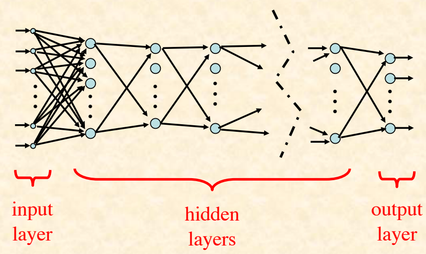
IV. Neural Networks and Learning

A. Artificial Neural Net Learning

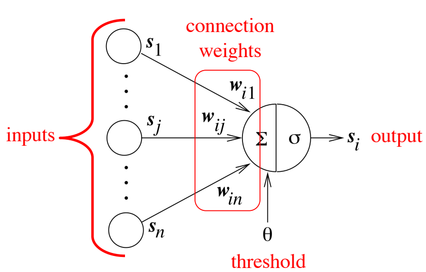
Supervised Learning

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

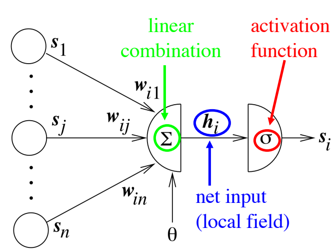
Feedforward Network



Typical Artificial Neuron



Typical Artificial Neuron



Equations

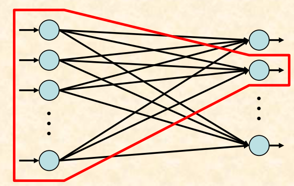
Net input: $h_i = \left(\sum_{j=1}^{n} w_{ij} s_j \right) - \theta$

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

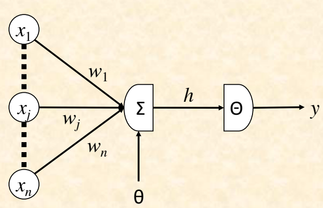
Neuron output: $s_i' = \sigma(h_i)$

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

Single-Layer Perceptron



Variables



Single Layer Perceptron Equations

Binary threshold activation function:

$$\sigma(h) = \Theta(h) = \begin{cases} 1, & \text{if } h > 0 \\ 0, & \text{if } h \le 0 \end{cases}$$

$$\text{Hence, } y = \begin{cases} 1, & \text{if } \sum_j w_j x_j > \theta \\ 0, & \text{otherwise} \end{cases}$$

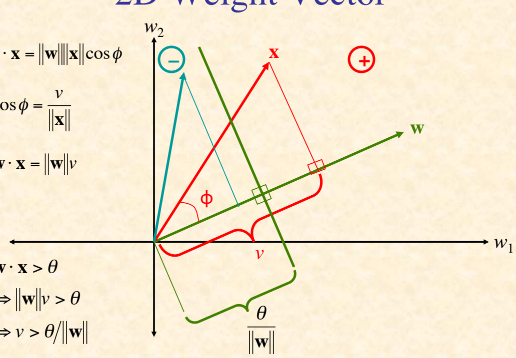
$$= \begin{cases} 1, & \text{if } \mathbf{w} \cdot \mathbf{x} > \theta \\ 0, & \text{if } \mathbf{w} \cdot \mathbf{x} \le \theta \end{cases}$$

2D Weight Vector

$\mathbf{w} \cdot \mathbf{x} = \|\mathbf{w}\|\|\mathbf{x}\|\cos\phi$

$\cos\phi = \frac{v}{\|\mathbf{x}\|}$

$\mathbf{w} \cdot \mathbf{x} = \|\mathbf{w}\| v$

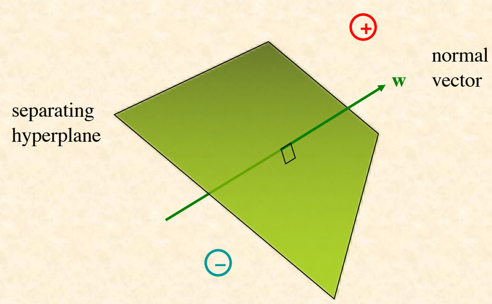


$\mathbf{w} \cdot \mathbf{x} > \theta$

$\Leftrightarrow \|\mathbf{w}\| v > \theta$

$\Leftrightarrow v > \theta / \|\mathbf{w}\|$

N-Dimensional Weight Vector



Goal of Perceptron Learning

- Suppose we have training patterns $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^P$ with corresponding desired outputs $y^1, y^2, \ldots, y^P$
- where $\mathbf{x}^p \in \{0, 1\}^n$, $y^p \in \{0, 1\}$
- We want to find $\mathbf{w}$, θ such that $y^p = \Theta(\mathbf{w} \cdot \mathbf{x}^p - \theta)$ for $p = 1, \ldots, P$

