Artificial Neural Networks

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Introduction

- Artificial Neural Networks (ANN)
  - Information processing paradigm inspired by biological nervous systems
  - ANN is composed of a system of neurons connected by synapses
  - ANN learn by example
    - Adjust synaptic connections between neurons

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History

- 1943: McCulloch and Pitts model neural networks based on their understanding of neurology.
  - Neurons embed simple logic functions:
    - a or b
    - a and b
- 1950s:
  - Farley and Clark
    - IBM group that tries to model biological behavior
    - Consult neuro-scientists at McGill, whenever stuck
  - Rochester, Holland, Haibit and Duda

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History

- Perceptron (Rosenblatt 1958)
  - Three layer system:
    - Input nodes
    - Output node
    - Association layer
  - Can learn to connect or associate a given input to a random output unit
- Minsky and Papert
  - Showed that a single layer perceptron cannot learn the XOR of two binary inputs
  - Lead to loss of interest (and funding) in the field

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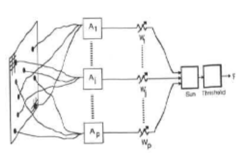
History

- Perceptron (Rosenblatt 1958)
  - Association units A_1, A_2, … extract features from user input
  - Output is weighted and associated
  - Function fires if weighted sum of input exceeds a threshold.



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History

- Back-propagation learning method (Werbos 1974)
  - Three layers of neurons
    - Input, Output, Hidden
  - Better learning rule for generic three layer networks
  - Regenerates interest in the 1980s
- Successful applications in medicine, marketing, risk management, … (1990)
- In need for another breakthrough.

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ANN

- Promises
  - Combine speed of silicon with proven success of carbon → artificial brains

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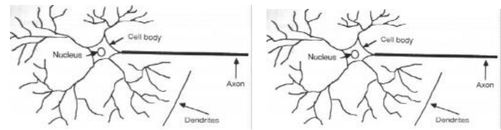
Neuron Model

- Natural neurons



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Neuron Model

- Neuron collects signals from *dendrites*
- Sends out spikes of electrical activity through an *axon*, which splits into thousands of branches.
- At end of each brand, a *synapses* converts activity into either exciting or inhibiting activity of a dendrite at another neuron.
- Neuron *fires* when exciting activity surpasses inhibitory activity
- Learning changes the effectiveness of the synapses

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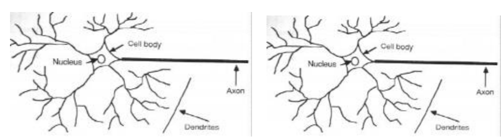
Neuron Model

- Natural neurons



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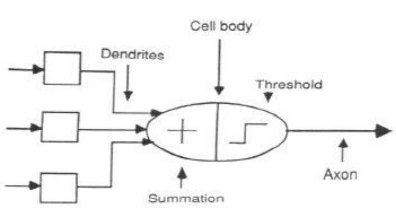
Neuron Model

- Abstract neuron model:



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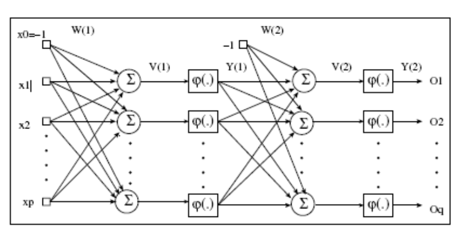
ANN Forward Propagation



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ANN Forward Propagation

- Bias Nodes
  - Add one node to each layer that has constant output
- Forward propagation
  - Calculate from input layer to output layer
  - For each neuron:
    - Calculate weighted average of input
    - Calculate activation function

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Neuron Model

- Firing Rules:
  - Threshold rules:
    - Calculate weighted average of input
    - Fire if larger than threshold
  - Perceptron rule
    - Calculate weighted average of input input
    - Output activation level is

$$\phi(\nu) = \begin{cases} 1 & \nu \geq \frac{1}{2} \\ \nu & 0 \leq \nu \leq \frac{1}{2} \\ 0 & \nu \leq 0 \end{cases}$$

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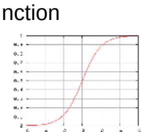
Neuron Model

