CS 4602

Introduction to Machine Learning

Neural Networks

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Roadmap

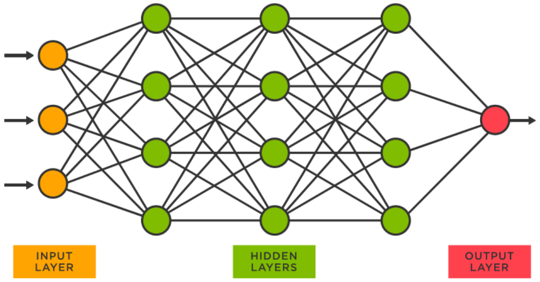
- Introduction and Basic Concepts
- Regression
- Bayesian Classifiers
- Decision Trees
- Linear Classifier
- Neural Networks
- Deep learning
- Convolutional Neural Networks
- Reinforcement Learning
- KNN
- Model Selection and Evaluation
- Clustering
- Data Exploration & Dimensionality reduction

Outline

- Motivation
- Multilayer perceptrons (MLP)
- Backpropogation

Connectionism

- A computer modeling approach based upon the architecture of the brain
- Multiple, individual “**nodes**” or “**units**” that operate at the same time (in parallel)
- A **network** that connects the nodes together
- Information is stored in a distributed fashion among the **links** that connect the nodes
- **Learning** can occur with gradual changes in connection strength



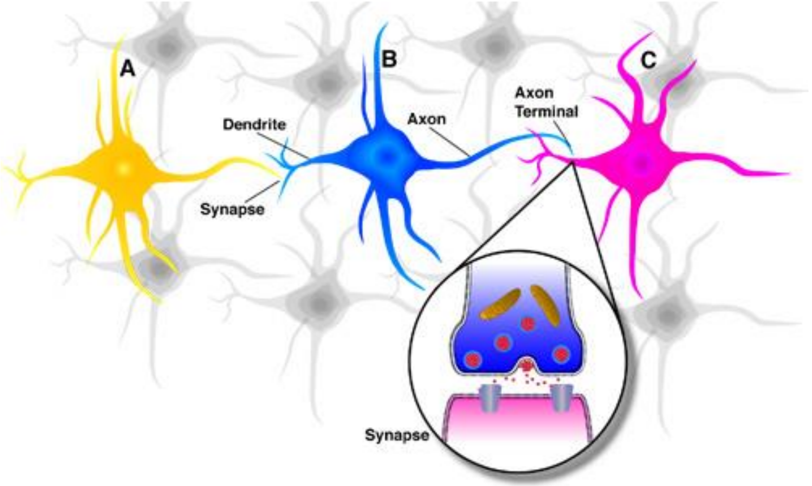
Brains vs Computers

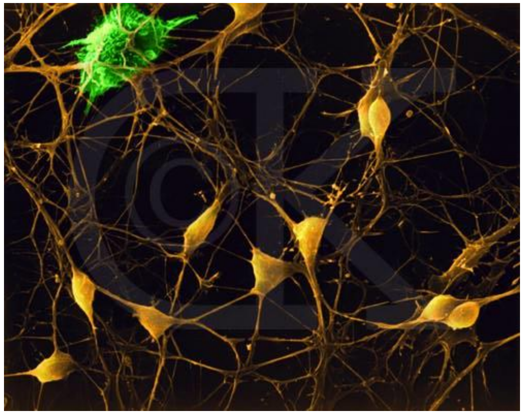
- 200 billion neurons, 32 trillion synapses
- Element size: 10^{-6} m
- Energy use: 25W
- Processing speed: 100 Hz
- Parallel, Distributed
- Fault Tolerant
- Learns: Yes
- Conscious: Usually

- 1 billion bytes RAM but trillions of bytes on disk
- Element size: 10^{-9} m
- Energy watt: 30-90W (CPU)
- Processing speed: 10^9 Hz
- Serial, Centralized
- Generally not Fault Tolerant
- Learns: Some
- Conscious: Generally No

Neurons in the Brain

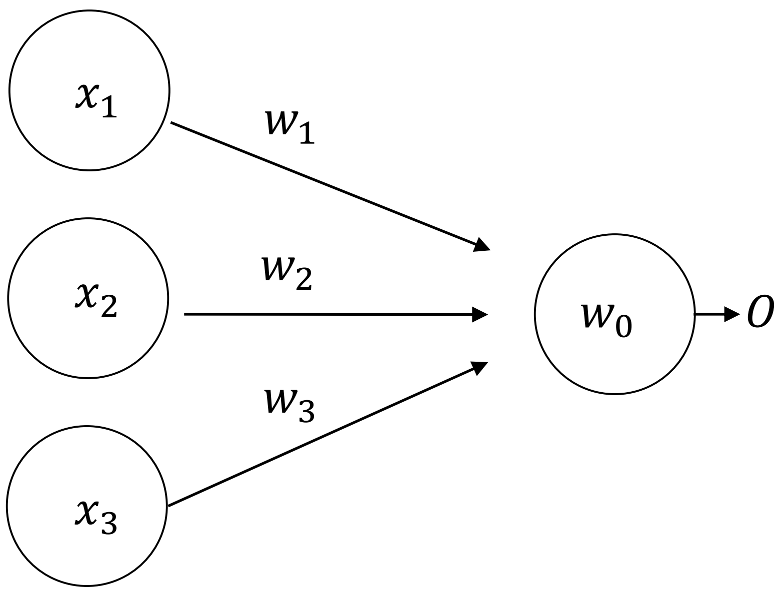
- A neuron receives input from other neurons (generally thousands) from its synapses
- Inputs are approximately summed
- When the input exceeds a threshold the neuron sends an electrical spike that travels that travels from the body, down the axon, to the next neuron(s)





Perceptron

- Initial proposal of connectionist networks
- Essentially a linear discriminant composed of nodes, weights

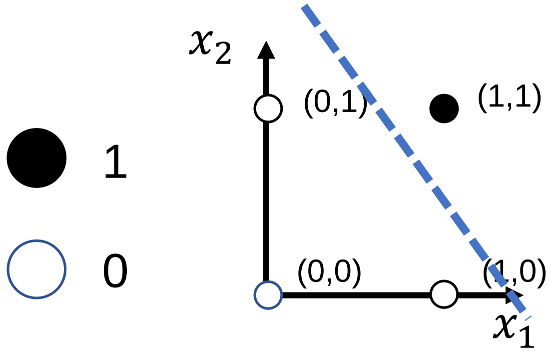


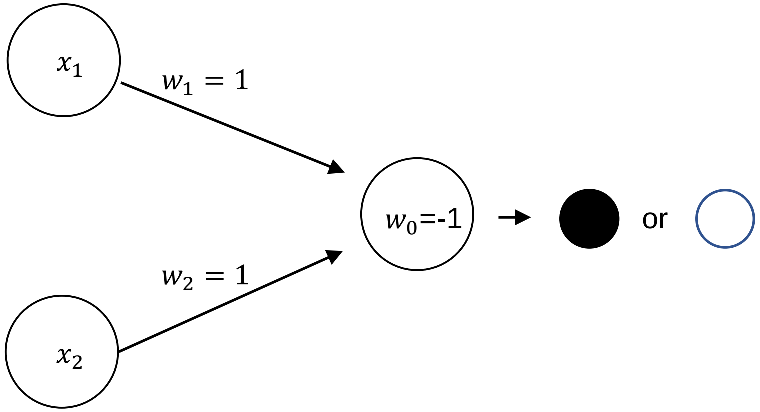
Activation Function

$$O = \begin{cases} 1 : \left(\sum_i w_i x_i \right) + w_0 > 0 \\ 0 : \quad otherwise \end{cases}$$

Linear separability

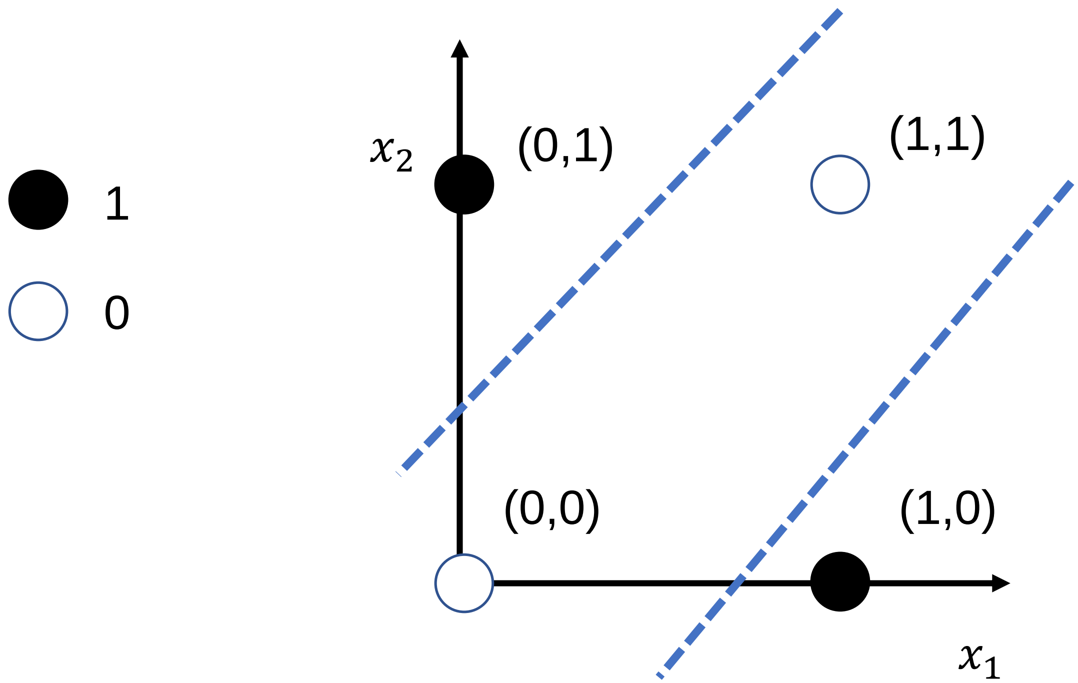
- Consider a single-layer perceptron
  - Assume threshold units
  - Assume binary inputs and outputs
  - Weighted sum forms a linear hyperplane $\sum_i w_i x_i = 0$
- Consider a single output network with two inputs
  - Only functions that are linearly separable can be computed
  - Example: AND is linearly separable





Linear inseparability

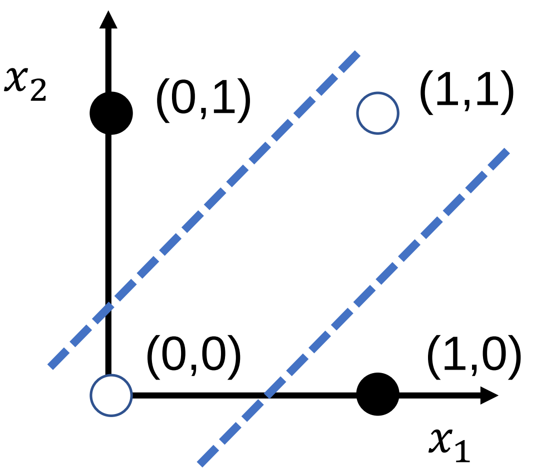
- Single-layer perceptron with threshold units fails if problem is not linearly separable
  - Example: XOR



Solution in 1980s: Multilayer perceptron (MLP)