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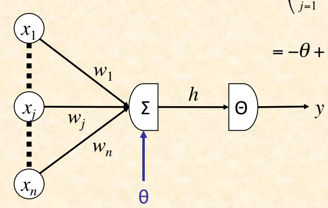
Treating Threshold as Weight



$$h = \left(\sum_{j=1}^{n} w_j x_j \right) - \theta$$

$$= -\theta + \sum_{j=1}^{n} w_j x_j$$

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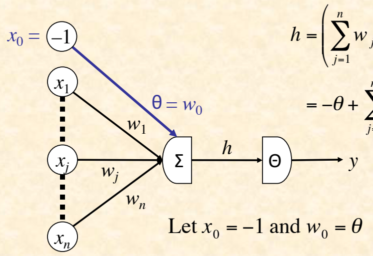
Treating Threshold as Weight



$$h = \left(\sum_{j=1}^{n} w_j x_j \right) - \theta$$

$$= -\theta + \sum_{j=1}^{n} w_j x_j$$

Let $x_0 = -1$ and $w_0 = \theta$

$$h = w_0 x_0 + \sum_{j=1}^{n} w_j x_j = \sum_{j=0}^{n} w_j x_j = \tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}$$

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Augmented Vectors

$$\tilde{\mathbf{w}} = \begin{pmatrix} \theta \\ w_1 \\ \vdots \\ w_n \end{pmatrix} \qquad \tilde{\mathbf{x}}^p = \begin{pmatrix} -1 \\ x_1^p \\ \vdots \\ x_n^p \end{pmatrix}$$

We want $y^p = \Theta\left(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}^p\right), \; p = 1, \ldots, P$

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Reformulation as Positive Examples

We have positive ($y^p = 1$) and negative ($y^p = 0$) examples

Want $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}^p > 0$ for positive, $\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}}^p \le 0$ for negative

Let $\mathbf{z}^p = \tilde{\mathbf{x}}^p$ for positive, $\mathbf{z}^p = -\tilde{\mathbf{x}}^p$ for negative

Want $\tilde{\mathbf{w}} \cdot \mathbf{z}^p \ge 0$, for $p = 1, \ldots, P$

Hyperplane through origin with all $\mathbf{z}^p$ on one side

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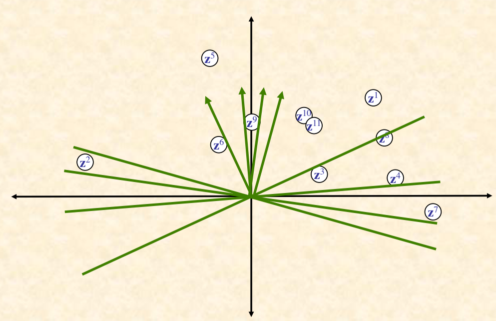
Adjustment of Weight Vector



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Outline of Perceptron Learning Algorithm

1. initialize weight vector randomly
2. until all patterns classified correctly, do:
   a) for $p = 1, \ldots, P$ do:
      1) if $\mathbf{z}^p$ classified correctly, do nothing
      2) else adjust weight vector to be closer to correct classification

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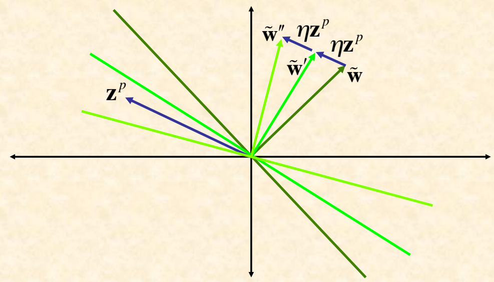
Weight Adjustment



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Improvement in Performance

$$\begin{aligned}\tilde{\mathbf{w}}' \cdot \mathbf{z}^p &= \left(\tilde{\mathbf{w}} + \eta\mathbf{z}^p\right) \cdot \mathbf{z}^p \\ &= \tilde{\mathbf{w}} \cdot \mathbf{z}^p + \eta\mathbf{z}^p \cdot \mathbf{z}^p \\ &= \tilde{\mathbf{w}} \cdot \mathbf{z}^p + \eta\left\|\mathbf{z}^p\right\|^2 \\ &> \tilde{\mathbf{w}} \cdot \mathbf{z}^p\end{aligned}$$