- Firing Rules: Sigmoid functions:
  - Hyperbolic tangent function

$$\varphi(\nu) = \tanh(\nu/2) = \frac{1-\exp(-\nu)}{1+\exp(-\nu)}$$

  - Logistic activation function

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



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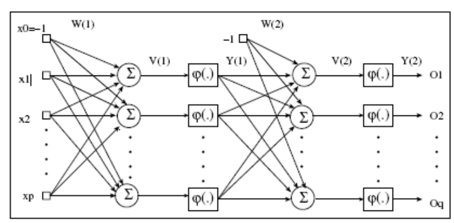
ANN Forward Propagation



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ANN Forward Propagation

- Apply input vector **X** to layer of neurons.
- Calculate

$$V_j(n) = \sum_{i=1}^{p} (W_{ji} X_i + Threshold)$$

  - where X_i is the activation of previous layer neuron i
  - W_{ji} is the weight of going from node i to node j
  - p is the number of neurons in the previous layer
- Calculate output activation

$$Y_j(n) = \frac{1}{1+\exp(-V_j(n))}$$

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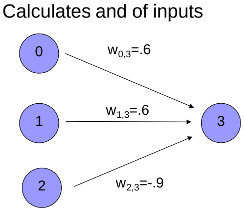
ANN Forward Propagation

- Example: ADALINE Neural Network
  - Calculates and of inputs



threshold function is step function

Bias Node

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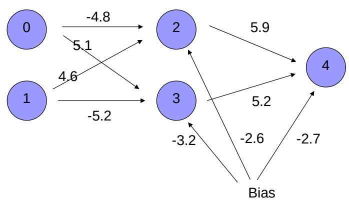
ANN Forward Propagation

- Example: Three layer network
  - Calculates xor of inputs



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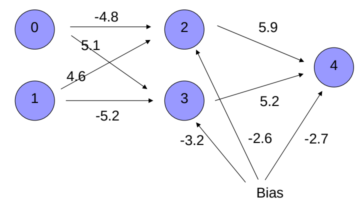
ANN Forward Propagation

- Input (0,0)



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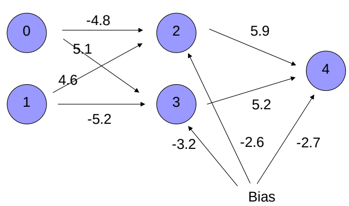
ANN Forward Propagation

$V_j(n)=\sum_{i=1}^{p}(W_{ji}X_i+Threshold)$

- Input (0,0)
  - Node 2 activation is φ(-4.8 · 0+4.6 · 0 - 2.6)= 0.0691



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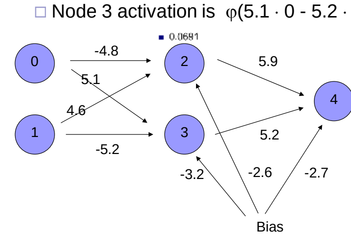
ANN Forward Propagation

$V_j(n)=\sum_{i=1}^{p}(W_{ji}X_i+Threshold)$

- Input (0,0)
  - Node 3 activation is φ(5.1 · 0 - 5.2 · 0 - 3.2)= 0.0392



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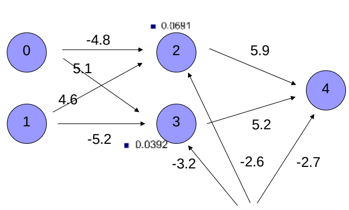
ANN Forward Propagation

$V_j(n)=\sum_{i=1}^{p}(W_{ji}X_i+Threshold)$

- Input (0,0)
  - Node 4 activation is φ(5.9 · 0.069 + 5.2 · 0.0392 – 2.7)= 0.110227



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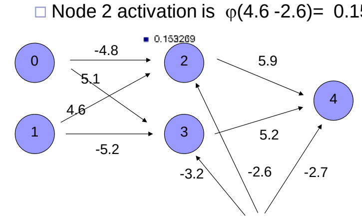
ANN Forward Propagation