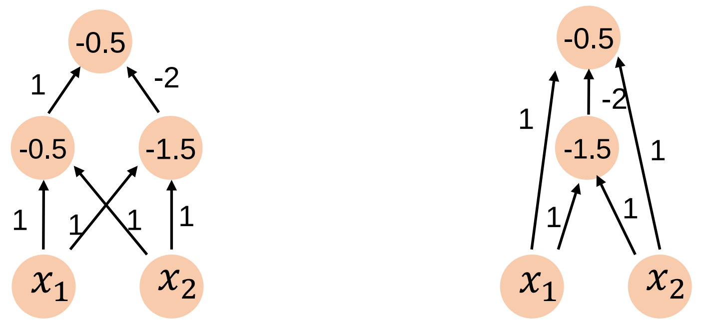
- Removes many limitations of single-layer networks
  - Can solve XOR

- How to Draw a two-layer perceptron that computes the XOR function?
  - 2 binary inputs x_1 and x_2
  - 1 binary output
  - One “hidden” layer
  - Find the appropriate weights and threshold



Multilayer perceptron

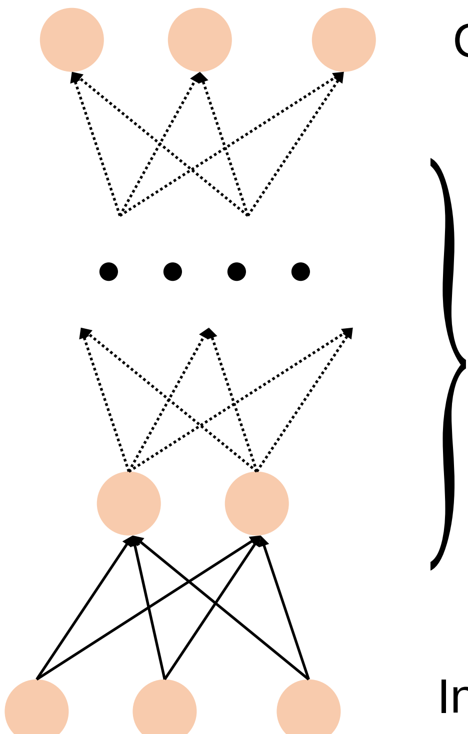
- Examples of two-layer perceptrons that compute XOR



- E.g. Right side network
  - Output is 1

  if and only if $x_1 + x_2 - 2(x_1 + x_2 - 1.5 > 0) - 0.5 > 0$

Multilayer perceptron



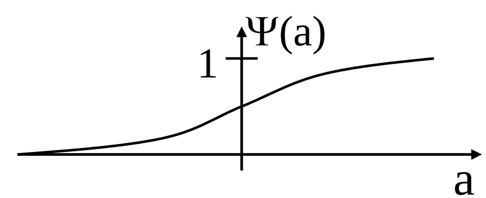
Output neurons

One or more layers of hidden units (hidden layers)

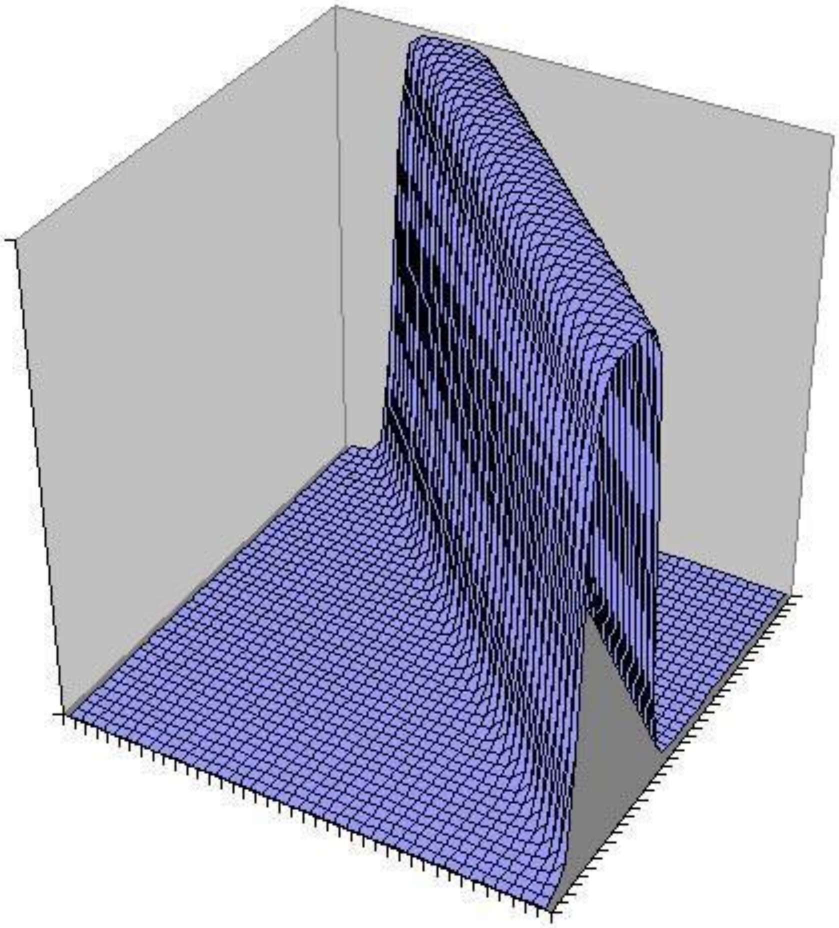
Input nodes

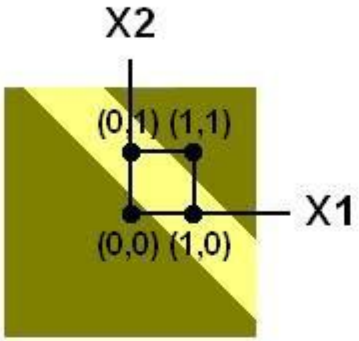
The most common output function (Sigmoid):

$$\Psi(a) = \frac{1}{1 + e^{-\beta a}}$$



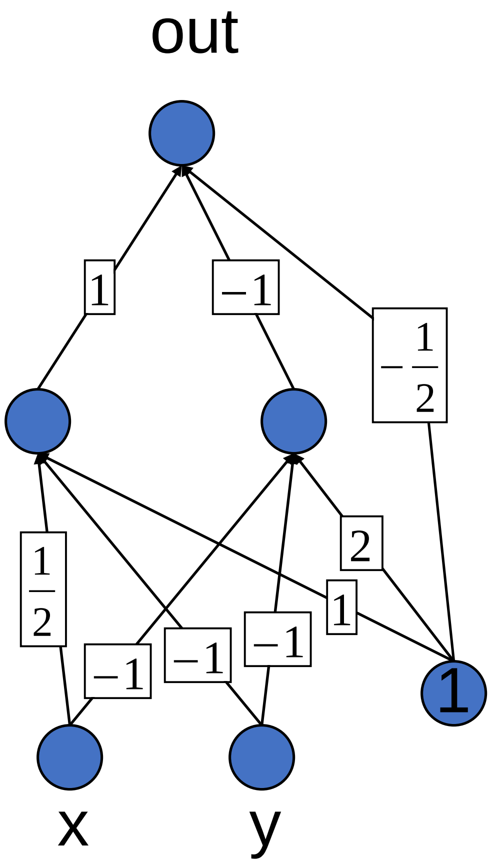
(non-linear function)