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Perceptron Learning Theorem

- If there is a set of weights that will solve the problem,
- then the PLA will eventually find it
- (for a sufficiently small learning rate)
- Note: only applies if positive & negative examples are linearly separable

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NetLogo Simulation of Perceptron Learning

Run Perceptron-Geometry.nlogo

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Classification Power of Multilayer Perceptrons

- Perceptrons can function as logic gates
- Therefore MLP can form intersections, unions, differences of linearly-separable regions
- Classes can be arbitrary *hyperpolyhedra*
- Minsky & Papert criticism of perceptrons
- No one succeeded in developing a MLP learning algorithm

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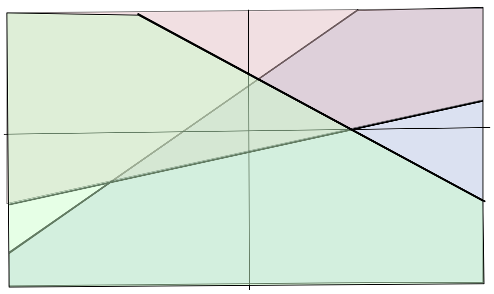
Hyperpolyhedral Classes



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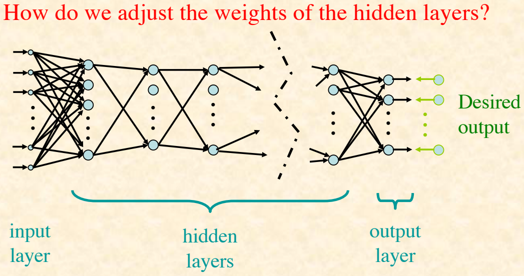
Credit Assignment Problem

How do we adjust the weights of the hidden layers?



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NetLogo Demonstration of Back-Propagation Learning

Run Artificial Neural Net.nlogo

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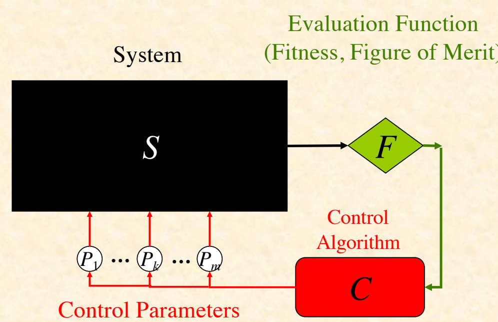
Adaptive System



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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 local increase in F

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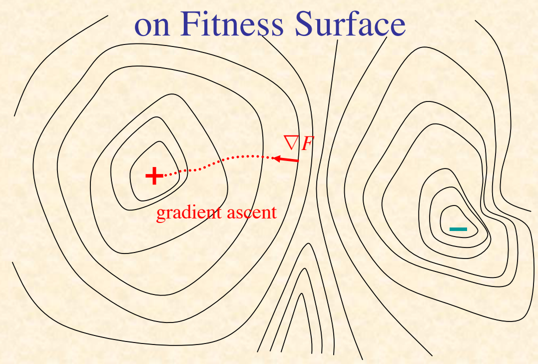
Gradient Ascent on Fitness Surface



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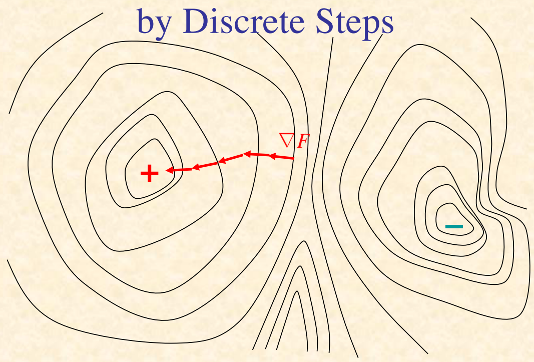
Gradient Ascent by Discrete Steps



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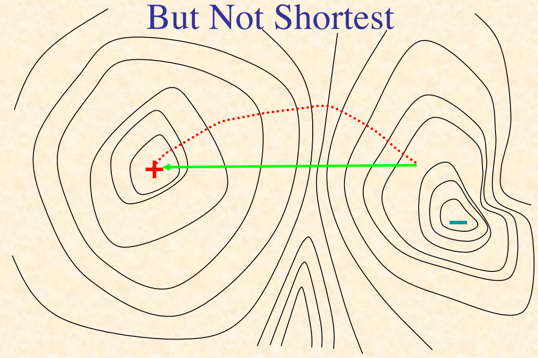
Gradient Ascent is Local But Not Shortest



