Regression & the LMS Algorithm

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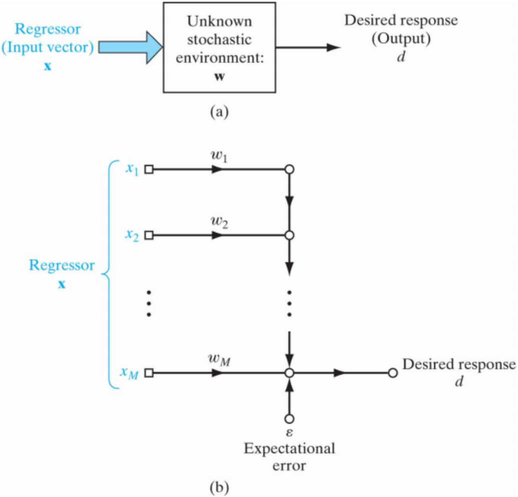
Problem statement



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

$$\begin{aligned} d_i &= y_i + \epsilon_i = \varphi(wx_i + b) + \varepsilon \\ &= wx_i + b + \varepsilon \end{aligned}$$

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

$$\varepsilon_i = d_i - y_i$$

is called the (expectational) regression error.

Linear regression

- 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

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

Linear regression

To minimize the two-variable square function, set

$$\begin{cases} \frac{\partial E}{\partial b} & = 0 \\ \frac{\partial E}{\partial w} & = 0 \end{cases}$$

$$\Rightarrow \begin{cases} -\sum_i (d_i - wx_i - n) & = 0 \\ -\sum_i (d_i - wx_i - b) x_i & = 0 \end{cases}$$

Analytic solution approaches

- Solve one equation for b in terms of w
  - Substitute into other equation, solve for w
  - Substitute solution for w back into equation for b

$$\begin{cases} -\sum_i (d_i - wx_i - b) & = 0 \\ -\sum_i (d_i - wx_i - b)x_i & = 0 \end{cases}$$

$\Rightarrow$

Analytic solution approaches

- Solve one equation for b in terms of w
  - Substitute into other equation, solve for w
  - Substitute solution for w back into equation for b

$$\begin{cases} -\sum_i (d_i - wx_i - b) & = 0 \\ -\sum_i (d_i - wx_i - b)x_i & = 0 \end{cases}$$

$$\Rightarrow \quad b = \frac{\sum_i x_i^2 \sum_i d_i - \sum_i x_i \sum_i x_i d_i}{N \sum_i (x_i - \bar{x})^2}, \quad w = \frac{\sum_i (x_i - \bar{x})(d_i - \bar{d})}{\sum_i (x_i - \bar{x})^2}$$

, where an $\bar{x}$ indicates the mean

There may exist other forms, such as $w = \frac{\sum_i d_i (x_i - \bar{x})}{\sum_i x_i^2 - \frac{1}{m}(\sum_i x_i)^2}$,

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

Analytic solution approaches

- Solve one equation for b in terms of w
  - Substitute into other equation, solve for w
  - Substitute solution for w back into equation for b
- Setup system of equations in matrix notation
  - Solve matrix equation
- Rewrite problem in matrix form
  - Compute matrix gradient
  - Solve for w

Linear regression in matrix notation

Let $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_N]^T$, then the model predictions are $\mathbf{y} = \mathbf{X}\mathbf{w}$. And the mean square error can be written as

$$E(\mathbf{w}) = \|\mathbf{d} - \mathbf{y}\|^2 = \|\mathbf{d} - \mathbf{X}\mathbf{w}\|^2$$

To find the optimal $\mathbf{w}$, set the gradient of the error *w.r.t.* $\mathbf{w}$ equal to 0 and solve for $\mathbf{w}$.

$$\partial E(\mathbf{w}) / \partial \mathbf{w} = 0$$

Linear regression in matrix notation

$$\begin{aligned}
\frac{\partial}{\partial \mathbf{w}} E(\mathbf{w}) &= \frac{\partial}{\partial \mathbf{w}} \|\mathbf{d} - \mathbf{X}\mathbf{w}\|^2 \\
&= \frac{\partial}{\partial \mathbf{w}} (\mathbf{d} - \mathbf{X}\mathbf{w})^T (\mathbf{d} - \mathbf{X}\mathbf{w}) \\
&= \frac{\partial}{\partial \mathbf{w}} \mathbf{d}^T\mathbf{d} - \mathbf{d}^T\mathbf{X}\mathbf{w} - \mathbf{w}^T\mathbf{X}^T\mathbf{d} + \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w} \\
&= 2\mathbf{X}^T\mathbf{X}\mathbf{w} - 2\mathbf{X}^T\mathbf{d} = 0
\end{aligned}$$