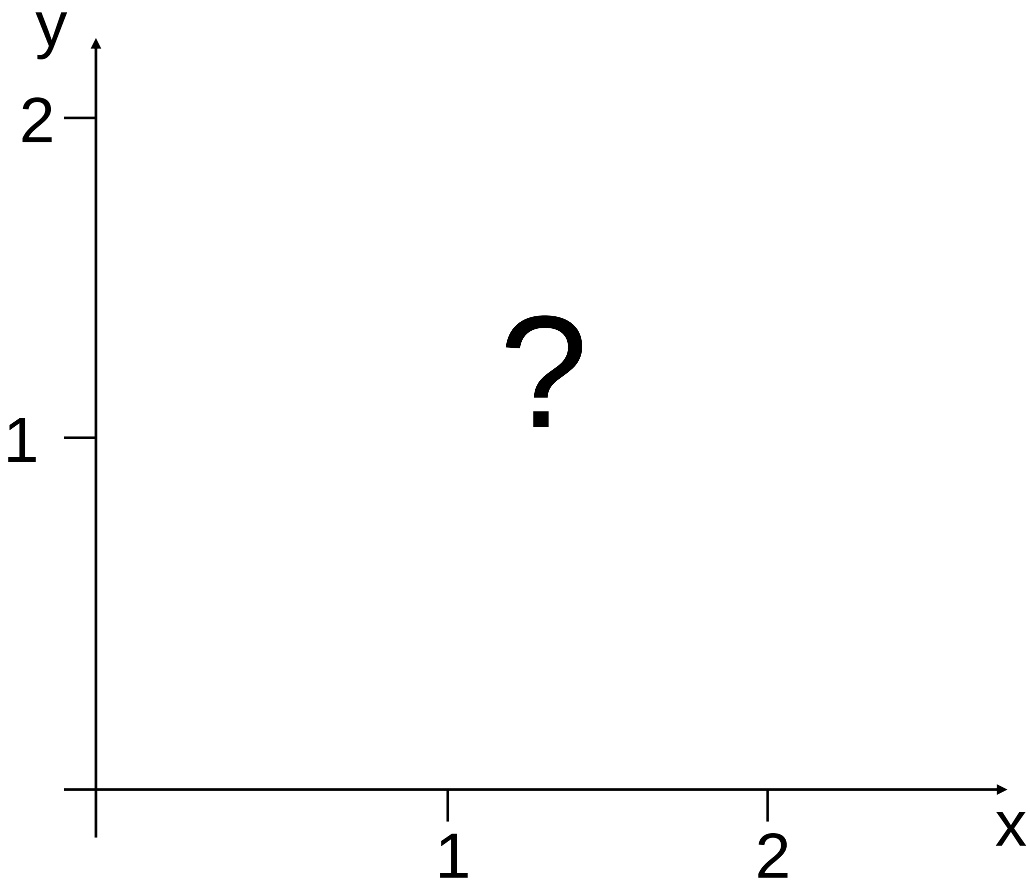




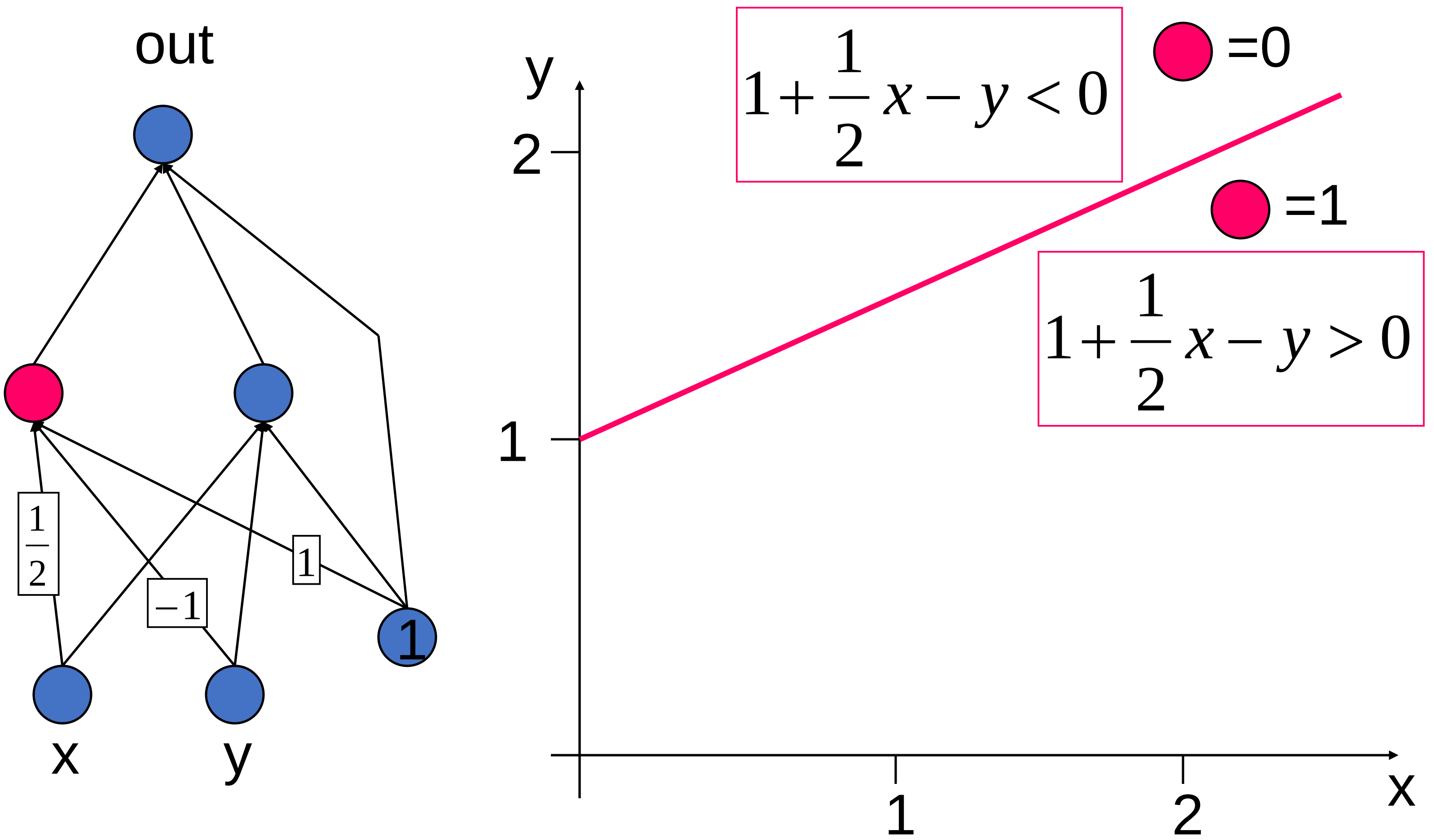
Source: http://colinfahey.com/

MLP separating patterns

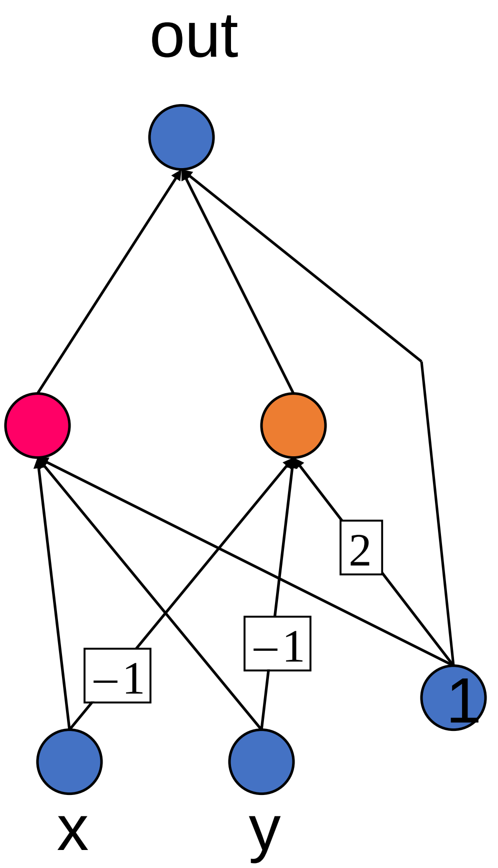


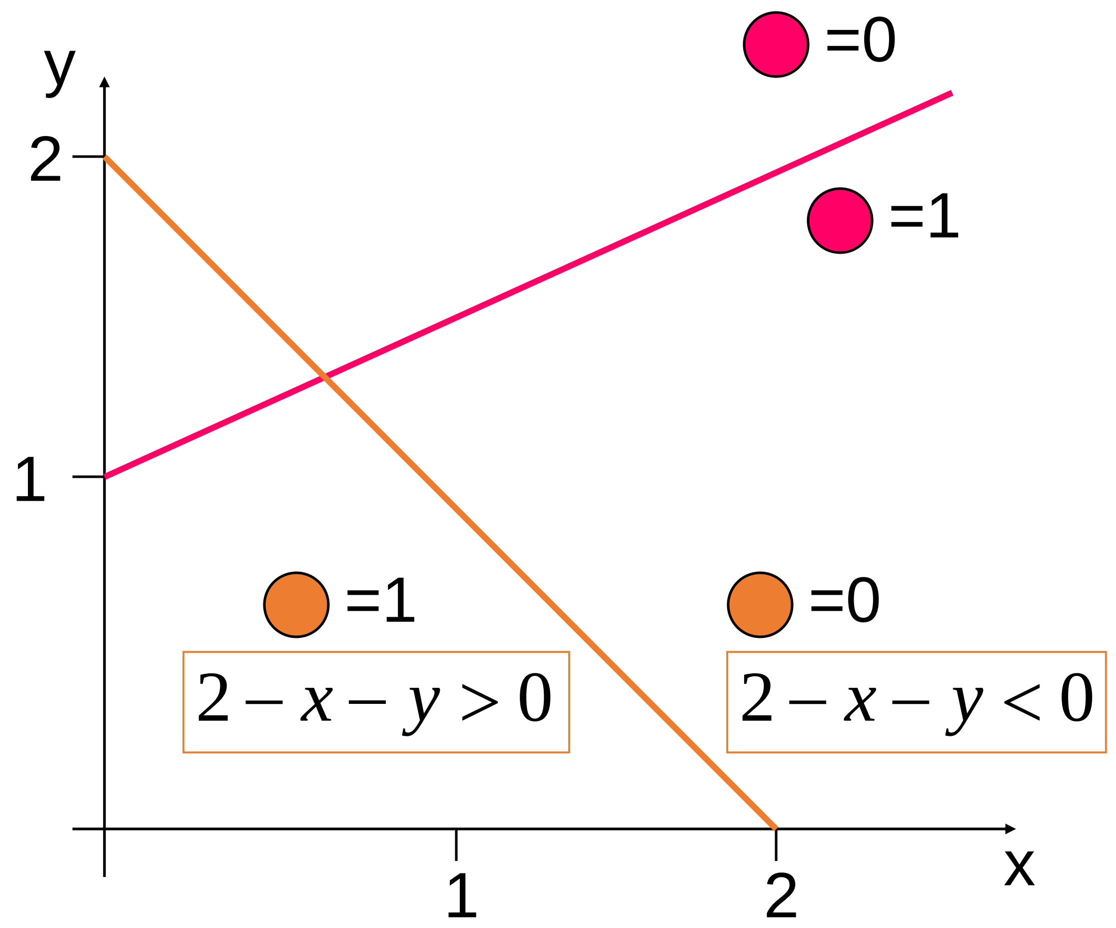


MLP separating patterns

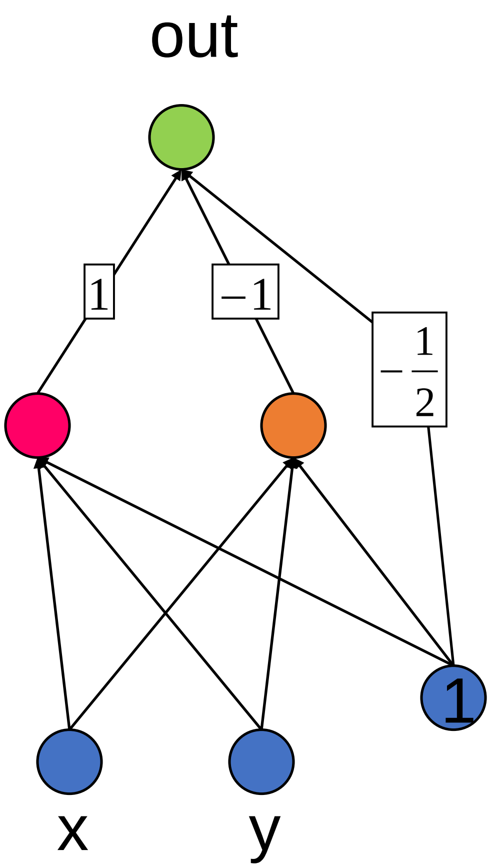


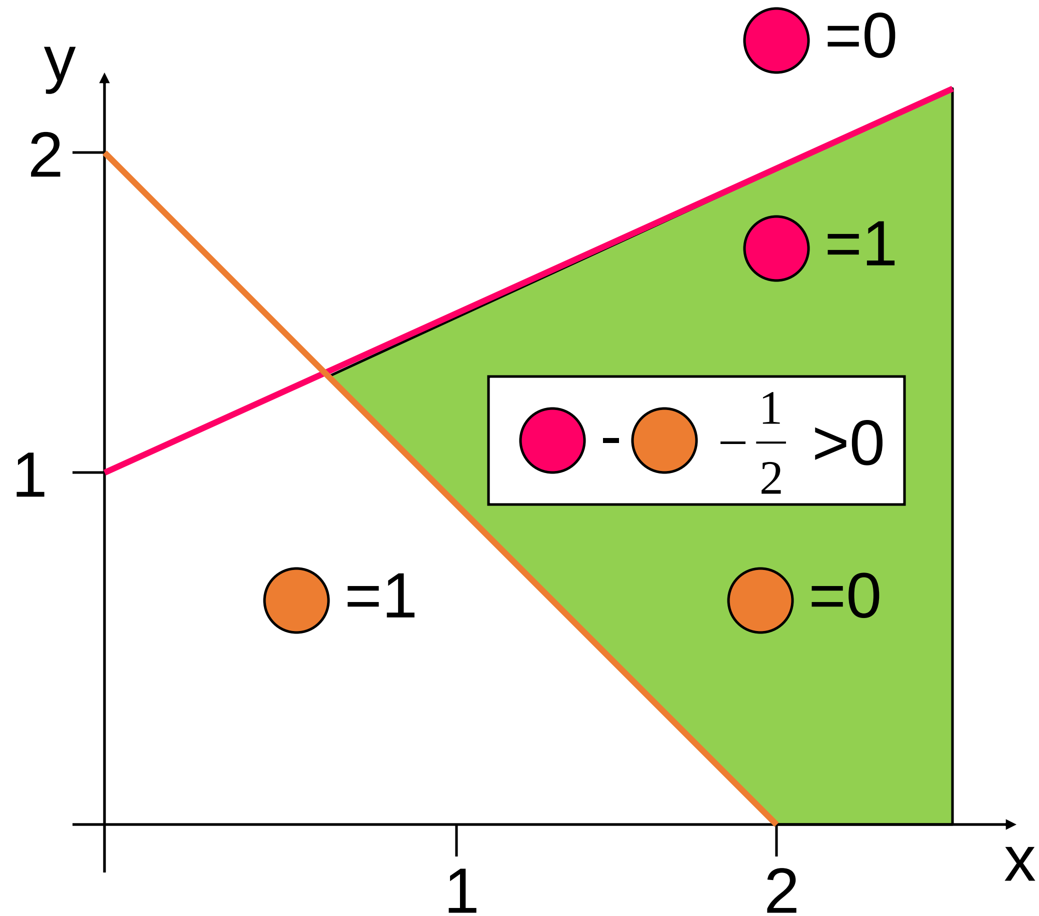
MLP separating patterns



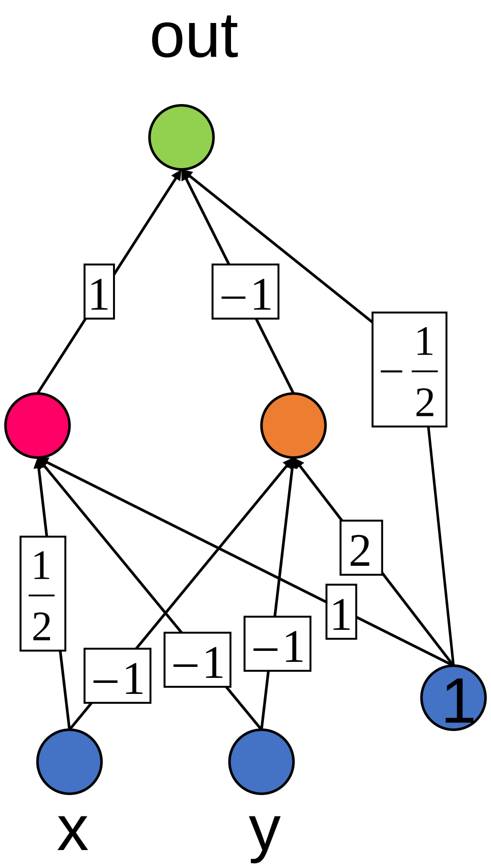


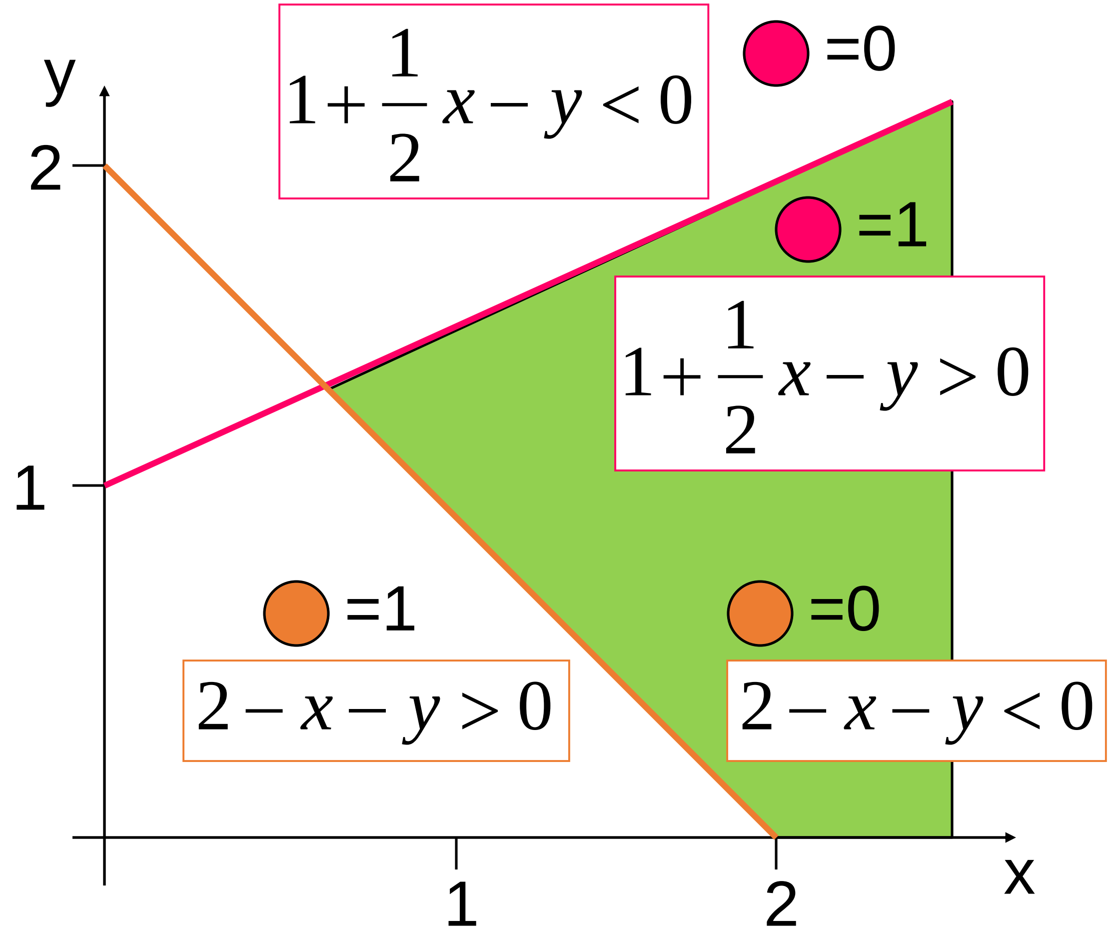
MLP separating patterns





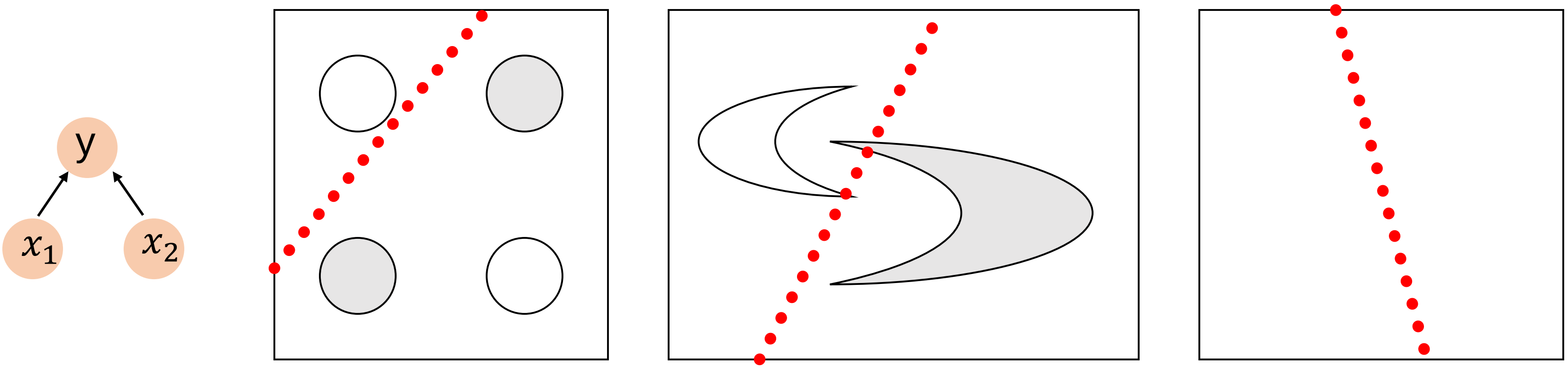
MLP separating patterns





Decision Boundary