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Gradient Ascent Process

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

Change in fitness:

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

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

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

Therefore gradient ascent increases fitness
(until reaches 0 gradient)

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General Ascent in Fitness

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

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

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

Hence we need $\cos\varphi > 0$

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

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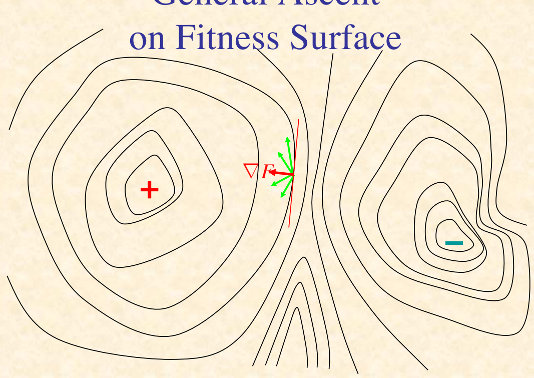
General Ascent on Fitness Surface



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

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Gradient of Fitness

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

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

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

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

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

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

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Derivative of Squared Euclidean Distance

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

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

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

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

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Gradient of Error on q^{th} Input

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

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

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

$$\nabla E^q = 2\left(\mathbf{J}^q\right)^{\mathrm{T}} \left(\mathbf{y}^q - \mathbf{t}^q\right)$$

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Recap

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

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

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

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

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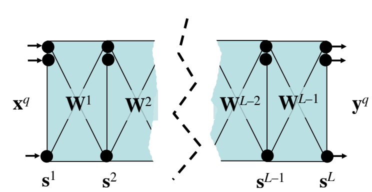
Multilayer Notation



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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 out how outputs y_i^q vary with weights W_{jk}^l (l = 1, …, L–1)

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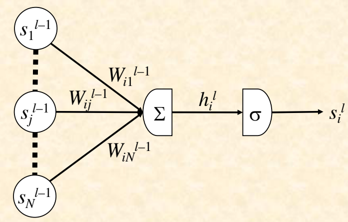
Typical Neuron



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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 ($l = L-2,\ldots,1$)

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

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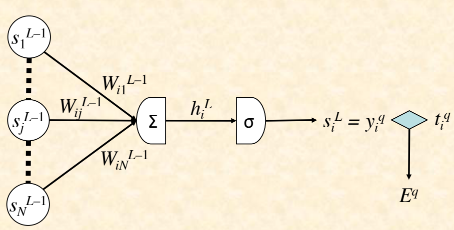
Output-Layer Neuron



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Output-Layer Derivatives (1)

$$\delta_i^L = \frac{\partial E^q}{\partial h_i^L} = \frac{\partial}{\partial h_i^L}\sum_k \left(s_k^L - t_k^q\right)^2$$

$$= \frac{\mathrm{d}\left(s_i^L - t_i^q\right)^2}{\mathrm{d}\,h_i^L} = 2\left(s_i^L - t_i^q\right)\frac{\mathrm{d}\,s_i^L}{\mathrm{d}\,h_i^L}$$

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

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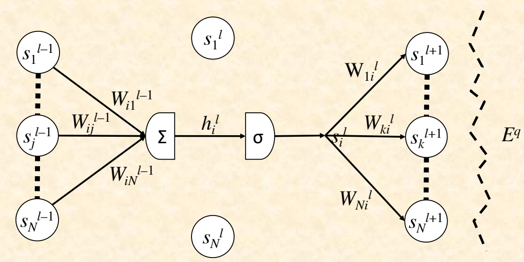
Output-Layer Derivatives (2)

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

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

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

$$\begin{aligned}
\mathrm{D}_h s &= \mathrm{D}_h\left[1+\exp(-\alpha h)\right]^{-1} = -\left[1+\exp(-\alpha h)\right]^{-2} \mathrm{D}_h\left(1+e^{-\alpha h}\right) \\
&= -\left(1+e^{-\alpha h}\right)^{-2}\left(-\alpha e^{-\alpha h}\right) = \alpha \frac{e^{-\alpha h}}{\left(1+e^{-\alpha h}\right)^2} \\
&= \alpha \frac{1}{1+e^{-\alpha h}} \frac{e^{-\alpha h}}{1+e^{-\alpha h}} = \alpha s\left(\frac{1+e^{-\alpha h}}{1+e^{-\alpha h}} - \frac{1}{1+e^{-\alpha h}}\right) \\
&= \alpha s(1-s)
\end{aligned}$$

