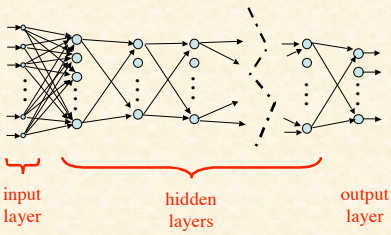
Neural Networks and Back-Propagation Learning

Supervised Learning

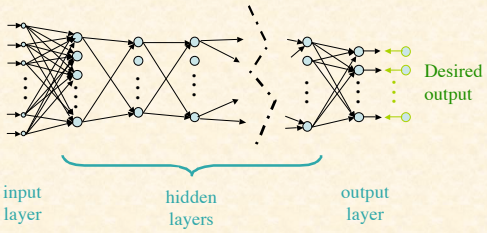
- Produce desired outputs for training inputs
- Generalize reasonably & appropriately to other inputs
- Good example: pattern recognition
- Feedforward multilayer networks

Feedforward Network

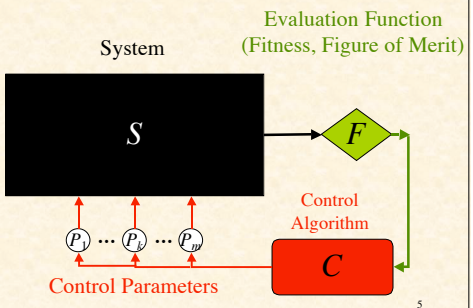


Credit Assignment Problem

How do we adjust the weights of the hidden layers?



Adaptive System



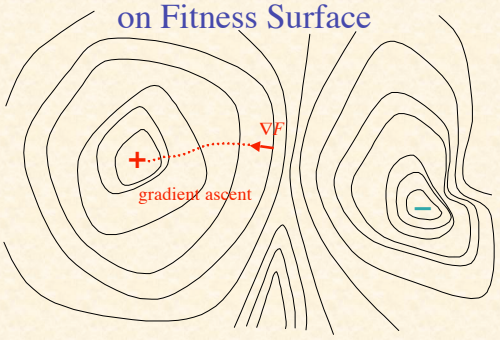
Gradient

$\frac{\partial F}{\partial P_k}$ measures how F is altered by variation of P_k

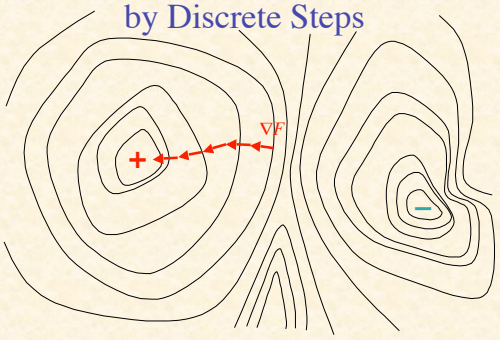
$$\nabla F = \begin{pmatrix} \partial F / \partial P_1 \\ \vdots \\ \partial F / \partial P_k \\ \vdots \\ \partial F / \partial P_m \end{pmatrix}$$

∇F points in direction of maximum increase in F

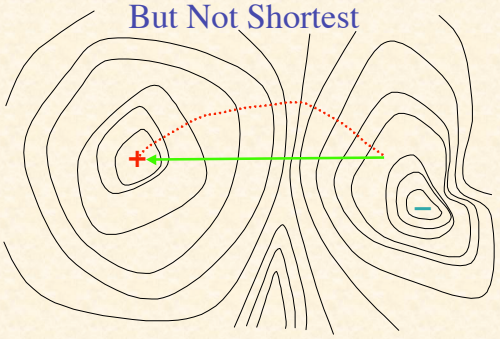
Gradient Ascent on Fitness Surface



Gradient Ascent by Discrete Steps



Gradient Ascent is Local But Not Shortest



Gradient Ascent Process

$$\dot{\mathbf{P}} = \eta \nabla F(\mathbf{P})$$

Change in fitness:

$$\dot{F} = \frac{\mathrm{d}F}{\mathrm{d}t} = \sum_{k=1}^{m} \frac{\partial F}{\partial P_k} \frac{\mathrm{d}P_k}{\mathrm{d}t} = \sum_{k=1}^{m} (\nabla F)_k \dot{P}_k$$

$$\dot{F} = \nabla F \cdot \dot{\mathbf{P}}$$

$$\dot{F} = \nabla F \cdot \eta \nabla F = \eta \left\| \nabla F \right\|^2 \geq 0$$

