output units
- An error vector of M dimensions for hidden units

Recurrent Network



Forward:
At time 1: present X1, 0
At time 2: present X2, y1
……

Backward:
Time t: back-propagate
Time t-1: back-propagate with
Output errors and errors from previous step

Recurrent Neural Network

1. Recurrent network is essentially a series of feed-forward neural networks sharing the same weights

2. Recurrent network is good for time series data and sequence data such as biological sequences.

Overfitting

- The training data contains information about the regularities in the mapping from input to output. But it also contains noise
  - The target values may be unreliable.
  - There is sampling error. There will be accidental regularities just because of the particular training cases that were chosen.
- When we fit the model, it cannot tell which regularities are real and which are caused by sampling error.
  - So it fits both kinds of regularity.
  - If the model is very flexible it can model the sampling error really well. This is a disaster.

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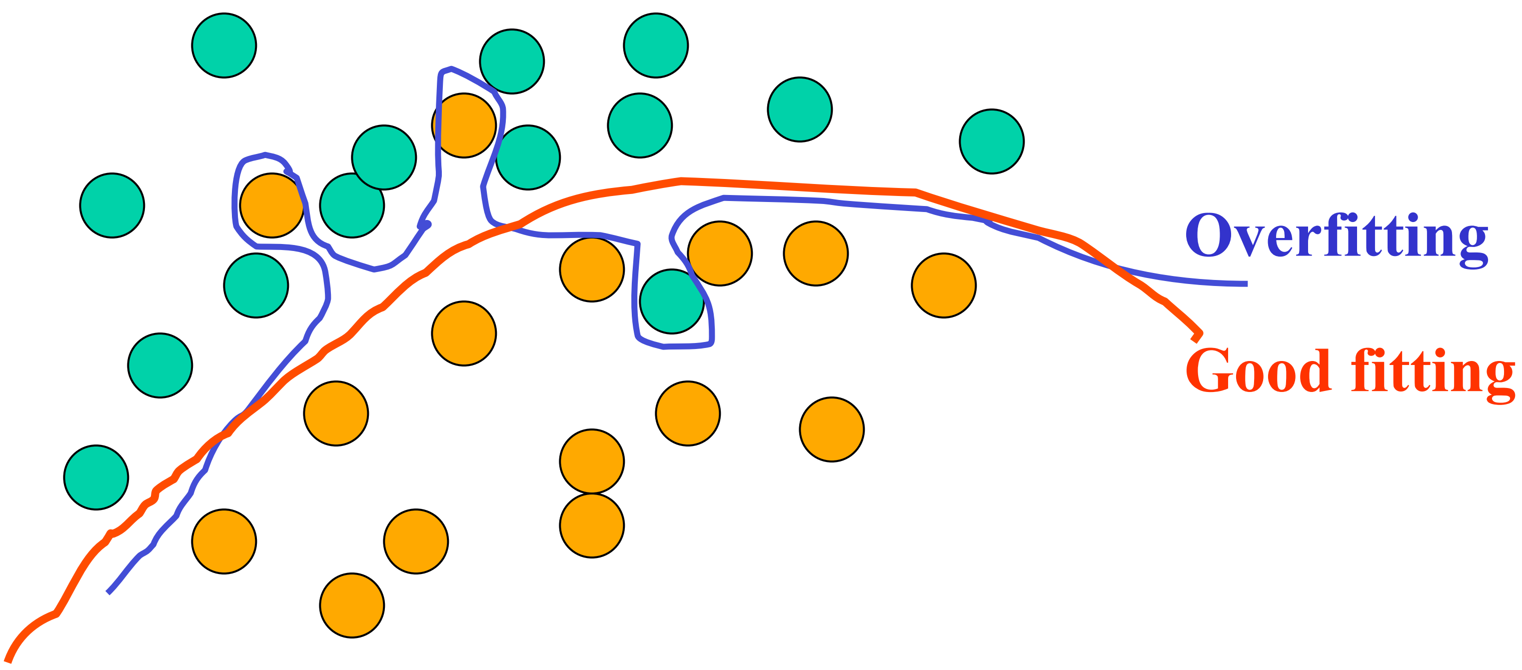
Example of Overfitting and Good Fitting



Overfitting function can not generalize well to unseen data.

