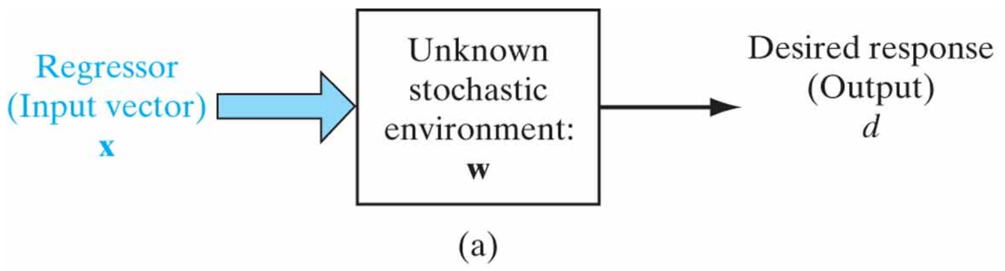
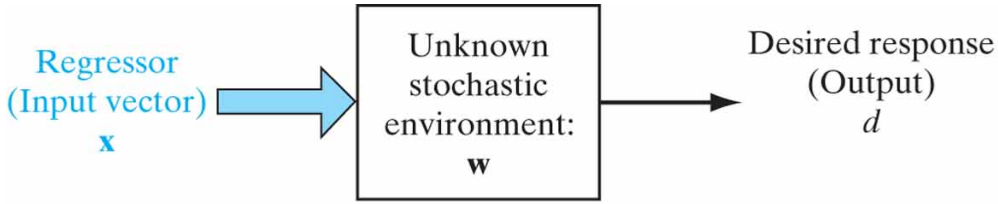
CSE 5526: Introduction to Neural Networks

Linear Regression

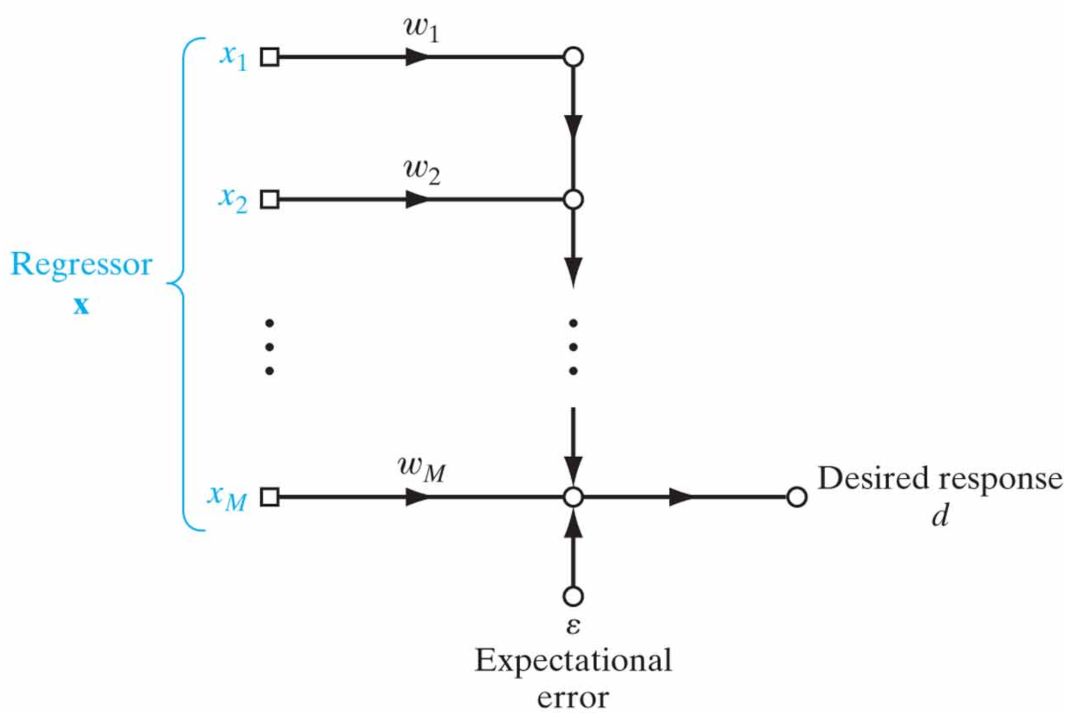
Problem statement



Problem statement



(a)



(b)

Linear regression with one variable

- Given a set of N pairs of data $< x_i, d_i >$, approximate d by a linear function of x (regressor)

  i.e.

$$d \approx wx + b$$

  or

$$d_i = y_i + \varepsilon_i = \varphi(wx_i + b) + \varepsilon_i$$
$$= wx_i + b + \varepsilon_i$$

  where the activation function $\varphi(x) = x$ is a linear function, and it corresponds to a linear neuron. y is the output of the neuron, and

$$\varepsilon_i = d_i - y_i$$

  is called the regression (expectational) error

Linear regression (cont.)