$$\Rightarrow \mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{d}$$

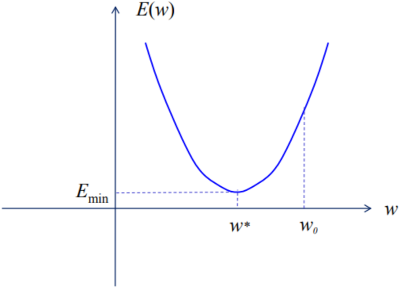
Finding optimal parameters via search

- Often there is no closed form solution for $\frac{\partial}{\partial \mathbf{w}} E(\mathbf{w}) = 0$
- We can still use the gradient in a numerical solution
- We will still use the same example to permit comparison
- For simplicity's sake, set $b = 0$

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

, where $E(w)$ is called cost function.

Cost function



Question: how can we update w from w_0 to minimize E?

Gradient and directional derivatives

Consider a two-variable function $f(x, y)$. Its gradient at the point $(x_0, y_0)^T$ is defined as

$$
\begin{aligned}
\nabla f &= \left(\partial f(x, y)/\partial x, \partial f(x, y)/\partial y\right)^T\Big|_{x=x_0, y=y_0} \\
&= f_x(x_0, y_0)\mathbf{u}_x + f_y(x_0, y_0)\mathbf{u}_y
\end{aligned}
$$

, 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

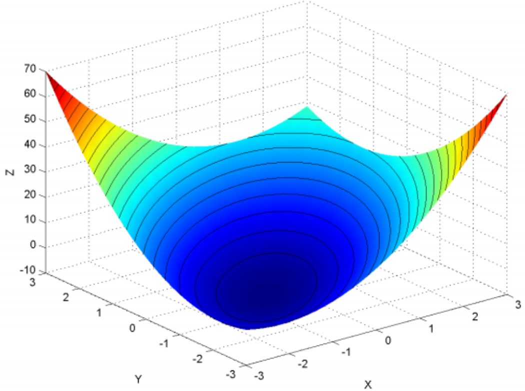
At any given direction, $\mathbf{u} = \alpha \mathbf{u}_x + b\mathbf{u}_y$, with $\sqrt{a^2 + b^2} = 1$, the directional derivative at $(x_0, y_0)^T$ along the unit vector $\mathbf{u}$ is

$$
\begin{aligned}
D_{\mathbf{u}} f(x_0, y_0) &= \lim_{h \to 0} \frac{f(x_0 + ha, y_0 + hb) - f(x_0, y_0)}{h} \\
&= \lim_{h \to 0} \left[f(x_0 + ha, y_0 + hb) - f(x_0, y_0 + hb) \right] / h \\
&\qquad + \left[f(x_0, y_0 + hb) - f(x_0, y_0) \right] / h \\
&= a f_x(x_0, y_0) + b f_y(x_0, y_0) \\
&= \nabla f(x_0, y_0)^T \mathbf{u}
\end{aligned}
$$

Which direction has the greatest slope? The gradient! Because of the dot product.

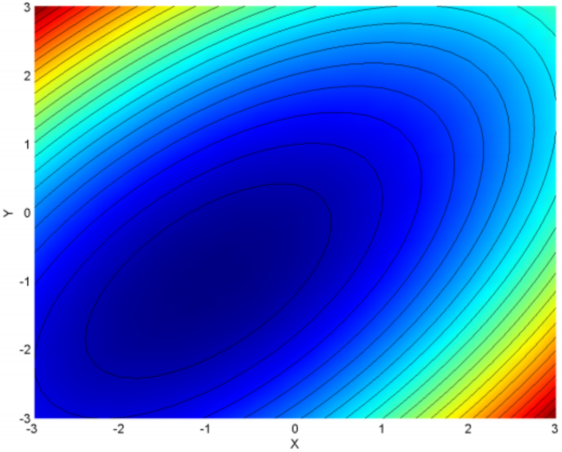
Gradient and directional derivatives

Example: $f(x,y) = 5/2x^2 - 3xy + 5/2y^2 + 2x + 2y$



Gradient and directional derivatives

Example: $f(x, y) = 5/2x^2 - 3xy + 5/2y^2 + 2x + 2y$



Gradient and directional derivatives (cont.)