Summary of Back-Propagation Algorithm

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

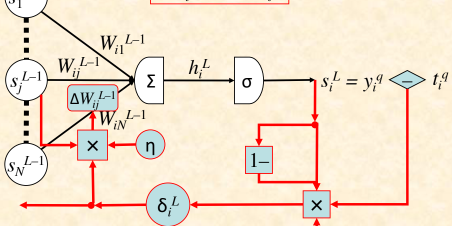
$$\frac{\partial E^q}{\partial W_{ij}^{L-1}} = \delta_i^L s_j^{L-1}$$

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

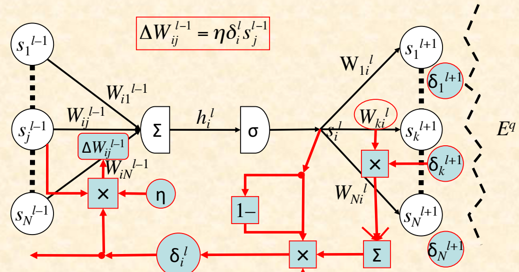
$$\Delta W_{ij}^{L-1} = \eta \delta_i^L s_j^{L-1}$$



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

Hidden-Layer Computation

$$\Delta W_{ij}^{l-1} = \eta \delta_i^l s_j^{l-1}$$

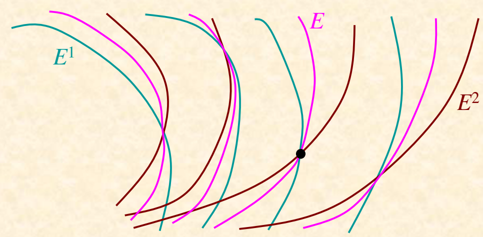


$$\delta_i^l = \alpha s_i^l \left(1 - s_i^l\right) \sum_k \delta_k^{l+1} W_{ki}^l$$

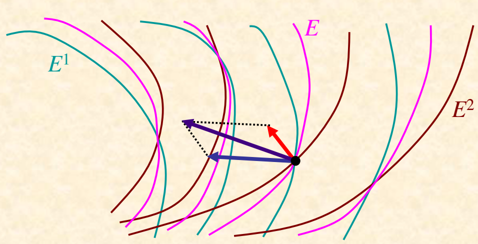
Training Procedures

- 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

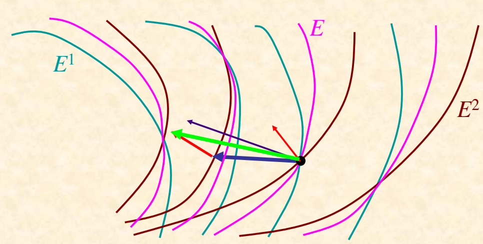
Summation of Error Surfaces



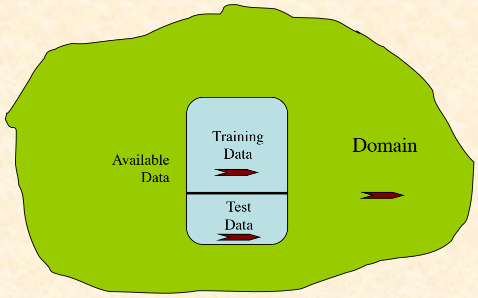
Gradient Computation in Batch Learning



Gradient Computation in Online Learning



Testing Generalization



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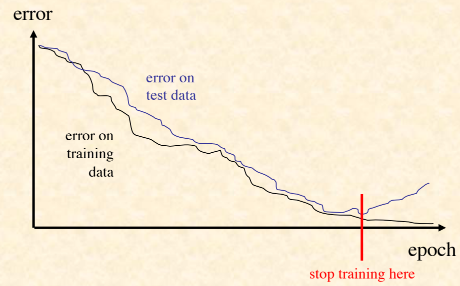
Problem of Rote Learning



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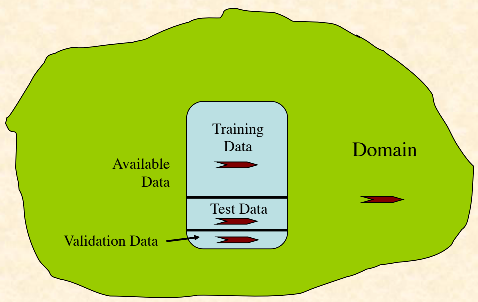
Improving Generalization