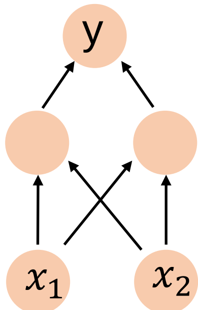
- 0 hidden layers: linear classifier
  - Hyperplanes

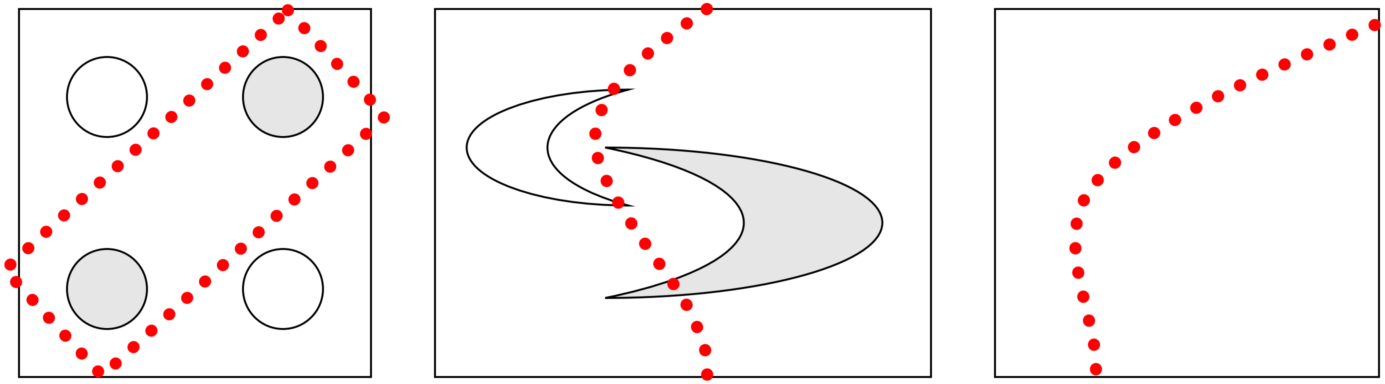


Example from to Eric Postma via Jason Eisner

Decision Boundary

- 1 hidden layer
  - Boundary of convex region (open or closed)

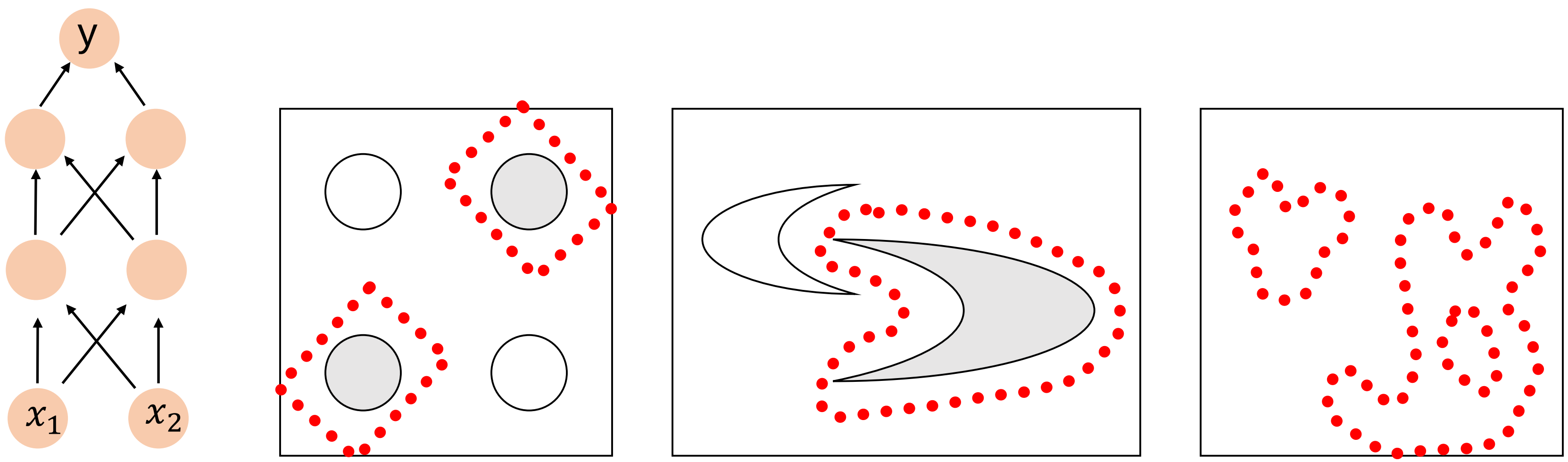




Example from to Eric Postma via Jason Eisner

Decision Boundary

- 2 hidden layers
  - Combinations of convex regions



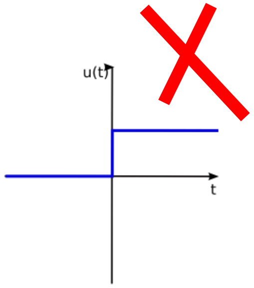
Example from to Eric Postma via Jason Eisner

Outline

- Motivation
- Multilayer perceptrons (MLP)
- Backpropogation (BP)