- The problem of regression with one variable is how to choose *w* and *b* to minimize the regression error

- The least squares method aims to minimize the square error *E*:

$$E = \frac{1}{2}\sum_{i=1}^{N}\varepsilon_i^2 = \frac{1}{2}\sum_{i=1}^{N}(d_i - y_i)^2$$

Linear regression (cont.)

- To minimize the two-variable square function, set

$$\begin{cases} \dfrac{\partial E}{\partial b} = 0 \\[2em] \dfrac{\partial E}{\partial w} = 0 \end{cases}$$

Linear regression (cont.)

$$\frac{\partial E}{\partial b} = \frac{1}{2}\sum_i \frac{\partial (d_i - wx_i - b)^2}{\partial b}$$

$$= -\sum_i (d_i - wx_i - b) = 0$$

$$\frac{\partial E}{\partial w} = \frac{1}{2}\sum_i \frac{\partial (d_i - wx_i - b)^2}{\partial w}$$

$$= -\sum_i (d_i - wx_i - b)x_i = 0$$

Linear regression (cont.)

- Hence

$$b = \frac{\sum_i x_i^2 \sum_i d_i - \sum_i x_i \sum_i x_i d_i}{N[\sum_i (x_i - \bar{x})^2]}$$

Derive yourself!

$$w = \frac{\sum_i (x_i - \bar{x})(d_i - \bar{d})}{\sum_i (x_i - \bar{x})^2}$$

where an overbar (i.e. $\bar{x}$) indicates the mean

Linear regression (cont.)

- This method gives an optimal solution, but it can be time- and memory-consuming as a batch solution