Preventing Overfitting

- Use a model that has the right capacity:
  - enough to model the true regularities
  - not enough to also model the spurious regularities (assuming they are weaker).
- Standard ways to limit the capacity of a neural net:
  - Limit the number of hidden units.
  - Limit the size of the weights.
  - Stop the learning before it has time to overfit.

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Limiting the Size of the Weights

- Weight-decay involves adding an extra term to the cost function that penalizes the squared weights.
  - Keeps weights small unless they have big error

$$C = E + \frac{\lambda}{2}\sum_i w_i^2$$

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$$\frac{\partial C}{\partial w_i} = \frac{\partial E}{\partial w_i} + \lambda w_i$$

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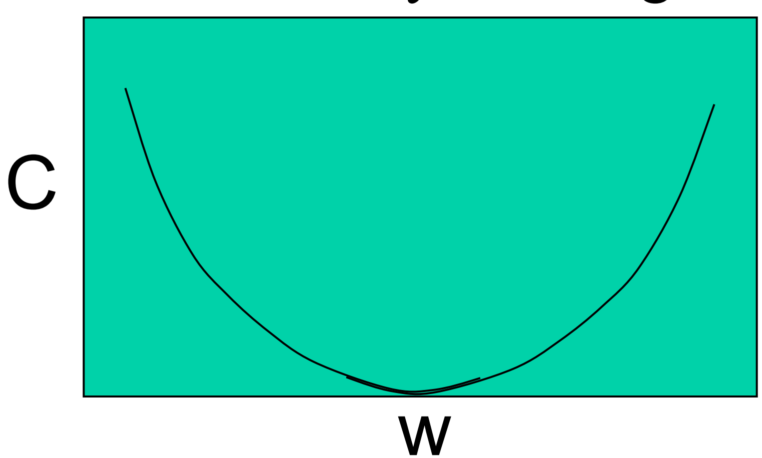
$$when \quad \frac{\partial C}{\partial w_i} = 0, \quad w_i = -\frac{1}{\lambda}\frac{\partial E}{\partial w_i}$$



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The Effect of Weight-Decay

- It prevents the network from using weights that it does not need.
  - This can often improve generalization a lot.
  - It helps to stop it from fitting the sampling error.
  - It makes a smoother model in which the output changes more slowly as the input changes.
- If the network has two very similar inputs it prefers to put half the weight on each rather than all the weight on one.

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Deciding How Much to Restrict the Capacity

- How do we decide which limit to use and how strong to make the limit?
  - If we use the test data we get an unfair prediction of the error rate we would get on new test data.
  - Suppose we compared a set of models that gave random results, the best one on a particular dataset would do better than chance. But it wont do better than chance on another test set.
- So use a separate validation set to do model selection.

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Using a Validation Set

- Divide the total dataset into three subsets:
  - Training data is used for learning the parameters of the model.
  - Validation data is not used of learning but is used for deciding what type of model and what amount of regularization works best.
  - Test data is used to get a final, unbiased estimate of how well the network works. We expect this estimate to be worse than on the validation data.
- We could then re-divide the total dataset to get another unbiased estimate of the true error rate.

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Preventing Overfitting by Early Stopping

- If we have lots of data and a big model, its very expensive to keep re-training it with different amounts of weight decay.
- It is much cheaper to start with very small weights and let them grow until the performance on the validation set starts getting worse (but don't get fooled by noise!)
- The capacity of the model is limited because the weights have not had time to grow big.

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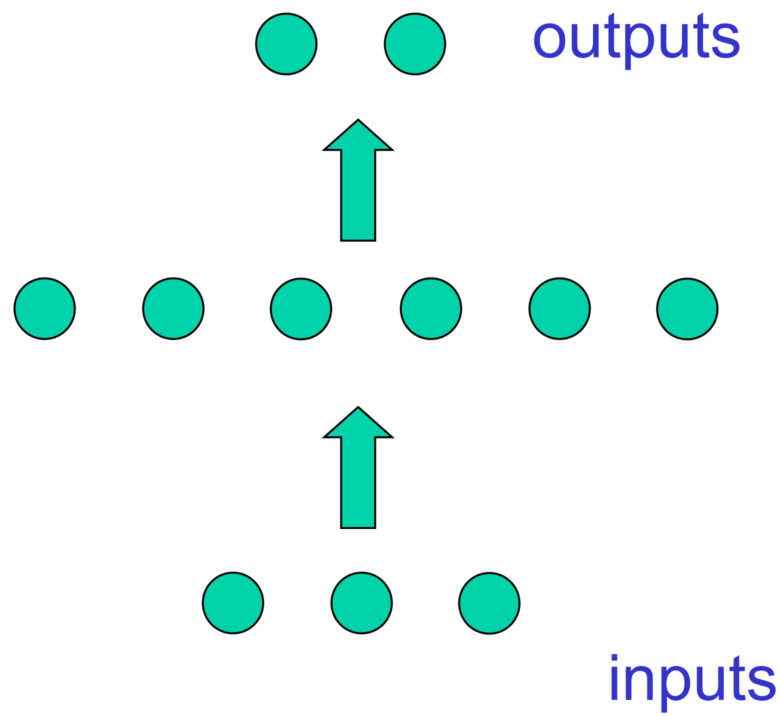
Why Early Stopping Works