Perceptron Alg. vs. Gradient Descent Rule

Not differentiable



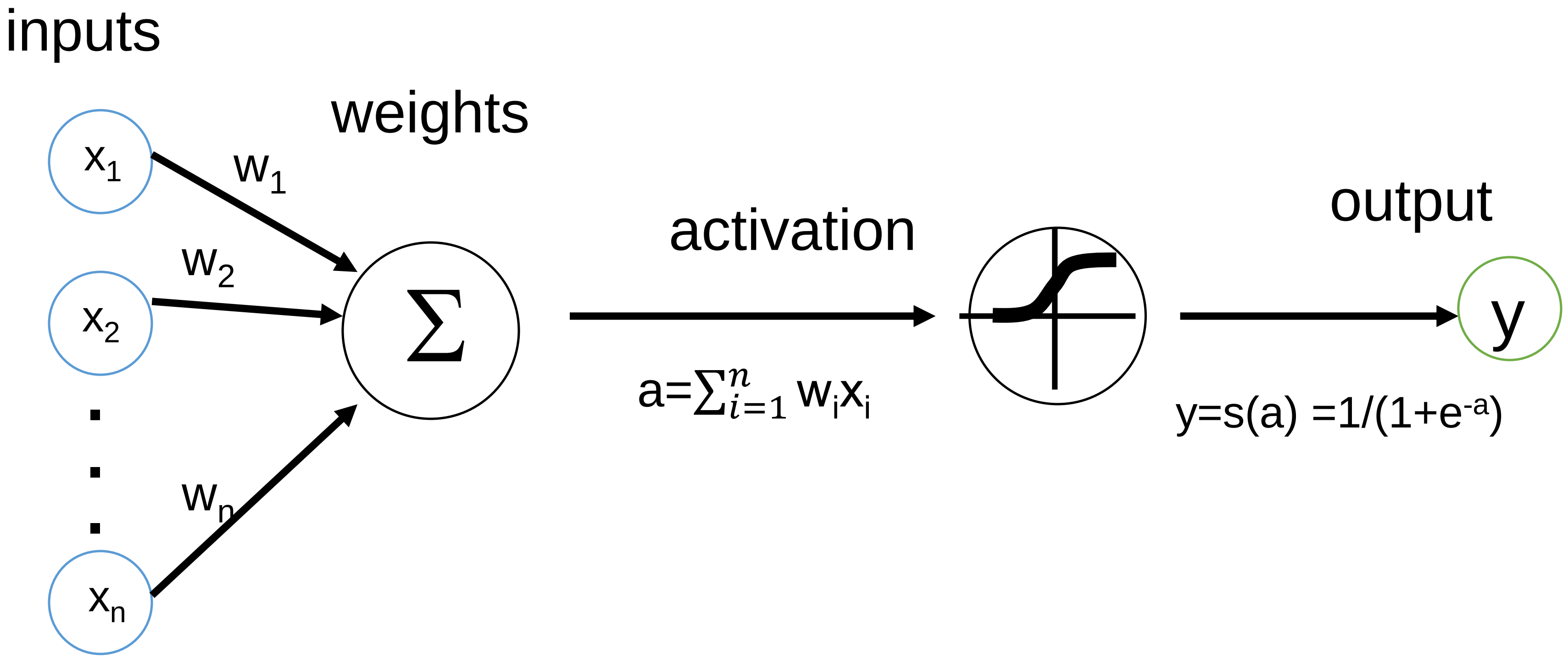
Perceptron learning rule guaranteed to succeed if

- Training examples are linearly separable
- Sufficiently small learning rate α

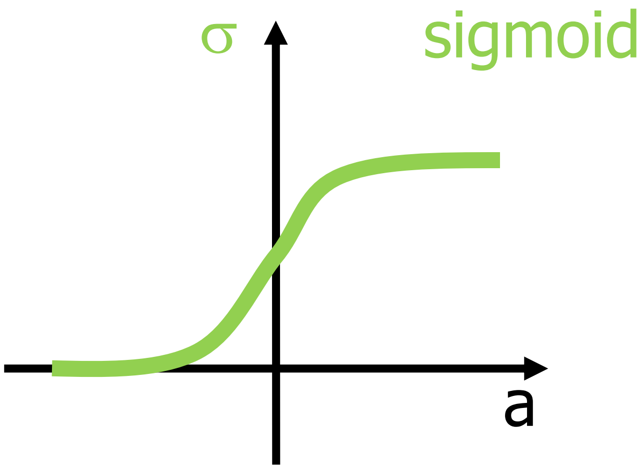
Linear unit training rules uses gradient descent

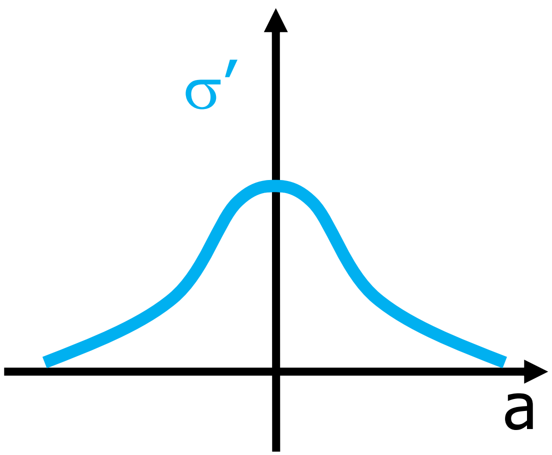
- Use a differentiable activation function
- Guaranteed to converge to hypothesis with minimum squared error
- Given sufficiently small learning rate α
- Even when training data contains noise
- Even when training data not separable by H

Neuron with Sigmoid Function



Gradient Descent for Sigmoid Function





$$E[w_1,\ldots,w_n] = \tfrac{1}{2}\,(t-y)^2$$

$$\partial E/\partial w_i = \partial/\partial w_i\ \tfrac{1}{2}\,(t-y)^2$$

$$= \partial/\partial w_i\ \tfrac{1}{2}\,(t-\sigma(\textstyle\sum_i w_i\, x_i))^2$$

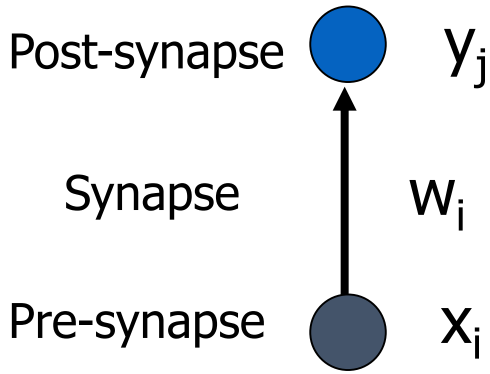
$$= (t-y)\ \sigma'(\textstyle\sum_i w_i\, x_i)\ (-x_i)$$

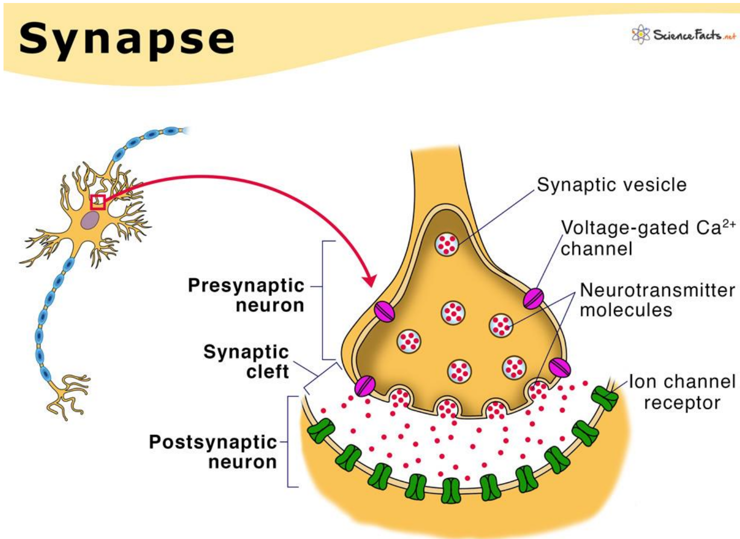
for $y=\sigma(a) = 1/(1+e^{-a})$

$\sigma'(a)= e^{-a}/(1+e^{-a})^2=\sigma(a)\ (1-\sigma(a))$

$$\Delta w_i = \alpha\ y\,(1-y)(t-y)\ x_i$$

Gradient Descent Learning Rule





https://www.sciencefacts.net/synapse.html

$$\Delta w_i = \alpha \;\; y_j(1-y_j) \;\; (t_j-y_j) \;\; x_i$$

learning rate

derivative of activation function

error of post-synaptic neuron

activation of pre-synaptic neuron

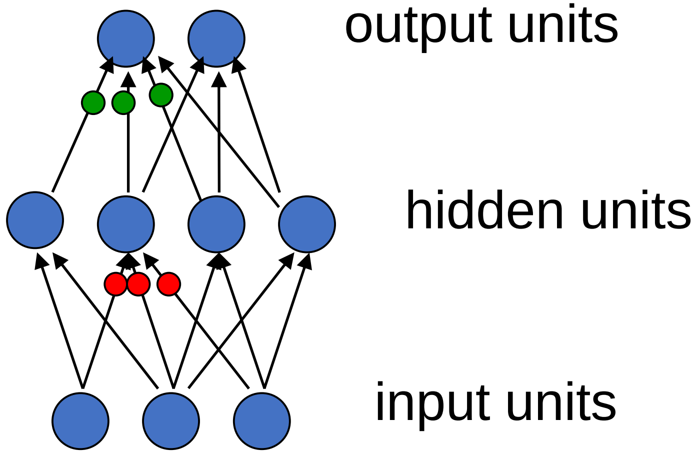
Learning with hidden units

- We need multiple layers of adaptive non-linear hidden units. But how can we train such networks?
  - We need an efficient way of adapting all the weights, not just the last layer.
  - Learning the weights going into hidden units is equivalent to learning **features**.
  - It's hard to tell directly what hidden units should do.

Learning by perturbing weights

- Randomly perturb one weight and see if it improves performance. If so, save the change.
  - Very inefficient. We need to do multiple forward passes to change one weight.
- Randomly perturb all the weights in parallel and correlate the performance gain with the weight changes.
  - We need lots of trials to “see” the effect of changing one weight through the noise created by all the others.

Learning the hidden to output weights is easy.

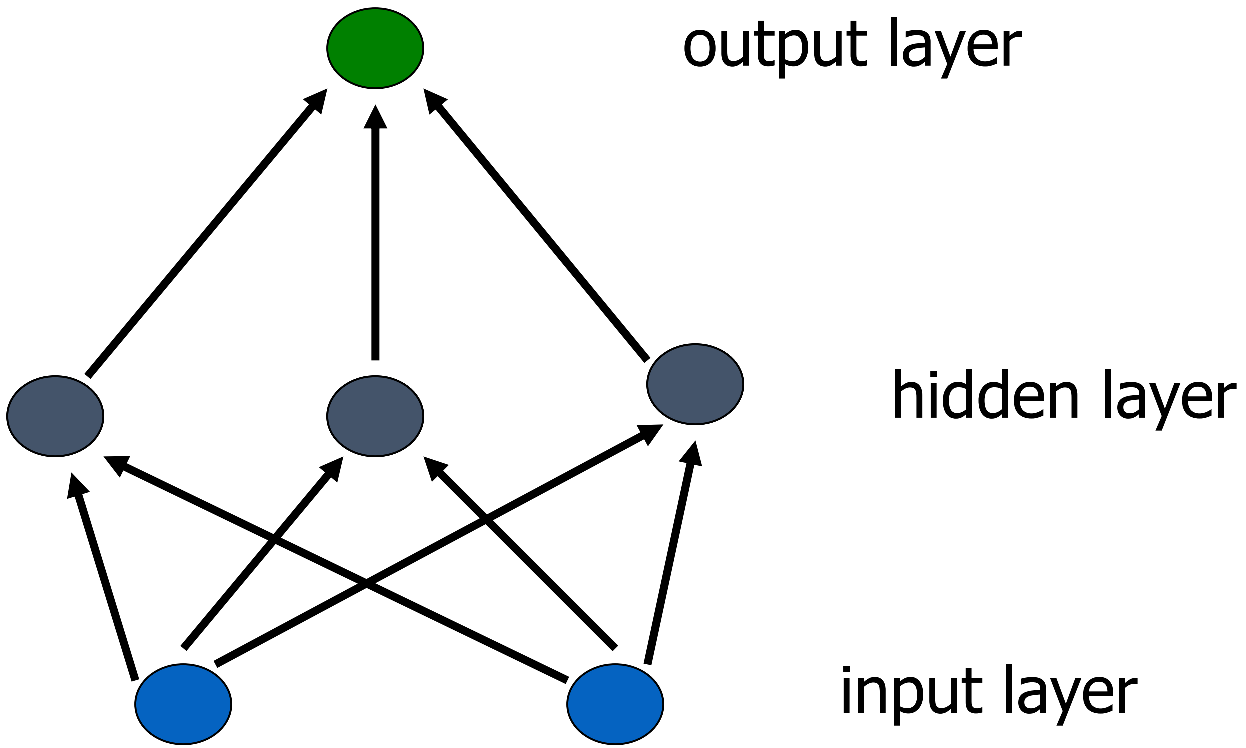


Learning the input to hidden weights is hard.