- The level curves of a function $f(x, y)$ are curves such that $f(x, y) = k$
- Thus, the directional derivative along a level curve is 0

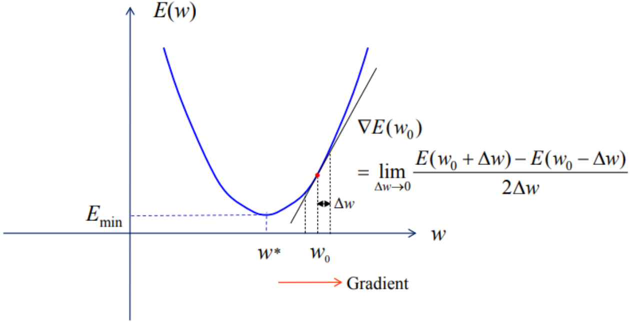
$$D_{\mathbf{u}} = \nabla f(x_0, y_0)^T \mathbf{u} = 0$$

- And the gradient vector is perpendicular to the level curve

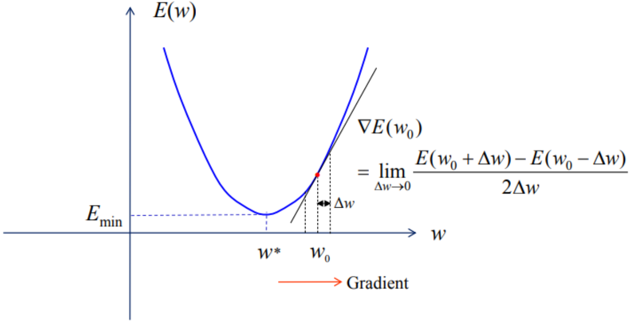
Gradient and directional derivatives (cont.)

- 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

Gradient descent (cont.)

- For the mean-square-error cost function and linear neurons

$$\begin{aligned} E(n) &= \frac{1}{2}e^2(n) = \frac{1}{2}[d(n) - y(n)]^2 \\ &= \frac{1}{2}[d(n) - w(n)x(n)]^2 \\ \nabla E(n) &= \frac{\partial E}{\partial w(n)} = \frac{\partial e^2(n)}{2\partial w(n)} \\ &= -e(n)x(n) \end{aligned}$$

Gradient descent (cont.)

- Hence

$$
\begin{aligned}
w(n+1) &= w(n) + \eta e(n)x(n) \\
&= w(n) + \eta[d(n) - y(n)]x(n)
\end{aligned}
$$

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

Stochastic gradient descent

- If the cost function is of the form

$$E(w) = \sum_{n=1}^{N} E_n(w)$$

- Then one gradient descent step requires computing

$$\Delta = \frac{\partial}{\partial w} E(w) = \sum_{n=1}^{N} \frac{\partial}{\partial w} E_n(w)$$

- Which means computing $E(w)$ or its gradient for every data point
- Many steps may be required to reach an optimum

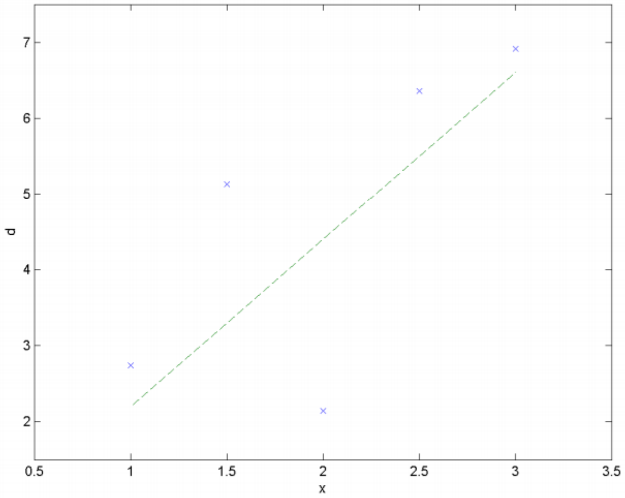
Stochastic gradient descent

- It is generally much more computationally efficient to use

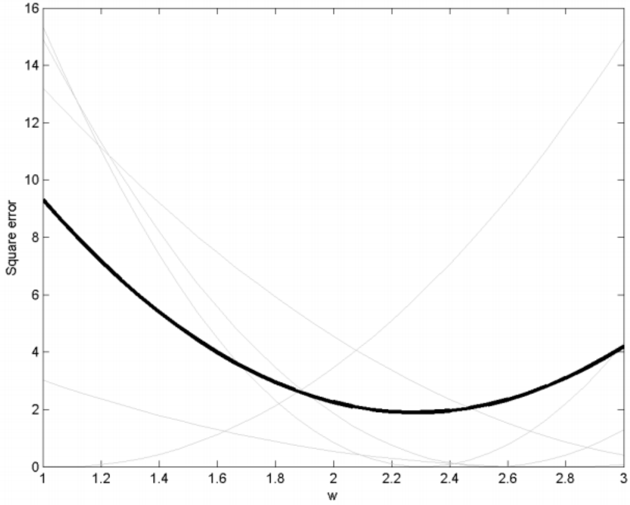
$$\Delta = \sum_{n=n_i}^{n_i+n_b-1} \frac{\partial}{\partial w} E_n(w)$$