$V_j(n)=\sum_{i=1}^{p}(W_{ji}X_i+Threshold)$

- Input (0,1)
  - Node 2 activation is φ(4.6 -2.6)= 0.153269



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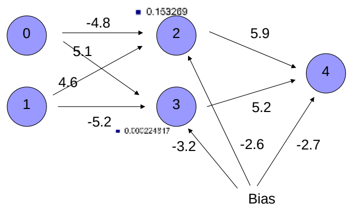
ANN Forward Propagation

$$V_j(n)=\sum_{i=1}^{p}(W_{ji}X_i+Threshold)$$

- Input (0,1)
  - Node 3 activation is φ(-5.2 -3.2)= 0.000224817



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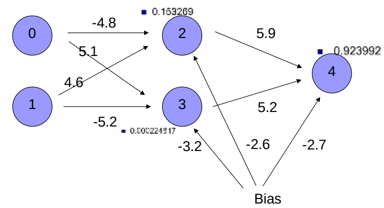
ANN Forward Propagation

$$V_j(n)=\sum_{i=1}^{p}(W_{ji}X_i+Threshold)$$

- Input (0,1)
  - Node 4 activation is φ(5.9 · 0.153269 + 5.2 · 0.000224817 -2.7)= 0.923992



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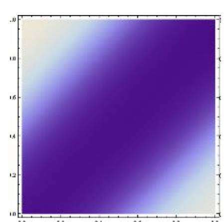
ANN Forward Propagation

- Density Plot of Output



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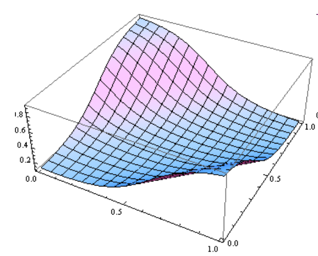
ANN Forward Propagation



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ANN Forward Propagation

- Network can learn a non-linearly separated set of outputs.
- Need to map output (real value) into binary values.

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ANN Training

- Weights are determined by *training*
  - Back-propagation:
    - On given input, compare actual output to desired output.
    - Adjust weights to output nodes.
    - Work backwards through the various layers
  - Start out with initial random weights
    - Best to keep weights close to zero (<<10)

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ANN Training

- Weights are determined by *training*
  - Need a training set
    - Should be representative of the problem
  - During each training epoch:
    - Submit training set element as input
    - Calculate the error for the output neurons
    - Calculate average error during epoch
    - Adjust weights

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ANN Training

- Error is the mean square of differences in output layer

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

y – observed output

t – target output

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ANN Training

- Error of training epoch is the average of all errors.

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ANN Training

- Update weights and thresholds using
  - Weights $w_{j,k} = w_{j,k} + (-\eta)\frac{\partial E(\vec{x})}{\partial w_{jk}}$
  - Bias $\theta_k = \theta_k + (-\eta)\frac{\partial E(\vec{x})}{\partial \theta_k}$
  - η is a possibly time-dependent factor that should prevent overcorrection

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ANN Training

- Using a sigmoid function, we get

$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

  - Logistics function φ has derivative $\varphi'(t) = \varphi(t)(1-\varphi(t))$

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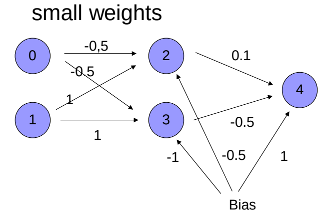
ANN Training Example

- Start out with random, small weights



x1	x2	y
0	0	0.687349
0	1	0.667459
1	0	0.698070
1	1	0.676727

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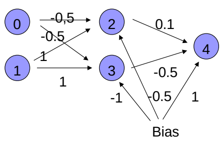
ANN Training Example



x1	x2	y	Error
0	0	0.69	0.472448
0	1	0.67	0.110583
1	0	0.70	0.0911618
1	1	0.68	0.457959

Average Error is 0.283038

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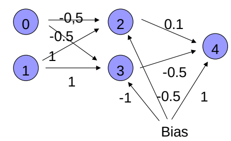
ANN Training Example



x1	x2	y	Error
0	0	0.69	0.472448
0	1	0.67	0.110583
1	0	0.70	0.0911618
1	1	0.68	0.457959

Average Error is 0.283038

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ANN Training Example

- Calculate the derivative of the error with respect to the weights and bias into the output layer neurons

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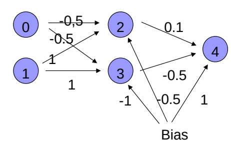
ANN Training Example



New weights going into node 4

We do this for all training inputs, then average out the changes

net_4 is the weighted sum of input going into neuron 4:

$net_4(0,0)$= 0.787754

net4(0,1)= 0.696717

net4(1,0)= 0.838124

net4(1,1)= 0.73877

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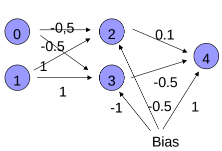
ANN Training Example



New weights going into node 4

We calculate the derivative of the activation function at the point given by the net-input.