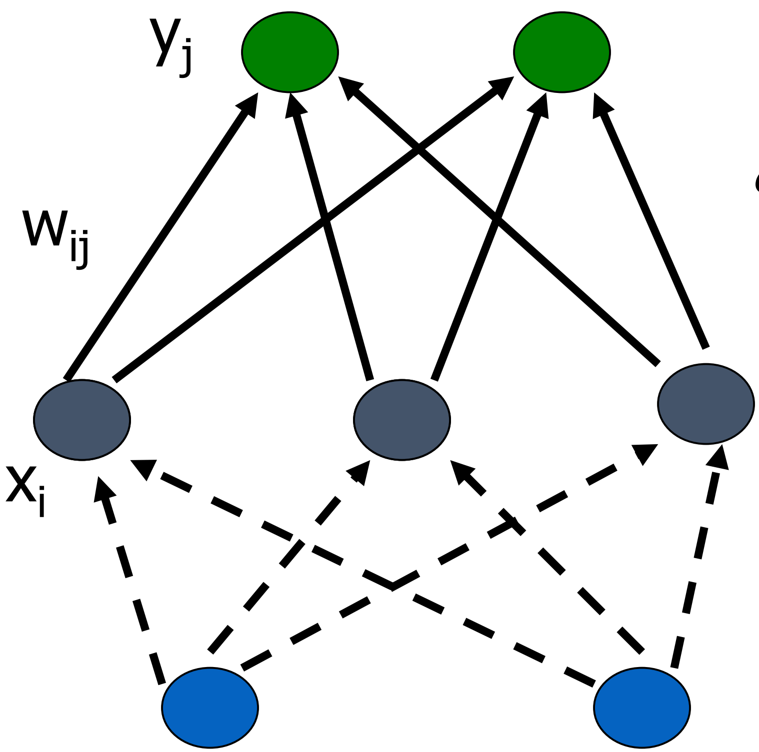
The idea behind backpropagation

- We don't know what the hidden units ought to do, but we can compute how fast the error changes as we change a hidden activity.
  - Instead of using desired activities to train the hidden units, use error derivatives w.r.t. hidden activities.
  - Each hidden activity can affect many output units.
  - Compute error derivatives for all the hidden units efficiently.
  - Once we have the error derivatives for the hidden activities, its easy to get the error derivatives for the weights going into a hidden unit.

Training Rule



Training Rule for Weights to the Output Layer



$E[w_{ij}] = ½ \Sigma_j (t_j-y_j)^2$

$$\partial E/\partial w_{ij} = \partial /\partial w_{ij}\ ½ \Sigma_j (t_j-y_j)^2$$
$$= \ldots$$
$$= - y_j(1-y_j)(t_j-y_j)\ x_i$$

Derivative of activation function

Learning rate

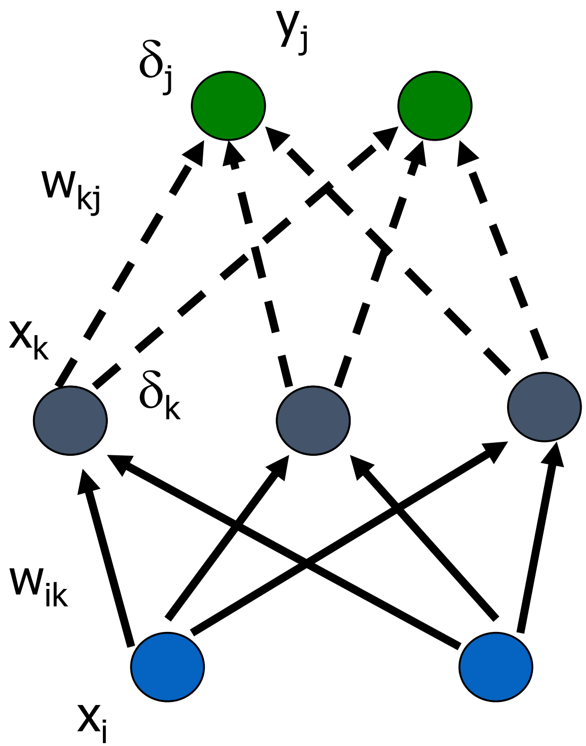
Error of post-synaptic neuron

$$\Delta w_{ij} = \alpha\ \ y_j(1-y_j)\ (t_j-y_j)\ x_i$$
$$= \alpha\ \ \delta_j\ x_i$$

Activation of pre-synaptic neuron

with $\delta_j := y_j(1-y_j)\ (t_j-y_j)$

Training Rule for Weights to the Hidden Layer



$E[w_{ik}] = \frac{1}{2} \Sigma_j (t_j - y_j)^2$

$\partial E/\partial w_{ik} = \partial/\partial w_{ik} \, \frac{1}{2} \Sigma_j (t_j - y_j)^2$

$= \partial/\partial w_{ik} \, \frac{1}{2} \Sigma_j (t_j - \sigma(\Sigma_k w_{kj} \, x_k))^2$

$= \partial/\partial w_{ik} \, \frac{1}{2} \Sigma_j (t_j - \sigma(\Sigma_k w_{kj} \, \sigma(\Sigma_i w_{ik} \, x_i)))^2$

$= -\Sigma_j (t_j - y_j) \, \sigma'_j(a) \, w_{kj} \, \sigma'_k(a) \, x_i$

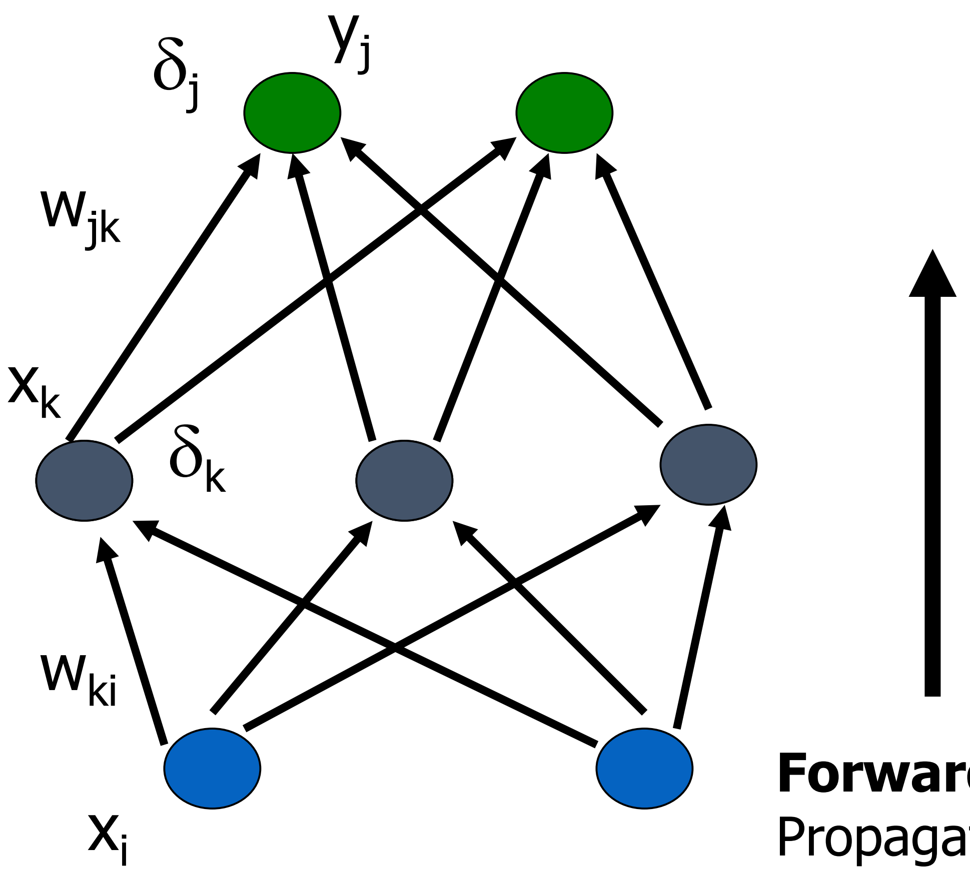
$= -\Sigma_j \delta_j \, w_{kj} \, \sigma'_k(a) \, x_i$

$= -\Sigma_j \delta_j \, w_{kj} \, x_k (1 - x_k) \, x_i$

$\Delta w_{ik} = \alpha \, \delta_k \, x_i$

with $\delta_k = \Sigma_j \delta_j \, w_{kj} \, x_k (1 - x_k)$

Backpropagation



Backward pass:
propagate errors from
output to hidden layer

Forward pass:
Propagate activation
from input to output layer

Backpropagation Algorithm

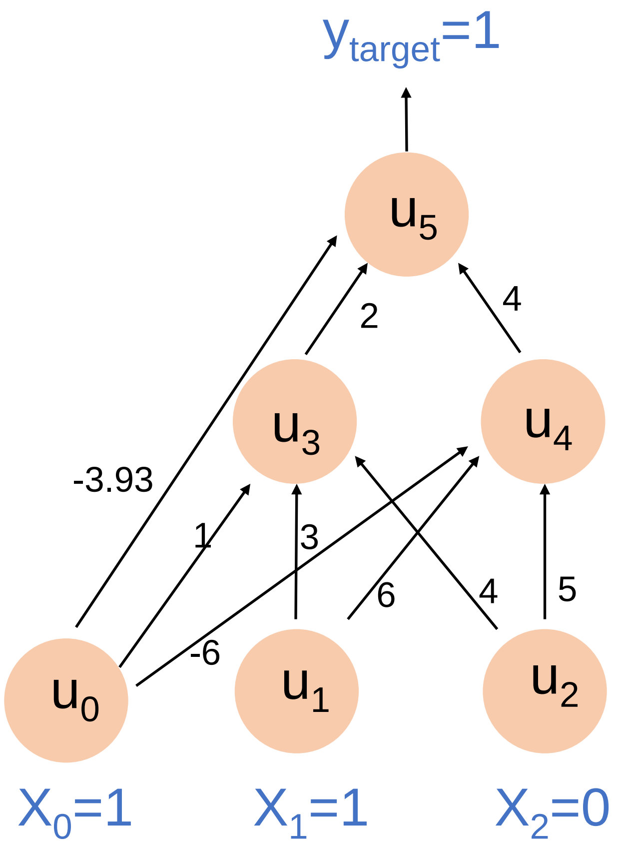
- Initialize each w_i to some small random value
- Until the termination condition is met, Do
  - For each training example <$(x_1,\ldots x_n),t$> Do
    - Input the instance $(x_1,\ldots,x_n)$ to the network and compute the network outputs y_k Forward Pass
    - For each output unit k

      $$\delta_k = y_k(1-y_k)(t_k-y_k)$$ Backward Pass
    - For each hidden unit h

      $$\delta_h = y_h(1-y_h) \sum_k w_{h,k}\, \delta_k$$
    - For each network weight $w_{i,j}$ Do Update