- For small values of n_b
- This update rule may converge in many fewer passes through the data (epochs)

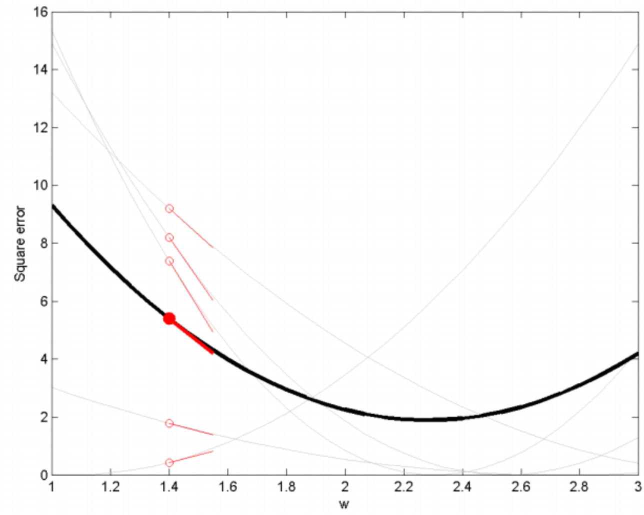
Stochastic gradient descent example



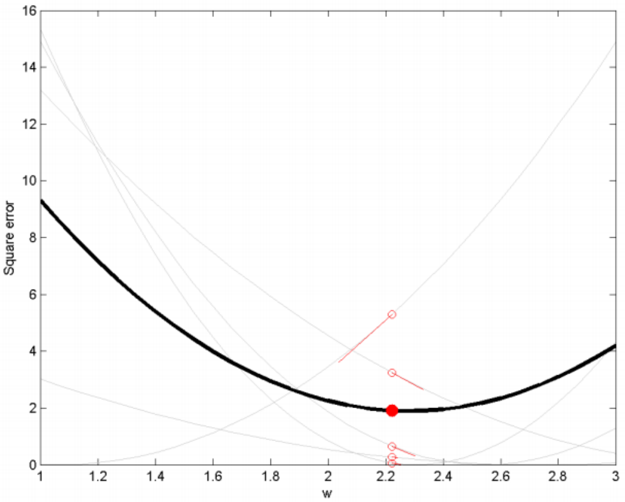
Stochastic gradient descent error functions



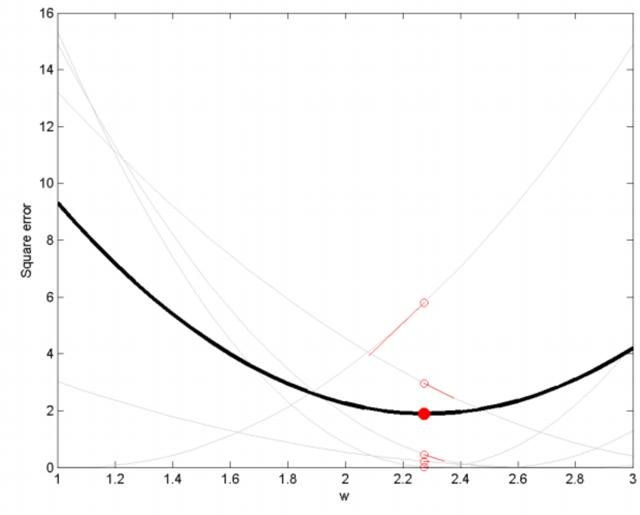
Stochastic gradient descent gradients



Stochastic gradient descent animation



Gradient descent animation



Multi-variable LMS

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

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

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

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

Multi-variable LMS (cont.)