Recall our cool formula

$\varphi'(t) = \varphi(t)(1- \varphi(t))$

$\varphi'(net_4(0,0)) = \varphi'(0.787754) =$ 0.214900

$\varphi'(net_4(0,1)) = \varphi'(0.696717) =$ 0.221957

$\varphi'(net_4(1,0)) = \varphi'(0.838124) =$ 0.210768

$\varphi'(net_4(1,1)) = \varphi'(0.738770) =$ 0.218768

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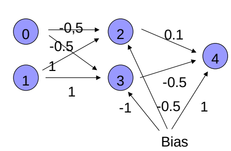
ANN Training Example



$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\mathrm{net}_j)(t_j - y_j)$$

New weights going into node 4

We now obtain δ values for each input separately:

Input 0,0:

$\delta_4 = \varphi'(net_4(0,0)) *(0-y_4(0,0)) =$ -0.152928

Input 0,1:

$\delta_4 = \varphi'(net4(0,1)) *(1-y_4(0,1)) =$ 0.0682324

Input 1,0:

$\delta_4 = \varphi'(net_4(1,0)) *(1-y_4(1,0)) =$ 0.0593889

Input 1,1:

$\delta_4 = \varphi'(net_4(1,1)) *(0-y_4(1,1)) =$ -0.153776

Average: $\delta_4 =$ -0.0447706

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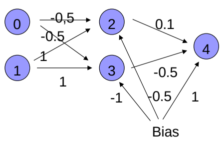
ANN Training Example



New weights going into node 4

Average: δ_4 = -0.0447706

We can now update the weights going into node 4:

Let's call: E_{ji} the derivative of the error function with respect to the weight going from neuron *i* into neuron *j*.

We do this for every possible input:

$E_{4,2}$ = - output(neuron(2)* δ_4

For (0,0): $E_{4,2}$ = 0.0577366

For (0,1): $E_{4,2}$ = -0.0424719

For(1,0): $E_{4,2}$ = -0.0159721

For(1,1): $E_{4,2}$ = 0.0768878

Average is 0.0190451

$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

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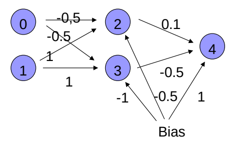
ANN Training Example



New weight from 2 to 4 is now going to be 0.1190451.

$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

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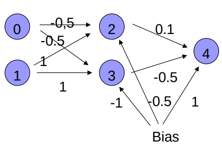
ANN Training Example



New weights going into node 4

For (0,0): $E_{4,3}$ = 0.0411287

For (0,1): $E_{4,3}$ = -0.0341162

For(1,0): $E_{4,3}$ = -0.0108341

For(1,1): $E_{4,3}$ = 0.0580565

Average is 0.0135588

New weight is -0.486441

$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

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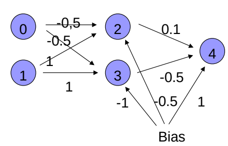
ANN Training Example



New weights going into node 4:

We also need to change the bias node

For (0,0): $E_{4,B}$ = 0.0411287

For (0,1): $E_{4,B}$ = -0.0341162

For(1,0): $E_{4,B}$ = -0.0108341

For(1,1): $E_{4,B}$ = 0.0580565

Average is 0.0447706

New weight is 1.0447706

$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

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ANN Training Example

- We now have adjusted all the weights into the output layer.
- Next, we adjust the hidden layer
- The target output is given by the delta values of the output layer
- More formally:
  - Assume that *j* is a hidden neuron
  - Assume that δ_k is the delta-value for an output neuron *k*.
  - While the example has only one output neuron, most ANN have more. When we sum over *k*, this means summing over all output neurons.
  - w_{kj} is the weight from neuron *j* into neuron *k*

$$\delta_j = \varphi'(\text{net}_j) \cdot \sum_k (\delta_k w_{kj})$$

$$\frac{\partial E}{\partial w_{ji}} = -y_i \delta_j$$

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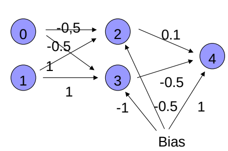
ANN Training Example



We now calculate the updates to the weights of neuron 2.

First, we calculate the net-input into 2.