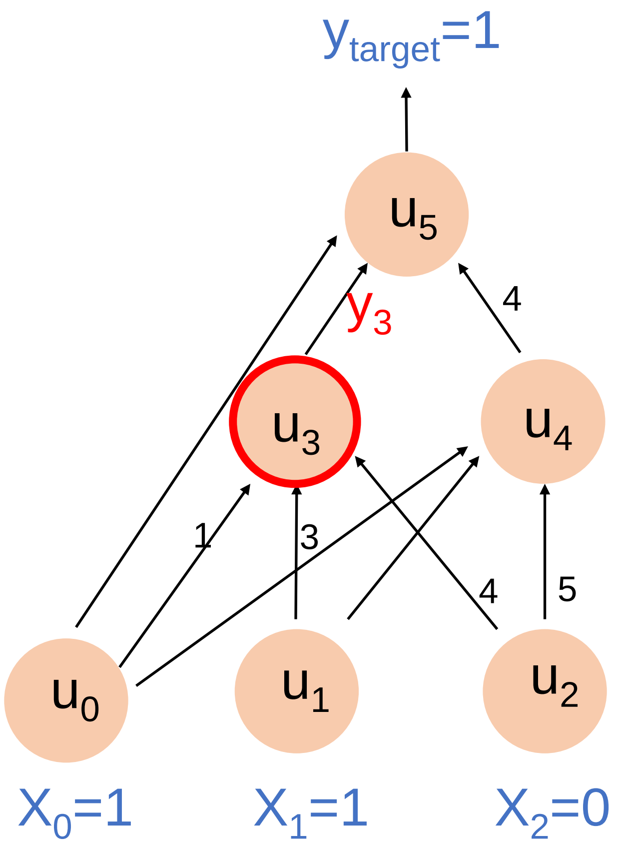
      $w_{i,j}=w_{i,j}+\Delta w_{i,j}$ where $\Delta w_{i,j}= \alpha\, \delta_j\, x_{i,j}$

BP: Example



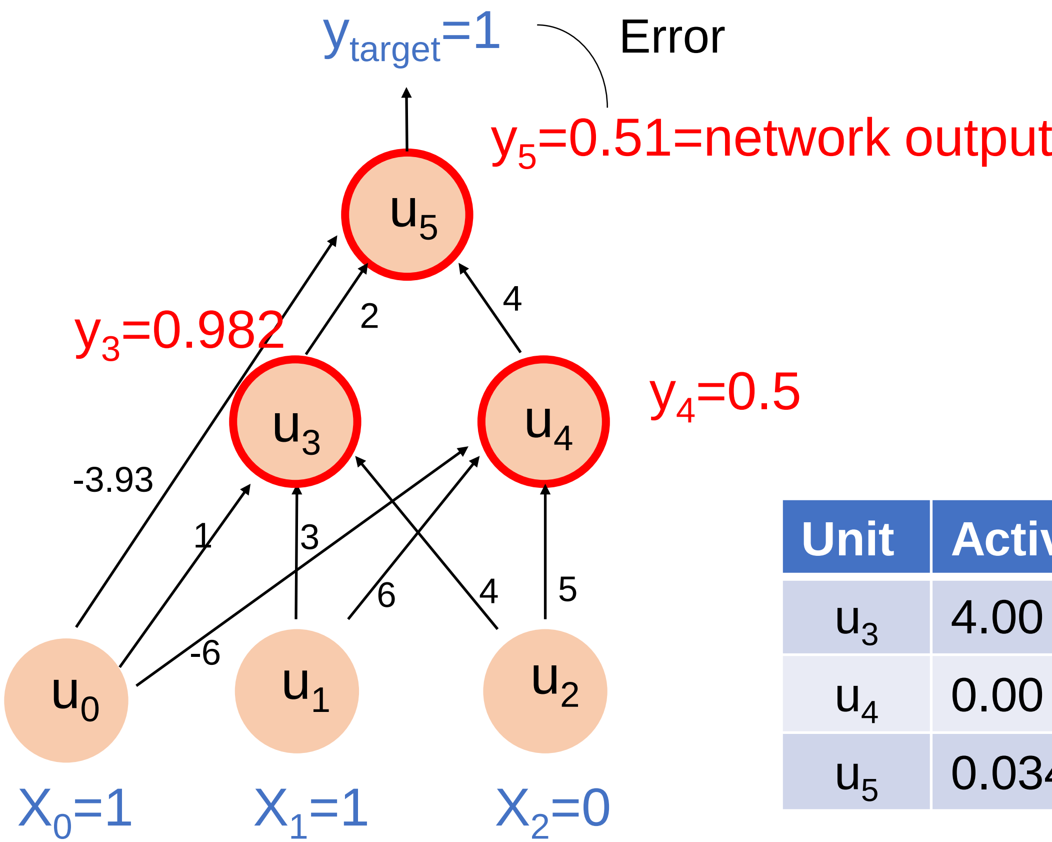
- Current state:
  - Weights: w_{13}=3, w_{35}=3, w_{24}=5…
  - Bias of u_4 is w_{04}=-6…
- Training data
  - X_1=1, X_2=0
  - Y_{target}=1

Example: Forward Pass



- Output for unit j is:
  - $a_j = \sum_i \; w_{ij} x_i$
  - $y_j = \sigma(a_j) = \frac{1}{1+e^{-a_j}}$
- E.g. Output for unit 3
  - a_3= 1*1+3*1+4*0 = 4
  - y_3= σ(4) = 0.982

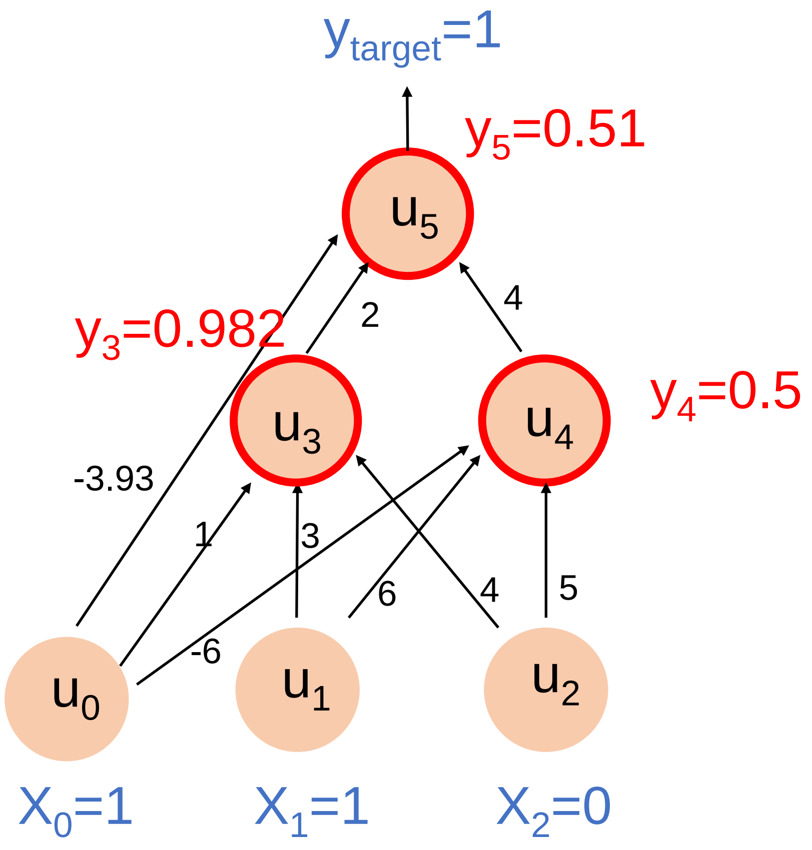
Example: Forward Pass



Unit	Activation a_i	Output y_i
u_3	4.00	0.982
u_4	0.00	0.50
u_5	0.034	**0.51**

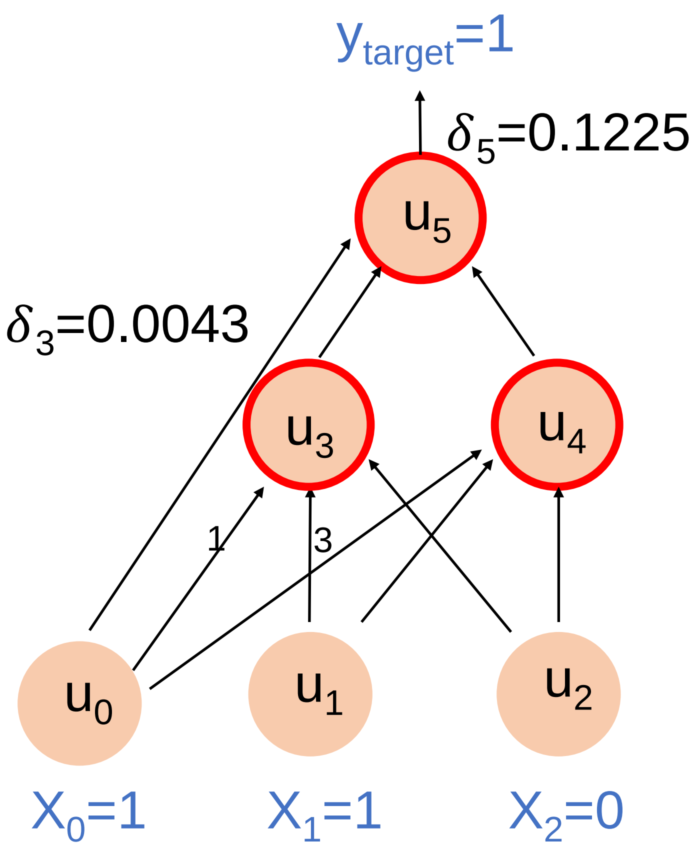
Error = $Y_{target} - y_5$ = 1-0.51 = 0.49

Example: Backward Pass



- Compute δ starting at output:
- $$\delta_5 = y_5(1-y_5)\left(y_{target} - y_5\right) \\ = 0.51(1-0.51) \times 0.49 \\ = 0.1225$$
- $$\delta_4 = y_4(1-y_4)\, w_{45}\delta_5 \\ = 0.5(1-0.5) \times 4 \times 0.122 \\ = 0.1225$$
- $$\delta_3 = y_3(1-y_3)\, w_{35}\delta_5 \\ = 0.982(1-0.982) \times 2 \times 0.122 \\ = 0.0043$$