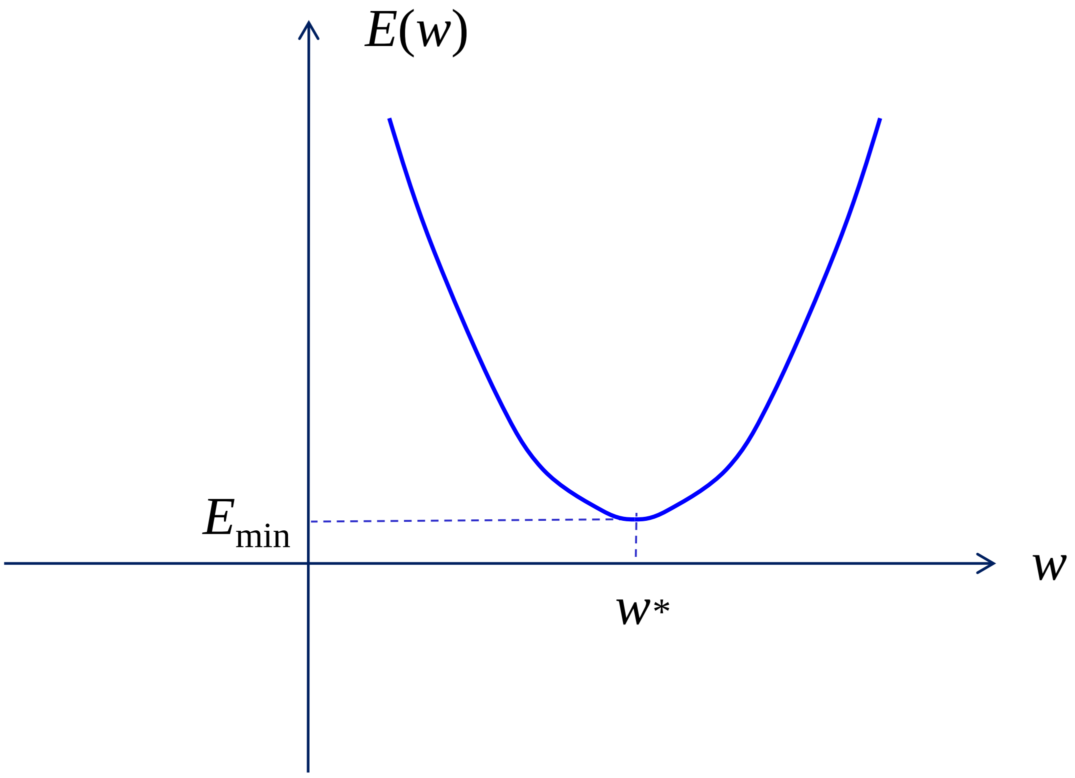
Finding optimal parameters via search

- Without loss of generality, set $b = 0$

$$E(w) = \frac{1}{2}\sum_{i=1}^{N}(d_i - wx_i)^2$$

$E(w)$ is called a cost function

Cost function



- Question: how can we update w to minimize E?

Gradient and directional derivatives

- Without loss of generality, consider a two-variable function $f(x, y)$. The gradient of $f(x, y)$ at a given point $(x_0, y_0)^T$ is

$$\nabla f = \left(\frac{\partial f(x,y)}{\partial x}, \frac{\partial f(x,y)}{\partial y}\right)^T \Bigg|_{\substack{x=x_0 \\ y=y_0}}$$

$$= f_x(x_0, y_0)\mathbf{u}_x + f_y(x_0, y_0)\mathbf{u}_y$$

where $\mathbf{u}_x$ and $\mathbf{u}_y$ are unit vectors in the x and y directions, and $f_x = \partial f / \partial x$ and $f_y = \partial f / \partial y$

Gradient and directional derivatives (cont.)

- At any given direction, $\mathbf{u} = a\mathbf{u}_x + b\mathbf{u}_y$, with $\sqrt{a^2+b^2}=1$, the directional derivative at $(x_0, y_0)^T$ along the unit vector $\mathbf{u}$ is

$$D_{\mathbf{u}} f(x_0, y_0) = \lim_{h\to 0} \frac{f(x_0+ha, y_0+hb) - f(x_0, y_0)}{h}$$

$$= \lim_{h\to 0} \frac{[f(x_0+ha, y_0+hb) - f(x_0, y_0+hb)] + [f(x_0, y_0+hb) - f(x_0, y_0)]}{h}$$

$$= af_x(x_0, y_0) + bf_y(x_0, y_0)$$

$$= \nabla f^T(x_0, y_0)\mathbf{u}$$

  - Which direction has the greatest slope?
    - **The gradient** because of the dot product!

Gradient and directional derivatives (cont.)

- Example: see blackboard

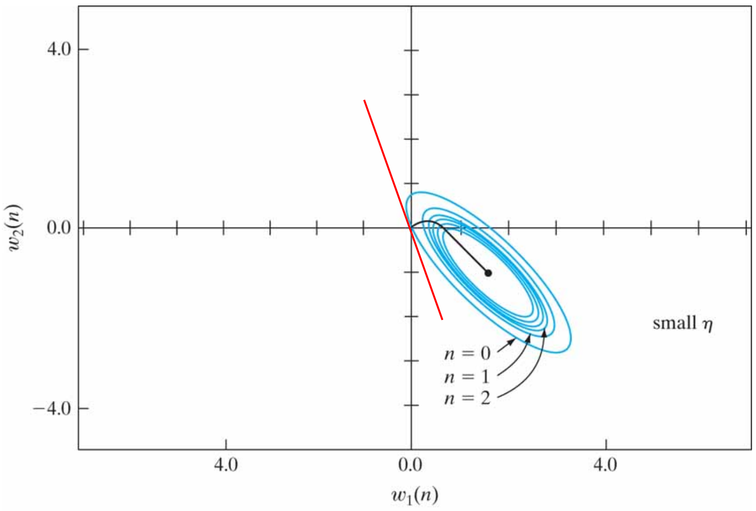
Gradient and directional derivatives (cont.)