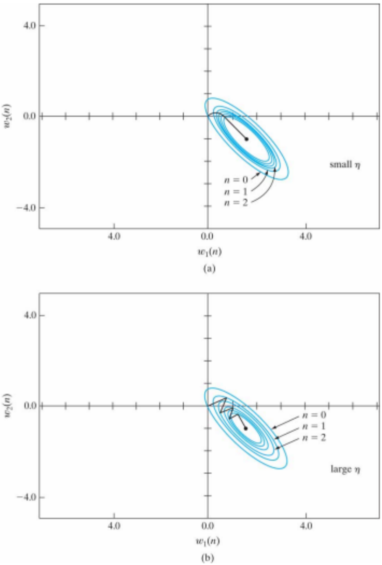
- The LMS algorithm

$$\begin{aligned}\mathbf{w}(n+1) &= \mathbf{w}(n) - \eta \nabla \mathbf{E}(n) \\ &= \mathbf{w}(n) + \eta e(n)\mathbf{x}(n) \\ &= \mathbf{w}(n) + \eta[d(n) - y(n)]\mathbf{x}(n)\end{aligned}$$

LMS algorithm remarks

- The LMS rule is exactly the same equation as the perceptron learning rule
- Perceptron learning is for nonlinear (M-P) neurons, whereas LMS learning is for linear neurons.
  - *i.e.*, 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
- Newtons method changes weights in the direction of the minimum $E(w)$ and leads to fast convergence.
  - But it is not online and is computationally expensive

Stability of adaptation



- When η is too small, learning converges slowly
- When η is too large, learning does not converge

Learning rate annealing

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

$$\eta(n) = c/n$$

c is a positive parameter

Learning rate annealing (cont.)

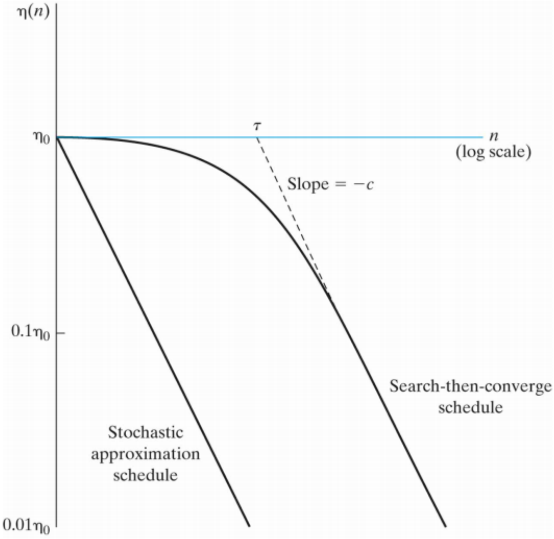
- Search-then-converge

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

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 rule schedule roughly follows stochastic approximation

Rate annealing illustration



Nonlinear neurons

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

$$
\begin{aligned}
E(n) &= 1/2\,[d(n) - y(n)]^2 \\
&= 1/2\left[d(n) - \varphi\left(\sum_j w_j x_j(n)\right)\right]^2
\end{aligned}
$$

Nonlinear neurons (cont.)

- By chain rule of differentiation

$$
\begin{aligned}
\frac{\partial E}{\partial w_j} &= \frac{\partial E}{\partial y}\frac{\partial y}{\partial v}\frac{\partial v}{\partial w_j} \\
&= -[d(n) - y(n)]\varphi'\left(v(n)\right) x_j(n) \\
&= -e(n)\varphi'(v(n))x_j(n)
\end{aligned}
$$

Nonlinear neurons (cont.)

- Gradient descent gives

$$\begin{aligned} w_j(n+1) &= w_j(n) + \eta e(n)\varphi'(v(n))x_j(n) \\ &= w_j(n) + \eta\delta(n)x_j(n) \end{aligned}$$

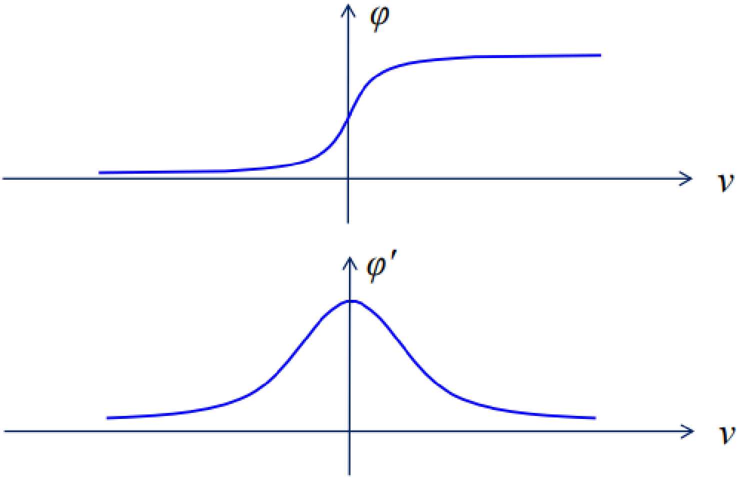
  - The above is called the delta (δ) rule
- If we choose a logistic sigmoid for

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

then

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

Role of activation function



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

Thank you!