Example: Update Weights

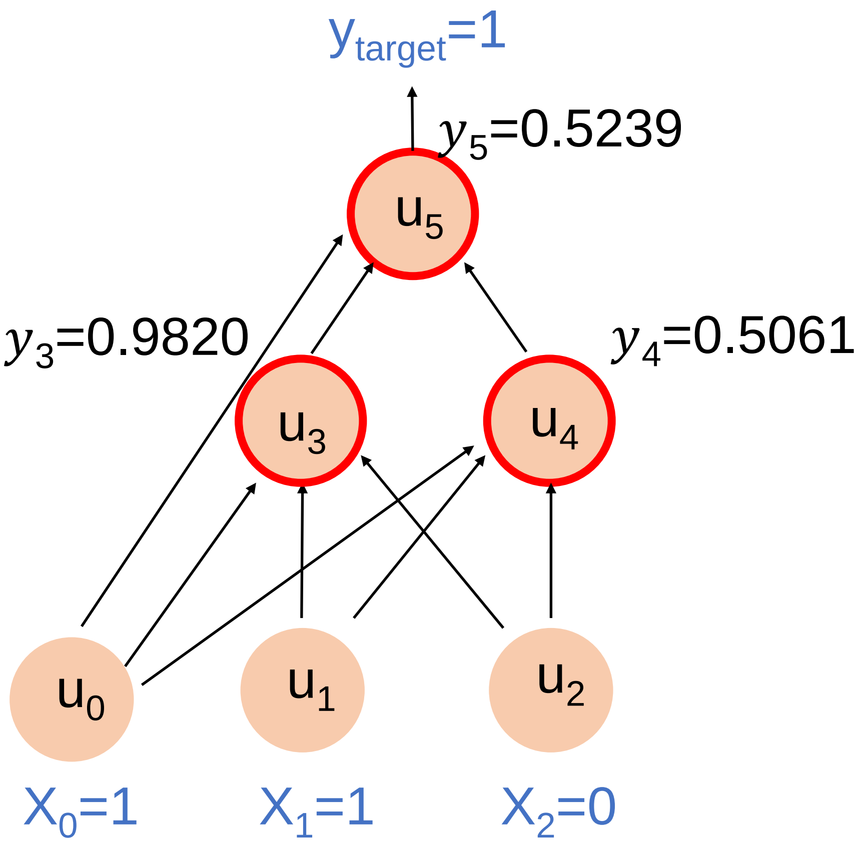


- Set learning rate α = 0.1
- Change weights by:
  - $\Delta w_{ij} = \alpha\delta_j y_i$
- E.g. Bias weight on u3:
  - $\Delta w_{03} = \alpha\delta_3 x_0 = 0.1 * 0.0043 * 1 = 0.0004$
- New $w_{03} = w_{03}(old) + \Delta w_{03} = 1 + 0.0004 = 1.0004$
- New $w_{13} = 3 + 0.0004 = 3.0004$

For the all weights w_{ij}:

i	j	w_{ij}	δ_j	y_i	New w_{ij}
0	3	1	0.0043	1.0	1.0004
1	3	3	0.0043	1.0	3.0004
2	3	4	0.0043	0.0	4.0000
0	4	-6	0.1225	1.0	-5.9878
1	4	6	0.1225	1.0	6.0123
2	4	5	0.1225	0.0	5.0000
0	5	-3.92	0.1225	1.0	-3.9078
3	5	2	0.1225	0.982	2.0120
4	5	4	0.1225	0.5	4.0061

Verification that it works



- On the next forward pass, the new activation are:
  - $y_3 = \sigma(4.0008) = 0.9820$
  - $y_4 = \sigma(0.0245) = 0.5061$
  - $y_5 = \sigma(0.0955) = \mathbf{0.5239}$
- The new error = 1-0.5239 = 0.476
- Error has been reduced from 0.49 to 0.476

Ref: "Neural Network Learning & Expert Systems" by Stephen Gallant

Backpropagation

- Gradient descent over entire *network* weight vector
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
- Often include weight *momentum* term

$$\Delta w_{i,j}(n) = \alpha\, \delta_j\, x_{i,j} + \eta\, \Delta w_{i,j}(n-1)$$

- Minimizes error training examples
  - Will it generalize well to unseen instances (over-fitting)?
- Training can be slow typical 1000-10000 iterations

Cross entropy

- Cross-entropy is a measure of the difference between two probability distributions.
- The first distribution consists of true values. The second distribution consists of estimated values.

$$-\sum_{i}^{N} p(i) \log q(i)$$

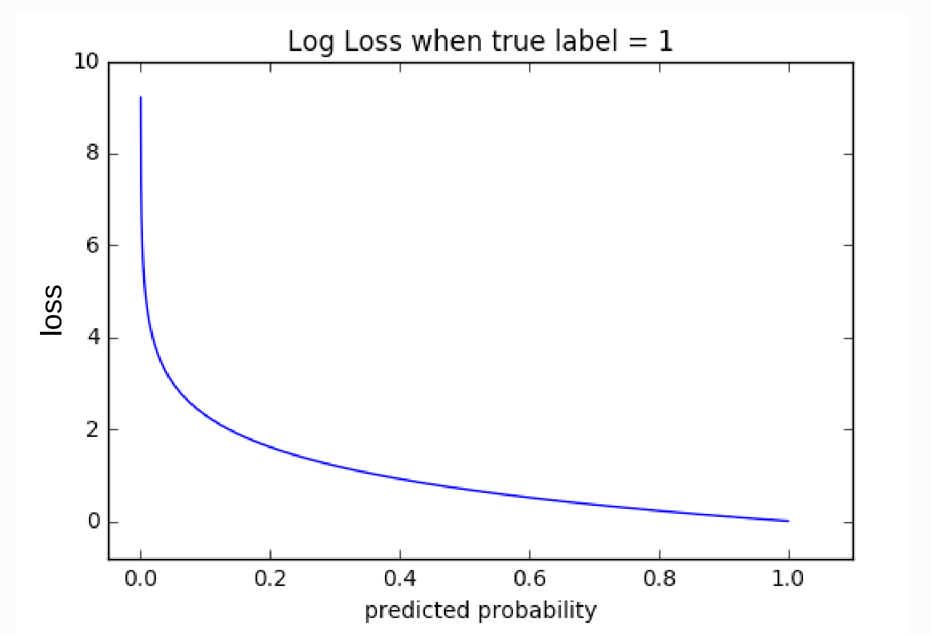
https://www.desmos.com/calculator/zytm2sf56e

Cross entropy (Cont.)

- Cross-entropy loss, or log loss, measures the performance of a classification model whose output is a probability value between 0 and 1

$Y_{predict}$	Y_{target}
0.8	1.0
0.2	0.0
0.1	0.0

$$L(Y_{predict}, Y_{target}) = -\sum_{i}^{N} Y_{target}^{i} \log(Y_{predict}^{i})$$

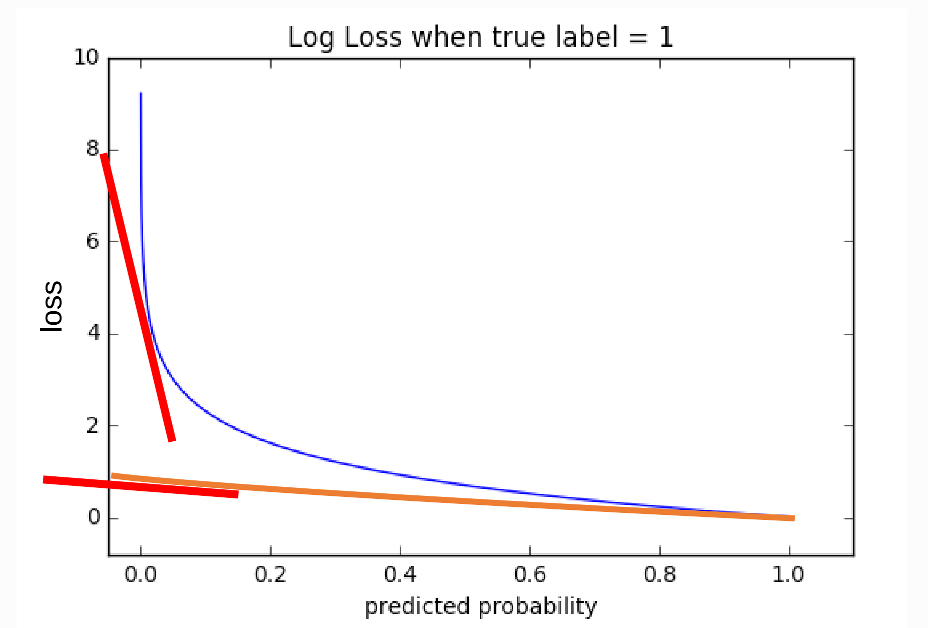


Why use cross entropy?

$$L(Y_{predict}, Y_{target}) = \text{Residual}^2 = \sum_i \left(Y^i_{target} - Y^i_{predict}\right)^2$$

$Y_{predict}$	Y_{target}
0.8	1.0
0.2	0.0
0.1	0.0

$$L(Y_{predict}, Y_{target}) = -\sum_i^N Y^i_{target} \log(Y^i_{predict})$$



Cross entropy (Cont.)

- Binary Cross-Entropy Loss(BCE) $-\sum_i^N\left(Y_{\text{target}}^i \log\left(Y_{\text{predict}}^i\right) + (1 - Y_{\text{target}}^i)\log(1 - Y_{\text{predict}}^i)\right)$
- Categorical Cross-Entropy Loss $-\sum_c^M\sum_i^N\left(Y_{\text{target}}^{i,c}\log\left(Y_{\text{predict}}^{i,c}\right)\right)$
  - More than 2 classes and outcomes are one hot encoded

```
[1,0,0]
[0,1,0]
[0,0,1]
```

- Sparse Categorical Cross-Entropy Loss
  - More than 2 classes and outcomes are **not** one hot encoded

```
1
2
3
```

TRUE	CLASS - 1	CLASS - 2
RECORD - 1	1	0
RECORD - 2	1	0
RECORD - 3	0	1

PREDICTED	CLASS - 1	CLASS - 2
RECORD - 1	0.9	0.1
RECORD - 2	0.7	0.3
RECORD - 3	0.4	0.6

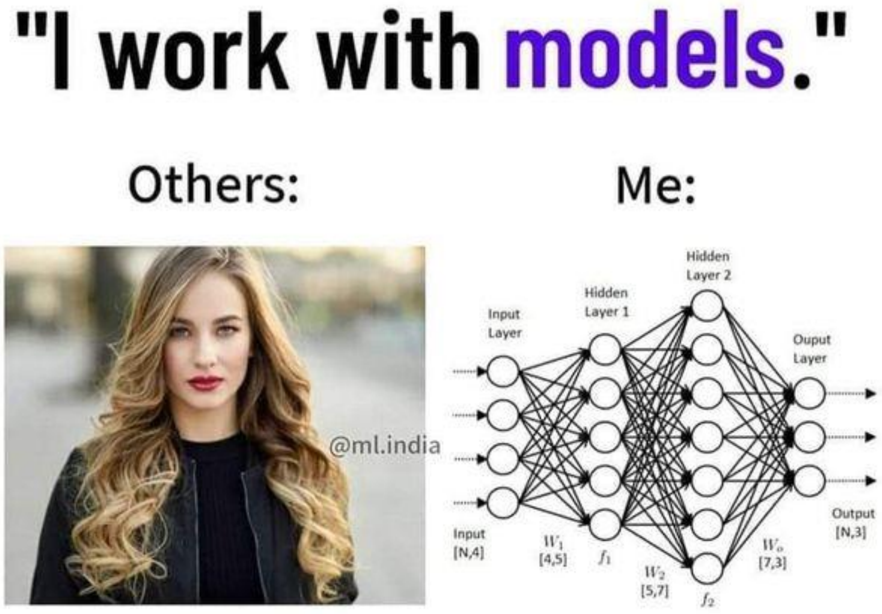
	CROSS-ENTROPY	CALCULATION
RECORD - 1	-(1 * log(0.9))	0.1053605157
RECORD - 2	-(1 * log(0.7))	0.3566749439
RECORD - 3	-(1 * log(0.6))	0.5108256238

0.3242870

Summary

- Many similarities between biology and neural networks
  - Information is contained in synaptic connections
  - Network learns to perform specific functions
  - Network generalizes to new inputs
- But NNs are woefully inadequate compared with biology
  - Simplistic model of neuron and synapse, implausible learning rules
  - Network construction (structure, learning rate etc.) is a heuristic art
  - Hard to train large networks => deep learning

Questions?



"I work with models."
Others:
Me:
@ml.india
Input Layer
Hidden Layer 1
Hidden Layer 2
Ouput Layer
Input [N,4]
W_1 [4,5]
f_1
W_2 [5,7]
f_2
W_o [7,3]
Output [N,3]