Therefore gradient ascent increases fitness (until reaches 0 gradient)

General Ascent in Fitness

Note that any adaptive process $\mathbf{P}(t)$ will increase fitness provided:

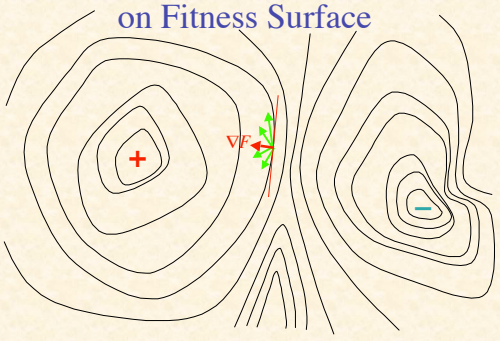
$$0 < \dot{F} = \nabla F \cdot \dot{\mathbf{P}} = \left\| \nabla F \right\| \left\| \dot{\mathbf{P}} \right\| \cos\varphi$$

where φ is angle between ∇F and $\dot{\mathbf{P}}$

Hence we need $\cos\varphi > 0$

or $|\varphi| < 90^\circ$

General Ascent on Fitness Surface



Fitness as Minimum Error

Suppose for Q different inputs we have target outputs $\mathbf{t}^1,\ldots,\mathbf{t}^Q$

Suppose for parameters $\mathbf{P}$ the corresponding actual outputs are $\mathbf{y}^1,\ldots,\mathbf{y}^Q$

Suppose $D(\mathbf{t},\mathbf{y}) \in [0,\infty)$ measures difference between target & actual outputs

Let $E^q = D(\mathbf{t}^q,\mathbf{y}^q)$ be error on qth sample

Let $F(\mathbf{P}) = -\sum_{q=1}^{Q} E^q(\mathbf{P}) = -\sum_{q=1}^{Q} D[\mathbf{t}^q,\mathbf{y}^q(\mathbf{P})]$

Gradient of Fitness

$$\nabla F = \nabla\left(-\sum_q E^q\right) = -\sum_q \nabla E^q$$

$$\frac{\partial E^q}{\partial P_k} = \frac{\partial}{\partial P_k} D(\mathbf{t}^q,\mathbf{y}^q) = \sum_j \frac{\partial D(\mathbf{t}^q,\mathbf{y}^q)}{\partial y_j^q}\frac{\partial y_j^q}{\partial P_k}$$

$$= \frac{\mathrm{d}\, D(\mathbf{t}^q,\mathbf{y}^q)}{\mathrm{d}\,\mathbf{y}^q}\cdot\frac{\partial \mathbf{y}^q}{\partial P_k}$$

$$= \nabla_{\mathbf{y}^q} D(\mathbf{t}^q,\mathbf{y}^q)\cdot \partial\mathbf{y}^q \Big/ \partial P_k$$

Jacobian Matrix

Define Jacobian matrix $\mathbf{J}^q = \begin{pmatrix} \partial y_1^q/\partial P_1 & \cdots & \partial y_1^q/\partial P_m \\ \vdots & \ddots & \vdots \\ \partial y_n^q/\partial P_1 & \cdots & \partial y_n^q/\partial P_m \end{pmatrix}$

Note $\mathbf{J}^q \in \Re^{n\times m}$ and $\nabla D(\mathbf{t}^q,\mathbf{y}^q) \in \Re^{n\times 1}$

Since $(\nabla E^q)_k = \frac{\partial E^q}{\partial P_k} = \sum_j \frac{\partial y_j^q}{\partial P_k}\frac{\partial D(\mathbf{t}^q,\mathbf{y}^q)}{\partial y_j^q}$,

$$\therefore \nabla E^q = (\mathbf{J}^q)^{\mathrm{T}} \nabla D(\mathbf{t}^q,\mathbf{y}^q)$$