This is really simple because it is just a linear functions of the arguments x_1 and x_2

$net_2 = -0.5\ x_1 + x2 - 0.5$

We obtain

δ_2 (0,0) = - 0.00359387

δ_2(0,1) = 0.00160349

δ_2(1,0) = 0.00116766

δ_2(1,1) = - 0.00384439

$$\delta_j = \varphi'(\text{net}_j) \cdot \sum_k (\delta_k w_{kj})$$

$$\frac{\partial E}{\partial w_{ji}} = -y_i \delta_j$$

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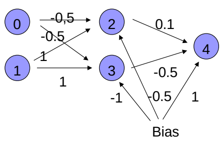
ANN Training Example



Call E_{20} the derivative of E with respect to w_{20}. We use the output activation for the neurons in the previous layer (which happens to be the input layer)

$E_{20}(0,0) = -\varphi(0)\cdot\delta_2(0,0) =$ 0.00179694

$E_{20}(0,1) =$ 0.00179694

$E_{20}(1,0) =$ -0.000853626

$E_{20}(1,1) =$ 0.00281047

$$\delta_j = \varphi'(\mathrm{net}_j)\cdot\sum_k(\delta_k w_{kj})$$

$$\frac{\partial E}{\partial w_{ji}} = -y_i\delta_j$$

The average is 0.00073801 and the new weight is -0.499262

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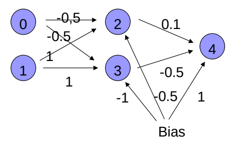
ANN Training Example



Call E_{21} the derivative of E with respect to w_{21}. We use the output activation for the neurons in the previous layer (which happens to be the input layer)

$E_{21}(0,0) = -\varphi(1)\cdot\delta_2(0,0) =$ 0.00179694

$E_{21}(0,1) =$ -0.00117224

$E_{21}(1,0) =$ -0.000583829

$E_{21}(1,1) =$ 0.00281047

$$\delta_j = \varphi'(\mathrm{net}_j)\cdot\sum_k(\delta_k w_{kj})$$

$$\frac{\partial E}{\partial w_{ji}} = -y_i\delta_j$$

The average is 0.000712835 and the new weight is 1.00071

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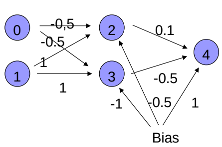
ANN Training Example



Call E_{2B} the derivative of E with respect to w_{2B}. Bias output is always -0.5

$E_{2B}(0,0) = - -0.5\cdot\delta_2(0,0) =$ 0.00179694

$E_{2B}(0,1) =$ -0.00117224

$E_{2B}(1,0) =$ -0.000583829

$E_{2B}(1,1) =$ 0.00281047

The average is 0.00058339 and the new weight is -0.499417

$$\delta_j = \varphi'(\mathrm{net}_j)\cdot\sum_k(\delta_k w_{kj})$$

$$\frac{\partial E}{\partial w_{ji}} = -y_i\delta_j$$

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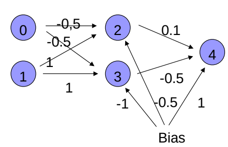
ANN Training Example



We now calculate the updates to the weights of neuron 3.

…

$$\delta_j = \varphi'(\mathrm{net}_j)\cdot\sum_k(\delta_k w_{kj})$$

$$\frac{\partial E}{\partial w_{ji}} = -y_i\delta_j$$

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ANN Training

- ANN Back-propagation is an empirical algorithm

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ANN Training

- XOR is too simple an example, since quality of ANN is measured on a finite sets of inputs.
- More relevant are ANN that are trained on a training set and unleashed on real data

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ANN Training

- Need to measure effectiveness of training
  - Need training sets
  - Need test sets.
- There can be no interaction between test sets and training sets.
  - Example of a Mistake:
    - Train ANN on training set.
    - Test ANN on test set.
    - Results are poor.
    - Go back to training ANN.
  - After this, there is no assurance that ANN will work well in practice.
    - In a subtle way, the test set has become part of the training set.