- When the weights are very small, every hidden unit is in its linear range.
  - So a net with a large layer of hidden units is linear.
  - It has no more capacity than a linear net in which the inputs are directly connected to the outputs!
- As the weights grow, the hidden units start using their non-linear ranges so the capacity grows.



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Combining Networks

- When the amount of training data is limited, we need to avoid overfitting.
  - Averaging the predictions of many different networks is a good way to do this.
  - It works best if the networks are as different as possible.
  - Combining networks reduces variance
- If the data is really a mixture of several different “regimes” it is helpful to identify these regimes and use a separate, simple model for each regime.
  - We want to use the desired outputs to help cluster cases into regimes. Just clustering the inputs is not as efficient.

How the Combined Predictor Compares with the Individual Predictors

- On any one test case, some individual predictors will be better than the combined predictor.
  - But different individuals will be better on different cases.
- If the individual predictors disagree a lot, the combined predictor is typically better than all of the individual predictors when we average over test cases.
  - So how do we make the individual predictors disagree? (without making them much worse individually).

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Ways to Make Predictors Differ

- Rely on the learning algorithm getting stuck in a different local optimum on each run.
  - A dubious hack unworthy of a true computer scientist (but definitely worth a try).
- Use lots of different kinds of models:
  - Different architectures
  - Different learning algorithms.
- Use different training data for each model:
  - Bagging: Resample (with replacement) from the training set: a,b,c,d,e -> a c c d d
  - Boosting: Fit models one at a time. Re-weight each training case by how badly it is predicted by the models already fitted.
    - This makes efficient use of computer time because it does not bother to "back-fit" models that were fitted earlier.

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How to Speedup Learning?
The Error Surface for a Linear Neuron

- The error surface lies in a space with a horizontal axis for each weight and one vertical axis for the error.
  - It is a quadratic bowl.
    - i.e. the height can be expressed as a function of the weights without using powers higher than 2. Quadratics have constant curvature (because the second derivative must be a constant)
  - Vertical cross-sections are parabolas.
  - Horizontal cross-sections are ellipses