Derivative of Squared Euclidean Distance

Suppose $D(\mathbf{t},\mathbf{y}) = \|\mathbf{t}-\mathbf{y}\|^2 = \sum_i (t_i - y_i)^2$

$$\frac{\partial D(\mathbf{t}-\mathbf{y})}{\partial y_j} = \frac{\partial}{\partial y_j}\sum_i (t_i - y_i)^2 = \sum_i \frac{\partial (t_i - y_i)^2}{\partial y_j}$$

$$= \frac{\mathrm{d}(t_j - y_j)^2}{\mathrm{d}\, y_j} = -2(t_j - y_j)$$

$$\therefore \frac{\mathrm{d}\, D(\mathbf{t},\mathbf{y})}{\mathrm{d}\,\mathbf{y}} = 2(\mathbf{y}-\mathbf{t})$$

Gradient of Error on q^{th} Input

$$\frac{\partial E^q}{\partial P_k} = \frac{\mathrm{d}\, D(\mathbf{t}^q,\mathbf{y}^q)}{\mathrm{d}\,\mathbf{y}^{\mathbf{q}}}\cdot\frac{\partial \mathbf{y}^q}{\partial P_k}$$

$$= 2(\mathbf{y}^q - \mathbf{t}^q)\cdot\frac{\partial \mathbf{y}^q}{\partial P_k}$$

$$= 2\sum_j (y_j^q - t_j^q)\frac{\partial y_j^q}{\partial P_k}$$

Recap

$$\dot{\mathbf{P}} = \eta \sum_q (\mathbf{J}^q)^{\mathrm{T}} (\mathbf{t}^q - \mathbf{y}^q)$$

To know how to decrease the differences between actual & desired outputs,

we need to know elements of Jacobian, $\partial y_j^q \big/ \partial P_k$,

which says how jth output varies with kth parameter (given the qth input)

The Jacobian depends on the specific form of the system, in this case, a feedforward neural network

Equations

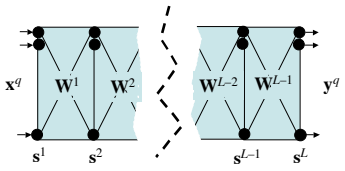
Net input: $h_i = \left(\sum_{j=1}^{n} w_{ij} s_j \right) - \theta$

$\mathbf{h} = \mathbf{W}\mathbf{s} - \theta$

Neuron output: $s_i' = \sigma(h_i)$

$\mathbf{s}' = \sigma(\mathbf{h})$

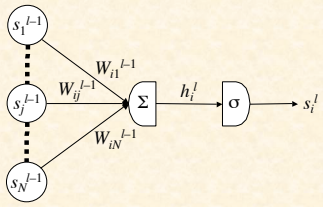
Multilayer Notation



Notation

- L layers of neurons labeled 1, …, L
- N_l neurons in layer l
- $\mathbf{s}^l$ = vector of outputs from neurons in layer l
- input layer $\mathbf{s}^1 = \mathbf{x}^q$ (the input pattern)
- output layer $\mathbf{s}^L = \mathbf{y}^q$ (the actual output)
- $\mathbf{W}^l$ = weights between layers l and l+1
- Problem: find how outputs y_i^q vary with weights W_{jk}^l (l = 1, …, L–1)

Typical Neuron



Error Back-Propagation

We will compute $\frac{\partial E^q}{\partial W_{ij}^l}$ starting with last layer ($l = L - 1$)

and working back to earlier layers ($l = L - 2, \ldots, 1$)

Delta Values

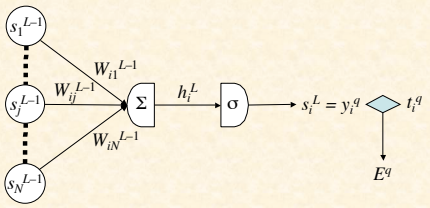
Convenient to break derivatives by chain rule:

$$\frac{\partial E^q}{\partial W_{ij}^{l-1}} = \frac{\partial E^q}{\partial h_i^l} \frac{\partial h_i^l}{\partial W_{ij}^{l-1}}$$