- To find the gradient at a particular point $(x_0, y_0)^T$, first find the level curve or contour of $f(x, y)$ at that point, $C(x_0, y_0)$. A tangent vector **u** to C satisfies

$$D_{\mathbf{u}} = \nabla f^T(x_0, y_0)\mathbf{u} = 0$$

because $f(x, y)$ is constant on a level curve. Hence the gradient vector is perpendicular to the tangent vector

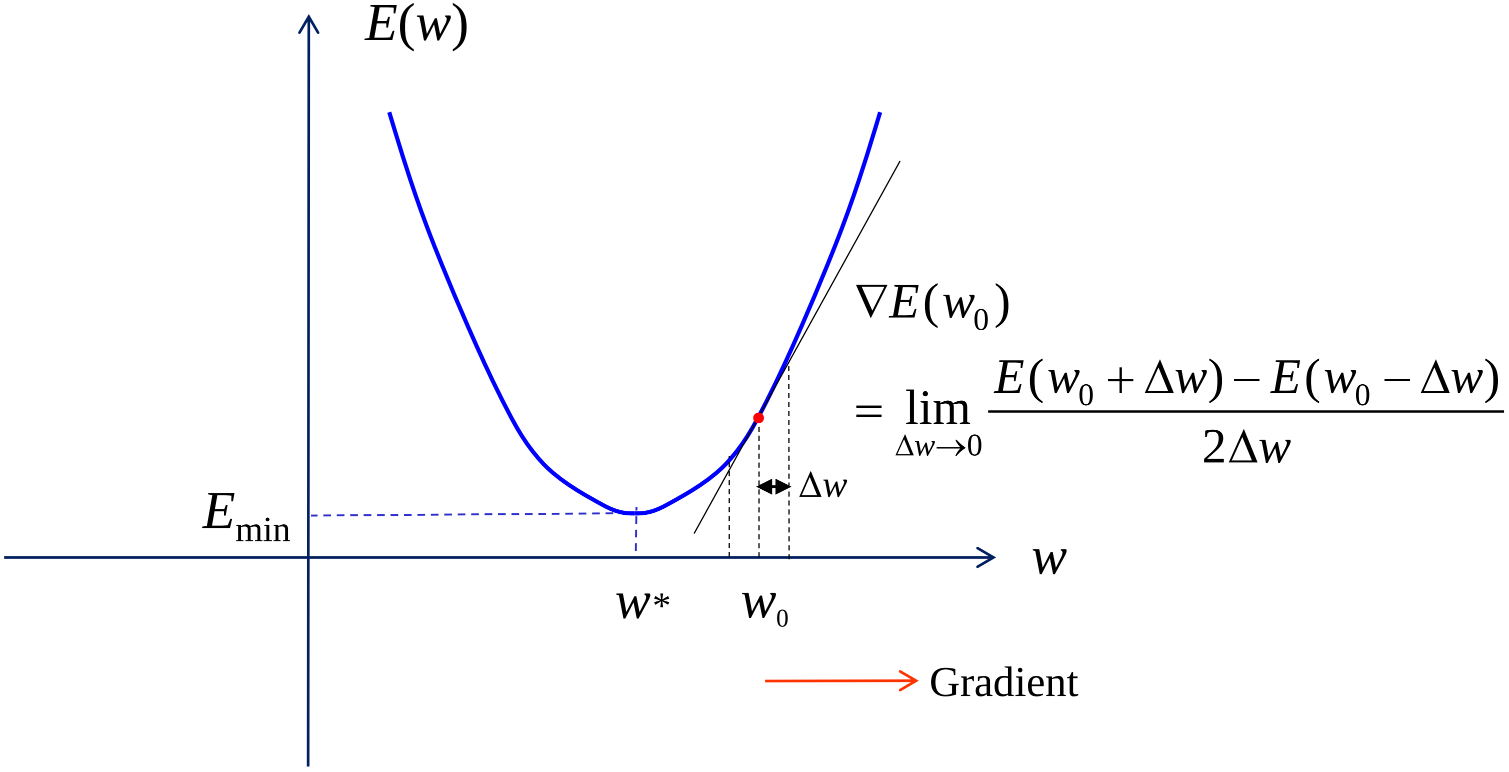
An illustration of level curves



Gradient and directional derivatives (cont.)

- The gradient of a cost function is a vector with the dimension of **w** that points to the direction of maximum *E* increase and with a magnitude equal to the slope of the tangent of the cost function along that direction
  - Can the slope be negative?

Gradient illustration



Gradient descent

- Minimize the cost function via gradient (steepest) descent – a case of hill-climbing

$$w(n+1) = w(n) - \eta \nabla E(n)$$

n: iteration number
η: learning rate

- See previous figure

Gradient descent (cont.)