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ANN Training

- Convergence
  - ANN back propagation uses gradient decent.
  - Naïve implementations can
    - overcorrect weights
    - undercorrect weights
  - In either case, convergence can be poor
- Stuck in the wrong place
  - ANN starts with random weights and improves them
  - If improvement stops, we stop algorithm
  - No guarantee that we found the best set of weights
  - Could be stuck in a local minimum

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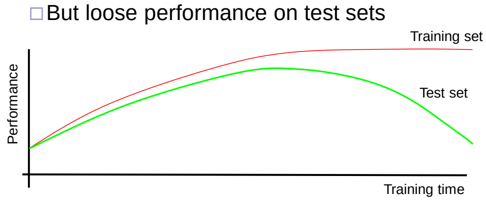
ANN Training

- Overtraining
  - An ANN can be made to work too well on a training set
  - But loose performance on test sets



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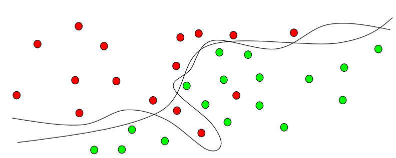
ANN Training

- Overtraining
  - Assume we want to separate the red from the green dots.
  - Eventually, the network will learn to do well in the training case
  - But have learnt only the particularities of our training set



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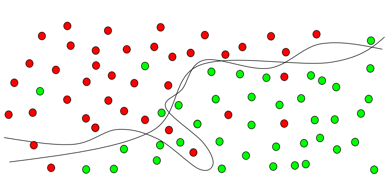
ANN Training

- Overtraining



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ANN Training

- Improving Convergence
  - Many Operations Research Tools apply
    - Simulated annealing
    - Sophisticated gradient descent

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ANN Design

- ANN is a largely empirical study
  - “Seems to work in almost all cases that we know about”
- Known to be statistical pattern analysis

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ANN Design

- Number of layers
  - Apparently, three layers is almost always good enough and better than four layers.
  - Also: fewer layers are faster in execution and training
- How many hidden nodes?
  - Many hidden nodes allow to learn more complicated patterns
  - Because of overtraining, almost always best to set the number of hidden nodes too low and then increase their numbers.

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ANN Design

- Interpreting Output
  - ANN’s output neurons do not give binary values.
    - Good or bad
    - Need to define what is an accept.
  - Can indicate *n* degrees of certainty with *n*-1 output neurons.
    - Number of firing output neurons is degree of certainty

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ANN Applications

- Pattern recognition
  - Network attacks
  - Breast cancer
  - …
  - handwriting recognition
- Pattern completion
- Auto-association
  - ANN trained to reproduce input as output
    - Noise reduction
    - Compression
    - Finding anomalies
- Time Series Completion

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ANN Future

- ANNs can do some things really well
- They lack in structure found in most natural neural networks

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Pseudo-Code

- phi – activation function
- phid – derivative of activation function

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Pseudo-Code

- Forward Propagation:
  - Input nodes i, given input x_i:
    - foreach inputnode i
      - $\text{output}_i = x_i$
  - Hidden layer nodes j
    - foreach hiddenneuron j
      - $\text{output}_j = \sum_i \text{phi}(w_{ji} \cdot \text{output}_i)$
  - Output layer neurons k
    - foreach outputneuron k
      - $\text{output}_k = \sum_k \text{phi}(w_{kj} \cdot \text{output}_j)$

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Pseudo-Code

```
ActivateLayer(input,output)
  foreach i inputneuron
     calculate output_i
  foreach j hiddenneuron
      calculate output_j
  foreach k hiddenneuron
      calculate output_k
  output = {output_k}
```

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Pseudo-Code

- Output Error

```
Error()   {
foreach input in InputSet
  Error_input = Σ_k output neuron (target_k-output_k)^2
return Average(Error_input,InputSet)
```

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Pseudo-Code

- Gradient Calculation
  - We calculate the gradient of the error with respect to a given weight w_{kj}.
  - The gradient is the average of the gradients for all inputs.
  - Calculation proceeds from the output layer to the hidden layer

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Pseudo-Code

For each output neuron *k* calculate:

$$\delta_k = \varphi'(\text{net}_k) \cdot (\text{target}_k - \text{output}_k)$$

For each output neuron *k* calculate and hidden layer neuron *j* calculate:

$$\frac{\partial E}{\partial W_{kj}} = -\text{output}_j \cdot \delta_k$$

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Pseudo-Code

For each hidden neuron *j* calculate:

$$\delta_j = \varphi'(\text{net}_j) \cdot \sum_k (\delta_k W_{kj})$$

For each hidden neuron *j* and each input neuron *i* calculate:

$$\frac{\partial E}{\partial W_{ji}} = -\text{output}_i \cdot \delta_j$$

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Pseudo-Code

- These calculations were done for a single input.
- Now calculate the average gradient over all inputs (and for all weights).
- You also need to calculate the gradients for the bias weights and average them.