Let $\delta_i^l = \frac{\partial E^q}{\partial h_i^l}$

So $\frac{\partial E^q}{\partial W_{ij}^{l-1}} = \delta_i^l \frac{\partial h_i^l}{\partial W_{ij}^{l-1}}$

Output-Layer Neuron



Output-Layer Derivatives (1)

$$\delta_i^L = \frac{\partial E^q}{\partial h_i^L} = \frac{\partial}{\partial h_i^L}\sum_k \left(s_k^L - t_k^q\right)^2$$
$$= \frac{\mathrm{d}\left(s_i^L - t_i^q\right)^2}{\mathrm{d}\,h_i^L} = 2\left(s_i^L - t_i^q\right)\frac{\mathrm{d}\,s_i^L}{\mathrm{d}\,h_i^L}$$
$$= 2\left(s_i^L - t_i^q\right)\sigma'\left(h_i^L\right)$$

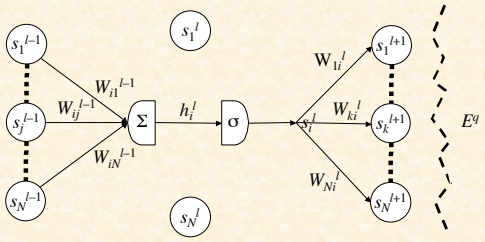
Output-Layer Derivatives (2)

$$\frac{\partial h_i^L}{\partial W_{ij}^{L-1}} = \frac{\partial}{\partial W_{ij}^{L-1}}\sum_k W_{ik}^{L-1} s_k^{L-1} = s_j^{L-1}$$

$$\therefore \frac{\partial E^q}{\partial W_{ij}^{L-1}} = \delta_i^L s_j^{L-1}$$

where $\delta_i^L = 2\left(s_i^L - t_i^q\right)\sigma'\left(h_i^L\right)$

Hidden-Layer Neuron



Hidden-Layer Derivatives (1)

Recall $\frac{\partial E^q}{\partial W_{ij}^{l-1}} = \delta_i^l \frac{\partial h_i^l}{\partial W_{ij}^{l-1}}$

$$\delta_i^l = \frac{\partial E^q}{\partial h_i^l} = \sum_k \frac{\partial E^q}{\partial h_k^{l+1}}\frac{\partial h_k^{l+1}}{\partial h_i^l} = \sum_k \delta_k^{l+1}\frac{\partial h_k^{l+1}}{\partial h_i^l}$$

$$\frac{\partial h_k^{l+1}}{\partial h_i^l} = \frac{\partial \sum_m W_{km}^l s_m^l}{\partial h_i^l} = \frac{\partial W_{ki}^l s_i^l}{\partial h_i^l} = W_{ki}^l \frac{\mathrm{d}\,\sigma\left(h_i^l\right)}{\mathrm{d}\,h_i^l} = W_{ki}^l \sigma'\left(h_i^l\right)$$

$$\therefore \delta_i^l = \sum_k \delta_k^{l+1} W_{ki}^l \sigma'\left(h_i^l\right) = \sigma'\left(h_i^l\right)\sum_k \delta_k^{l+1} W_{ki}^l$$

Hidden-Layer Derivatives (2)

$$\frac{\partial h_i^l}{\partial W_{ij}^{l-1}} = \frac{\partial}{\partial W_{ij}^{l-1}}\sum_k W_{ik}^{l-1} s_k^{l-1} = \frac{\mathrm{d}\,W_{ij}^{l-1} s_j^{l-1}}{\mathrm{d}\,W_{ij}^{l-1}} = s_j^{l-1}$$

$$\therefore \frac{\partial E^q}{\partial W_{ij}^{l-1}} = \delta_i^l s_j^{l-1}$$

where $\delta_i^l = \sigma'\left(h_i^l\right)\sum_k \delta_k^{l+1} W_{ki}^l$

Derivative of Sigmoid

Suppose $s = \sigma(h) = \dfrac{1}{1+\exp(-\alpha h)}$ (logistic sigmoid)