- For the mean-square-error cost function:

$$E(n) = \frac{1}{2}e^2(n) = \frac{1}{2}[d(n) - y(n)]^2$$

$$= \frac{1}{2}[d(n) - w(n)x(n)]^2 \qquad \text{linear neurons}$$

$$\nabla E(n) = \frac{\partial E}{\partial w(n)} = \frac{1}{2}\frac{\partial e^2(n)}{\partial w(n)}$$

$$= -e(n)x(n)$$

Gradient descent (cont.)

- Hence

$$w(n+1) = w(n) + \eta e(n) x(n)$$

$$= w(n) + \eta [d(n) - y(n)] x(n)$$

  - This is the least-mean-square (LMS) algorithm, or the Widrow-Hoff rule

Multi-variable case

- The analysis for the one-variable case extends to the multi-variable case

$$E(n) = \frac{1}{2}[d(n) - \mathbf{w}^T(n)\mathbf{x}(n)]^2$$

$$\nabla E(\mathbf{w}) = \left(\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \ldots, \frac{\partial E}{\partial w_m}\right)^T$$

where $w_0 = b$ (bias) and $x_0 = 1$, as done for perceptron learning

Multi-variable case (cont.)

- The LMS algorithm

$$\mathbf{w}(n+1) = \mathbf{w}(n) - \eta \nabla E(n)$$

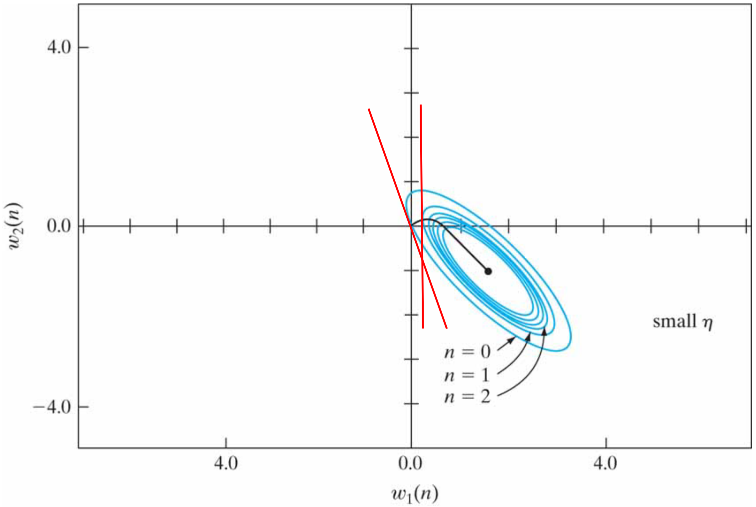
$$= \mathbf{w}(n) + \eta e(n)\mathbf{x}(n)$$

$$= \mathbf{w}(n) + \eta[d(n) - y(n)]\mathbf{x}(n)$$

LMS algorithm

- **Remarks**
  - The LMS rule is exactly the same in math form as the perceptron learning rule
  - Perceptron learning is for McCulloch-Pitts neurons, which are nonlinear, whereas LMS learning is for linear neurons. In other words, perceptron learning is for classification and LMS is for function approximation
  - LMS should be less sensitive to noise in the input data than perceptrons. On the other hand, LMS learning converges slowly
  - Newton's method changes weights in the direction of the minimum $E(\mathbf{w})$ and leads to fast convergence. But it is not an online version and computationally extensive

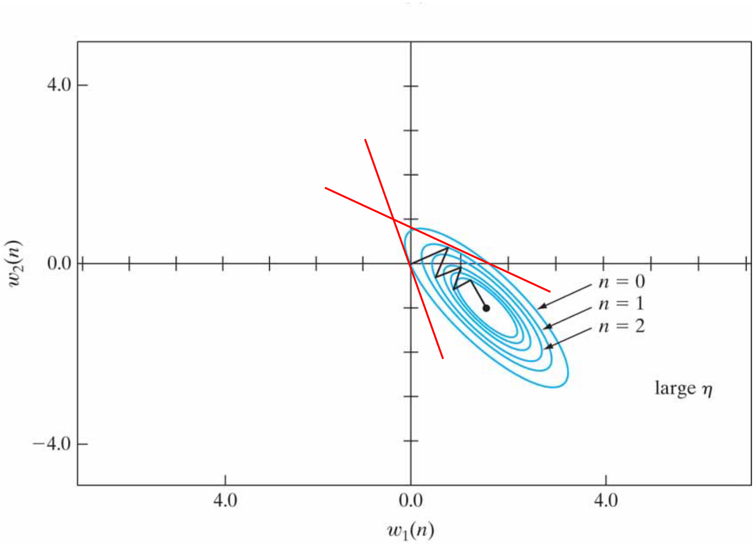
Stability of adaptation



(a)

- When η is too small, learning converges slowly

Stability of adaptation (cont.)