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Pseudo-Code

- Naïve back-propagation code:
  - Initialize weights to a small random value (between -1 and 1)
  - For a maximum number of iterations do
    - Calculate average error for all input. If error is smaller than tolerance, exit.
    - For each input, calculate the gradients for all weights, including bias weights and average them.
    - If length of gradient vector is smaller than a small value, then stop.
    - Otherwise:
      - Modify all weights by adding a negative multiple of the gradient to the weights.

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Pseudo-Code

- This naïve algorithm has problems with convergence and should only be used for toy problems.

0.337379

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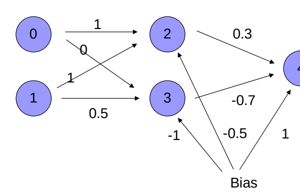
ANN Training Example 2

- Start out with random, small weights



Node 0: x_0
Node 1: x_1
Node 2: $o_2 = \varphi(x_0 + x_1 - 0.5)$
Node 3: $o_3 = \varphi(0.5\ x_1 - 1)$
Node 4: $o_4 = \varphi(0.3\ o_2 - 0.7\ o_3 + 1)$

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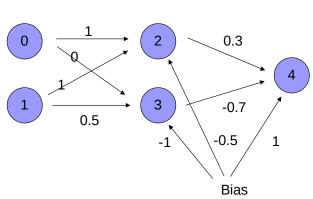
ANN Training Example 2

- Calculate outputs



x1	x2	$y=o_4$
0	0	0.7160
0	1	0.7155
1	0	0.7308
1	1	0.7273

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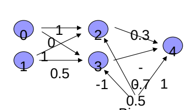
ANN Training Example 2

- Calculate average error to be E = 0.14939



x_0	x_1	y	t	$E=(y-t)^2/2$
0	0	0.7160	0	0.2564
0	1	0.7155	1	0.0405
1	0	0.7308	1	0.0362
1	1	0.7273	0	0.264487

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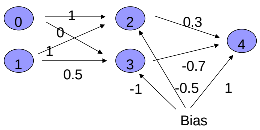
ANN Training Example 2

- Calculate the change for node 4



Need to calculate net_4, the weighted input of all input into node 4

$net_4(x_0,x_1) = 0.3\ o_2(x_0,x_1) – 0.7\ o_3(x0,x1) + 1$

$net_4 = (net_4(0,0) + net_4(0,1) + net_4(1,0) + net_4(1,1))/4$

This gives 0.956734

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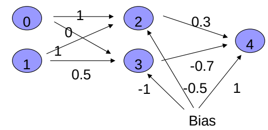
ANN Training Example 2

- Calculate the change for node 4



$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

We now calculate

$\delta_4(0,0) = \varphi'(net_4(0,0)(0 - o_4(0,0)) = - 0.14588$

$\delta_4(0,1) = \varphi'(net4(0,1)(1 - o4(0,1)) = 0.05790$

$\delta_4(1,1) = \varphi'(net4(1,0)(0 - o4(1,0)) = 0.05297$

$\delta_4(1,1) = \varphi'(net4(1,1)(0 - o4(1,1)) = -0.14425$

On average $\delta_4 = -0.044741$

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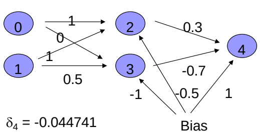
ANN Training Example 2

- Calculate the change for node 4



$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

$\delta_4 = -0.044741$

We can now update the weights for node 4

$E_{4,2}(0,0) = -o_2(0,0)^* \delta_4 = 0.01689$

$E_{4,2}(0,1) = -o_2(0,1)^* \delta_4 = 0.02785$

$E_{4,2}(1,0) = -o_2(1,0)^* \delta_4 = 0.02785$

$E_{4,2}(0,0) = -o_2(0,0)^* \delta_4 = 0.03658$

with average 0.00708

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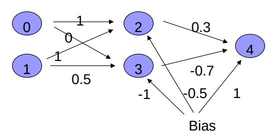
ANN Training Example 2

- Calculate the change for node 4



$$\frac{\partial E(\vec{x})}{\partial w_{jk}} = -y_j \delta_j$$

$$\delta_j = f'(\text{net}_j)(t_j - y_j)$$

$E_{4,2} = 0.00708$

Therefore, new weight w_{42} is 0.2993

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