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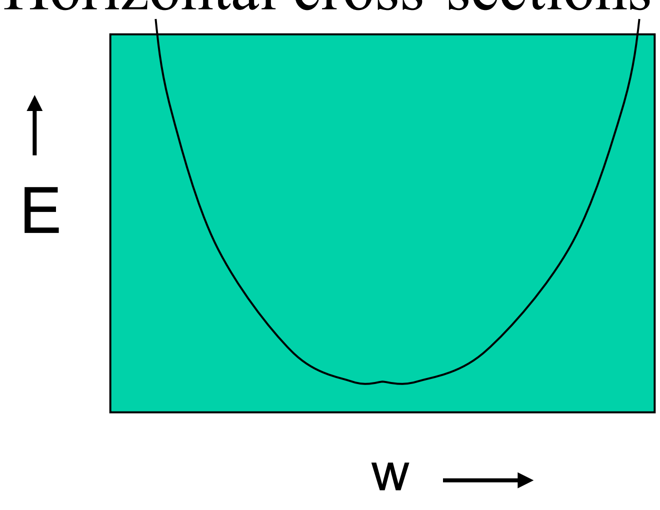
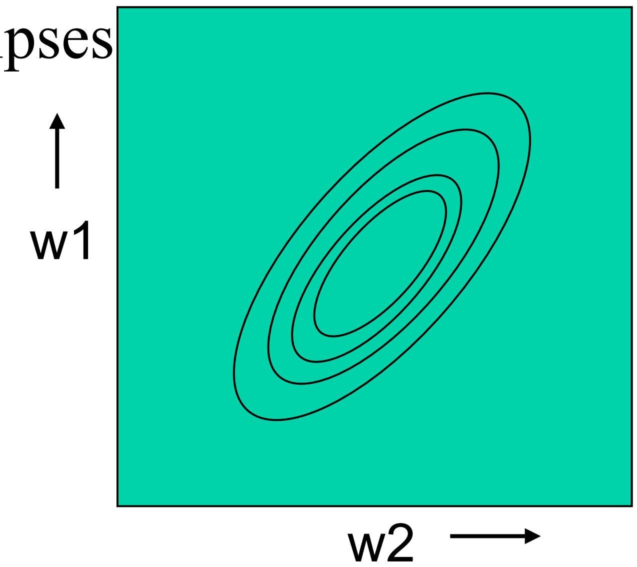
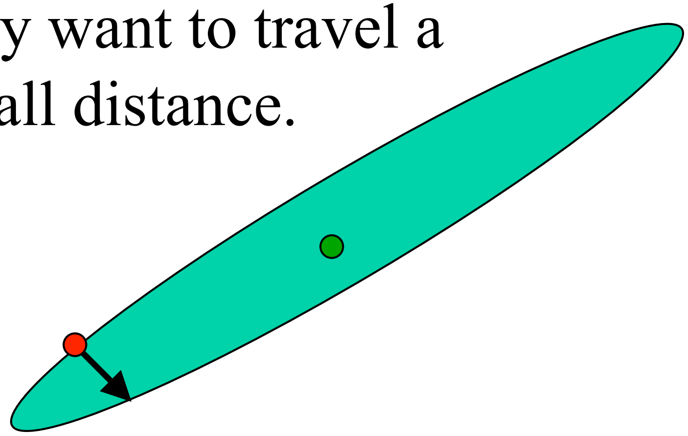




Convergence Speed

- The direction of steepest descent does not point at the minimum unless the ellipse is a circle.
  - The gradient is big in the direction in which we only want to travel a small distance.
  - The gradient is small in the direction in which we want to travel a large distance.



$$\Delta w_i = -\varepsilon \frac{\partial E}{\partial w_i}$$

This equation is sick. The RHS needs to be multiplied by a term of dimension w^2 to make the dimensions balance.

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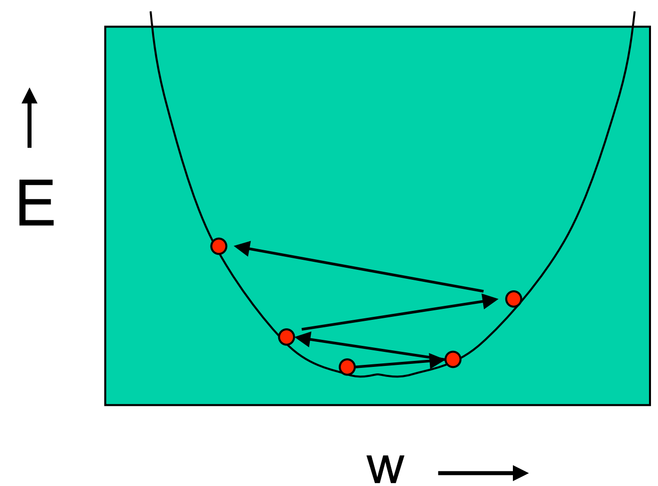
How the Learning Goes Wrong

- If the learning rate is big, it sloshes to and fro across the ravine. If the rate is too big, this oscillation diverges.
- How can we move quickly in directions with small gradients without getting divergent oscillations in directions with big gradients?



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Five Ways to Speed up Learning

- Use an adaptive global learning rate
  - Increase the rate slowly if its not diverging
  - Decrease the rate quickly if it starts diverging
- Use separate adaptive learning rate on each connection
  - Adjust using consistency of gradient on that weight axis
- Use momentum
  - Instead of using the gradient to change the position of the weight "particle", use it to change the velocity.
- Use a stochastic estimate of the gradient from a few cases
  - This works very well on large, redundant datasets.
- Don't go in the direction of steepest descent.
  - The gradient does not point at the minimum.
    - Can we preprocess the data or do something to the gradient so that we move directly towards the minimum?

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The Momentum Method

Imagine a ball on the error surface with velocity v.