(b)

- When η is too large, learning doesn't converge

Learning rate annealing

- Basic idea: start with a large rate but gradually decrease it
- **Stochastic approximation**

$$\eta(n) = \frac{c}{n}$$

c is a positive parameter

Learning rate annealing (cont.)

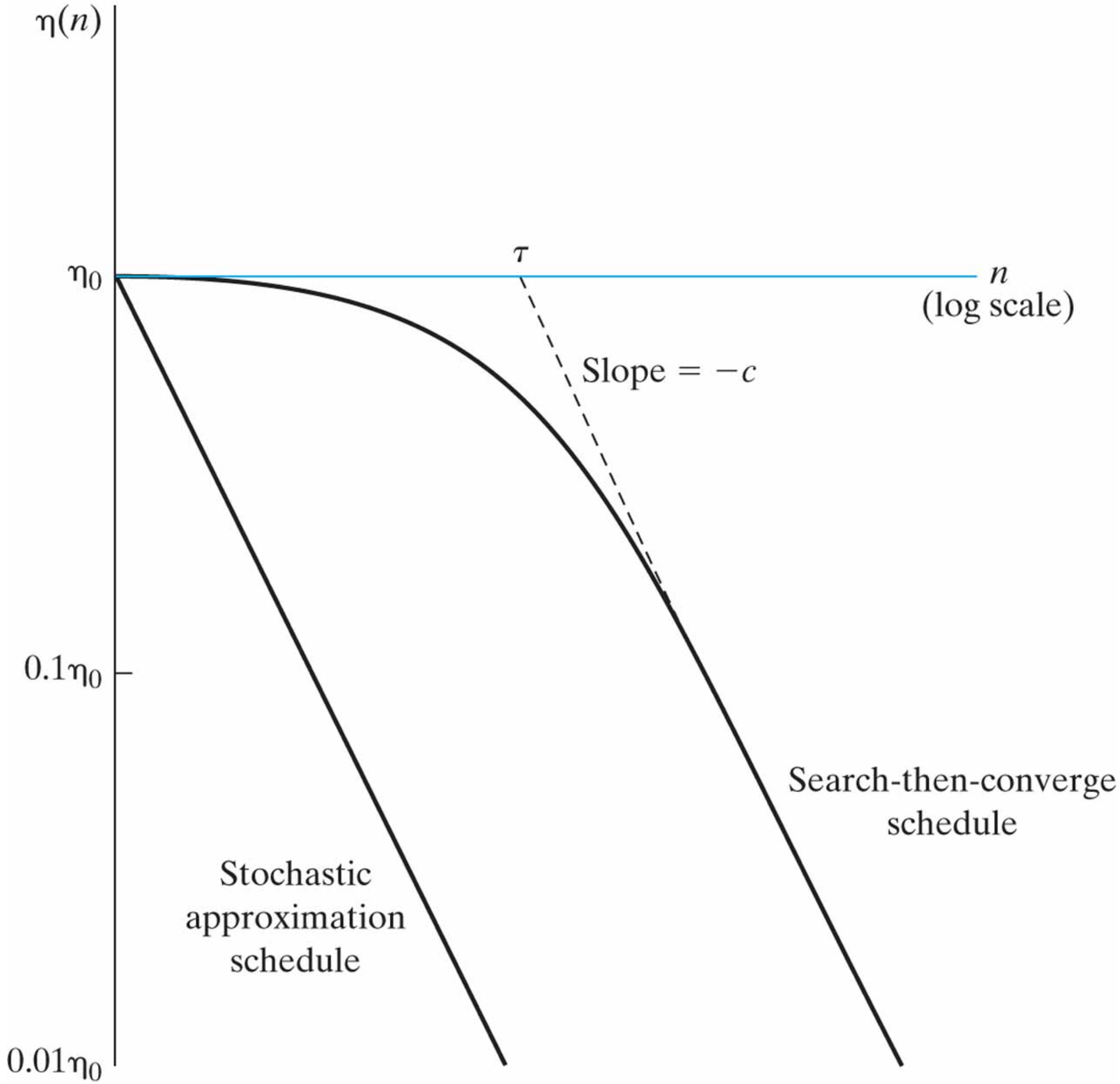
- **Search-then-converge**

$$\eta(n) = \frac{\eta_0}{1 + (n/\tau)}$$

η_0 and τ are positive parameters

- When n is small compared to τ, learning rate is approximately constant
- When n is large compared to τ, learning rate schedule roughly follows stochastic approximation