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A Few Random Tips

- Too few neurons and the ANN may not be able to decrease the error enough
- Too many neurons can lead to rote learning
- Preprocess data to:
  - standardize
  - eliminate irrelevant information
  - capture invariances
  - keep relevant information
- If stuck in local min., restart with different random weights

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Run Example BP Learning

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Beyond Back-Propagation

- Adaptive Learning Rate
- Adaptive Architecture
  - Add/delete hidden neurons
  - Add/delete hidden layers
- Radial Basis Function Networks
- Recurrent BP
- Etc., etc., etc.…

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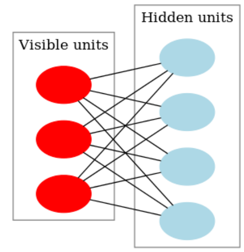
Deep Belief Networks

- Inspired by hierarchical representations in mammalian sensory systems
- Use "deep" (multilayer) feed-forward nets
- Layers self-organize to represent input at progressively more abstract, task-relevant levels
- Supervised training (e.g., BP) can be used to tune network performance.
- Each layer is a *Restricted Boltzmann Machine*

Restricted Boltzmann Machine

- Goal: hidden units become model of input domain
- Should capture statistics of input
- Evaluate by testing its ability to reproduce input statistics
- Change weights to decrease difference



(fig. from wikipedia)

Unsupervised RBM Learning

- Stochastic binary units
- Assume bias units $x_0 = y_0 = 1$
- Set y_i with probability $\sigma\left(\sum_j W_{ij} x_j\right)$
- Set x_j' with probability $\sigma\left(\sum_i W_{ij} y_i\right)$
- Set y_i' with probability $\sigma\left(\sum_j W_{ij} x_j'\right)$
- After several cycles of sampling, update weights based on statistics:

$$\Delta W_{ij} = \eta\left(\langle y_i x_j \rangle - \langle y_i' x_j' \rangle\right)$$

Training a DBN Network

- Present inputs and do RBM learning with first hidden layer to develop model
- When converged, do RBM learning between first and second hidden layers to develop higher-level model
- Continue until all weight layers trained
- May further train with BP or other supervised learning algorithms

What is the Power of Artificial Neural Networks?

- With respect to Turing machines?
- As function approximators?

Can ANNs Exceed the "Turing Limit"?

- There are many results, which depend sensitively on assumptions; for example:
- Finite NNs with real-valued weights have super-Turing power (Siegelmann & Sontag '94)
- Recurrent nets with Gaussian noise have sub-Turing power (Maass & Sontag '99)
- Finite recurrent nets with real weights can recognize <u>all</u> languages, and thus are super-Turing (Siegelmann '99)
- Stochastic nets with rational weights have super-Turing power (but only P/POLY, BPP/log*) (Siegelmann '99)
- But computing classes of functions is not a very relevant way to evaluate the capabilities of neural computation

A Universal Approximation Theorem

Suppose f is a continuous function on $[0,1]^n$
Suppose σ is a nonconstant, bounded, monotone increasing real function on $\Re$.
For any $\varepsilon > 0$, there is an m such that

$\exists \mathbf{a} \in \Re^m, \mathbf{b} \in \Re^n, \mathbf{W} \in \Re^{m \times n}$ such that if

$$F(x_1,\ldots,x_n) = \sum_{i=1}^{m} a_i \sigma\left(\sum_{j=1}^{n} W_{ij} x_j + b_j\right)$$

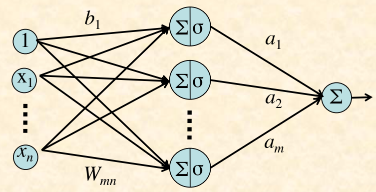
$$\left[\text{i.e., } F(\mathbf{x}) = \mathbf{a} \cdot \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})\right]$$

then $\left|F(\mathbf{x}) - f(\mathbf{x})\right| < \varepsilon$ for all $\mathbf{x} \in [0,1]^n$

(see, e.g., Haykin, *N.Nets* 2/e, 208–9)

One Hidden Layer is Sufficient

- Conclusion: One hidden layer is sufficient to approximate any continuous function arbitrarily closely



The Golden Rule of Neural Nets

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

IVB