- It starts off by following the gradient, but once it has velocity, it no longer does steepest descent.
  - It damps oscillations by combining gradients with opposite signs.
  - It builds up speed in directions with a gentle but consistent gradient.
  - On an inclined plane it reaches a terminal velocity.

$$v(t) = \alpha\, v(t-1) - \varepsilon \frac{\partial E}{\partial w}(t)$$

$$\begin{aligned} \Delta w(t) &= v(t) \\ &= \alpha\, v(t-1) - \varepsilon \frac{\partial E}{\partial w}(t) \\ &= \alpha\, \Delta w(t-1) - \varepsilon \frac{\partial E}{\partial w}(t) \end{aligned}$$

$$v(\infty) = \frac{1}{1-\alpha}\left(-\varepsilon \frac{\partial E}{\partial w}\right)$$

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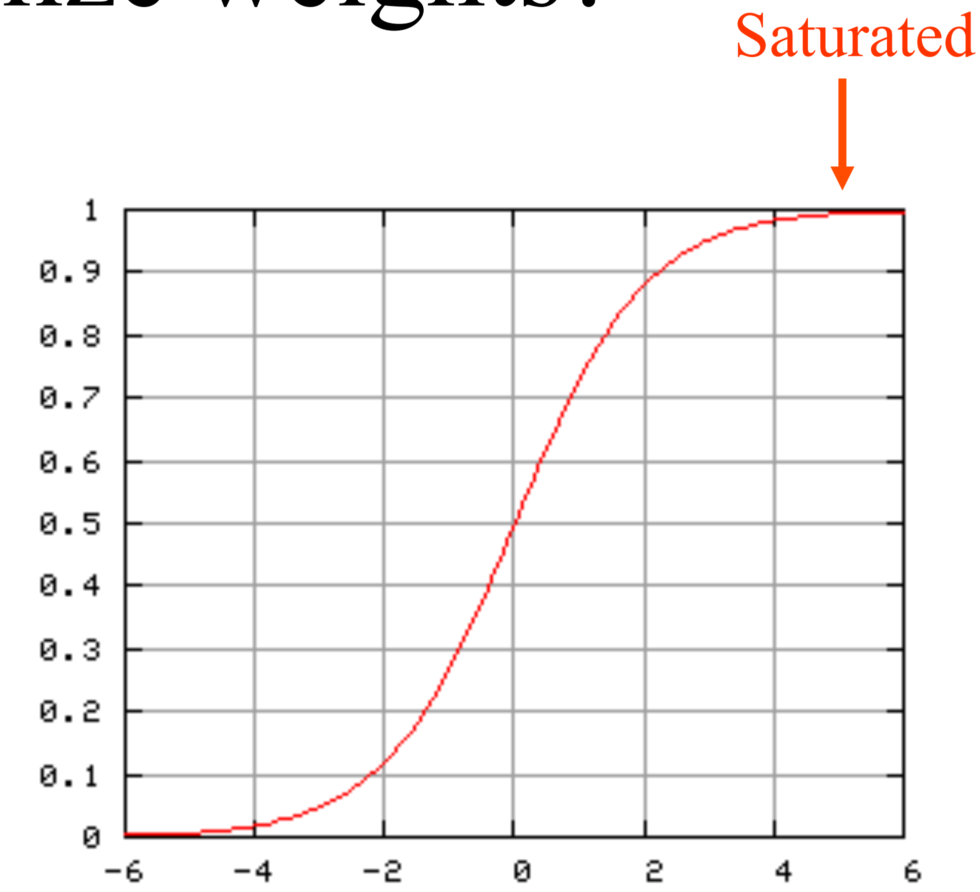
How to Initialize weights?

- Use small random numbers. For instance small numbers between [-0.2, 0.2].
- Some numbers are positive and some are negative.
- Why are the initial weights should be small?



$$\frac{1}{1+e^{-wx}}$$

Neural Network Software

- **Weka** (Java): http://www.cs.waikato.ac.nz/ml/weka/

- **NNClass** and **NNRank** (C++): http://www.eecs.ucf.edu/~jcheng/cheng_software.html

  J. Cheng, Z. Wang, G. Pollastri. A Neural Network Approach to Ordinal Regression. IJCNN, 2008

NNClass Demo

- Abalone data:
  http://archive.ics.uci.edu/ml/datasets/Abalone

UCI Machine Learning Repository

Abalone (from Spanish *Abulón*) are a group of shellfish (mollusks) in the family **Haliotidae** and the ***Haliotis*** genus. They are marine snails