$$D_h s = D_h\left[1+\exp(-\alpha h)\right]^{-1} = -\left[1+\exp(-\alpha h)\right]^{-2} D_h\left(1+e^{-\alpha h}\right)$$

$$= -\left(1+e^{-\alpha h}\right)^{-2}\left(-\alpha e^{-\alpha h}\right) = \alpha \frac{e^{-\alpha h}}{\left(1+e^{-\alpha h}\right)^2}$$

$$= \alpha \frac{1}{1+e^{-\alpha h}} \frac{e^{-\alpha h}}{1+e^{-\alpha h}} = \alpha s\left(\frac{1+e^{-\alpha h}}{1+e^{-\alpha h}} - \frac{1}{1+e^{-\alpha h}}\right)$$

$$= \alpha s(1-s)$$

Summary of Back-Propagation Algorithm

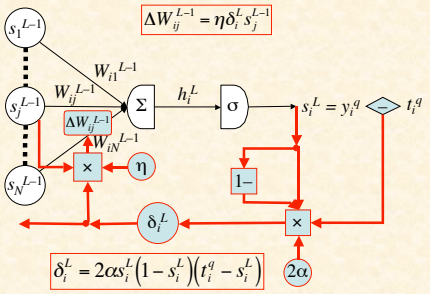
Output layer: $\delta_i^L = 2\alpha s_i^L\left(1-s_i^L\right)\left(s_i^L - t_i^q\right)$

$$\frac{\partial E^q}{\partial W_{ij}^{L-1}} = \delta_i^L s_j^{L-1}$$

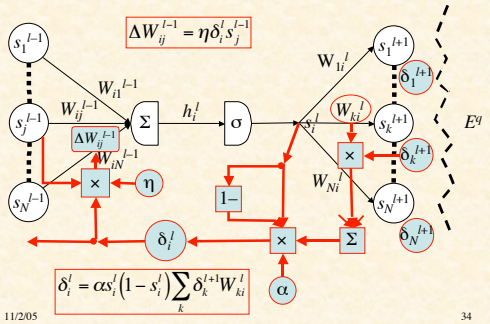
Hidden layers: $\delta_i^l = \alpha s_i^l\left(1-s_i^l\right)\sum_k \delta_k^{l+1} W_{ki}^l$

$$\frac{\partial E^q}{\partial W_{ij}^{l-1}} = \delta_i^l s_j^{l-1}$$

Output-Layer Computation



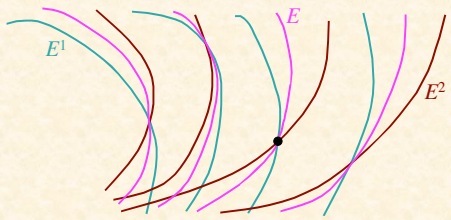
Hidden-Layer Computation



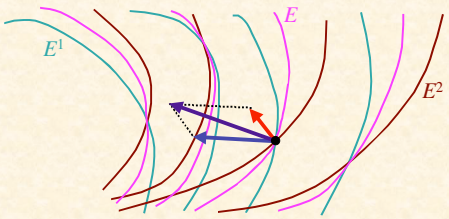
Training Procedures

- Batch Learning
  - on each *epoch* (pass through all the training pairs),
  - weight changes for all patterns accumulated
  - weight matrices updated at end of epoch
  - accurate computation of gradient
- Online Learning
  - weight are updated after back-prop of each training pair
  - usually randomize order for each epoch
  - approximation of gradient
- Doesn't make much difference

Summation of Error Surfaces

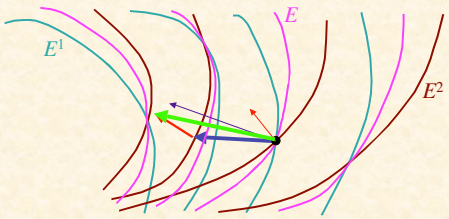


Gradient Computation in Batch Learning



11/2/05 37

Gradient Computation in Online Learning



11/2/05 38

The Golden Rule of Neural Nets

Neural Networks are the
second-best way
to do *everything*!

11/2/05 39