Rate annealing illustration



Nonlinear neurons

- To extend the LMS algorithm to nonlinear neurons, consider differentiable activation function φ at iteration n

$$E(n) = \frac{1}{2}[d(n) - y(n)]^2$$

$$= \frac{1}{2}[d(n) - \varphi(\sum_j w_j x_j(n))]^2$$

Nonlinear neurons (cont.)

- By chain rule of differentiation

$$\frac{\partial E}{\partial w_j} = \frac{\partial E}{\partial y}\frac{\partial y}{\partial v}\frac{\partial v}{\partial w_j}$$

$$= -[d(n) - y(n)]\varphi'(v(n))x_j(n)$$

$$= -e(n)\varphi'(v(n))x_j(n)$$

Nonlinear neurons (cont.)

- The gradient descent gives

$$w_j(n+1) = w_j(n) + \eta \underline{e(n)\varphi'(v(n))} x_j(n)$$
$$= w_j(n) + \eta \delta(n) x_j(n)$$

  - The above is called the delta (δ) rule
- If we choose a logistic sigmoid for φ

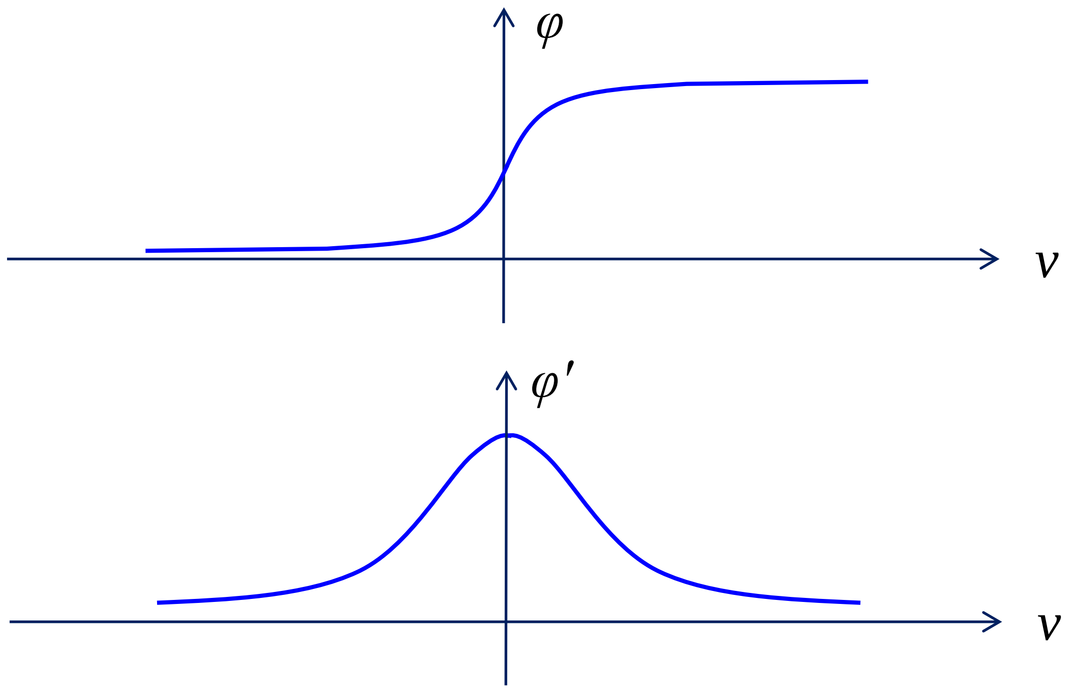
$$\varphi(v) = \frac{1}{1+\exp(-av)}$$

then

$$\varphi'(v) = a\varphi(v)[1-\varphi(v)]$$

(see textbook)

Role of activation function



- The role of φ': weight update is most sensitive when v is near zero