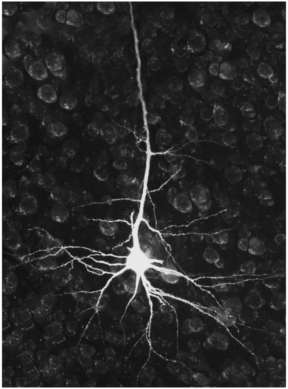
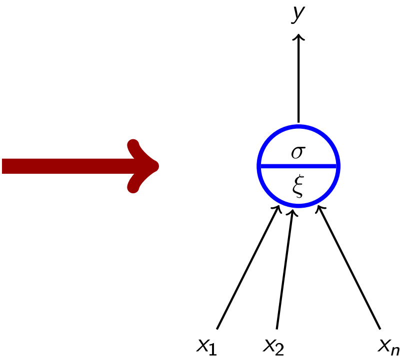
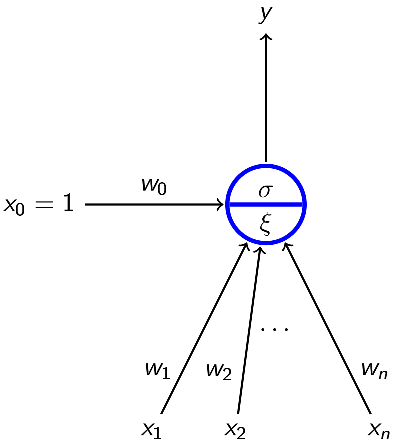
(Primitive) Mathematical Model of Neuron





Formal neuron



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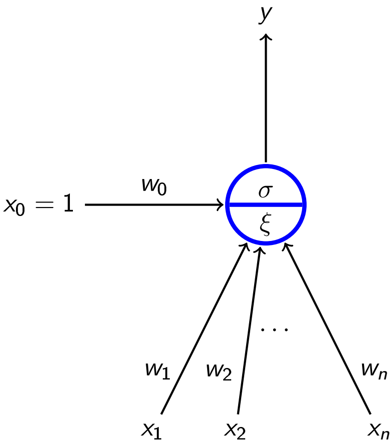

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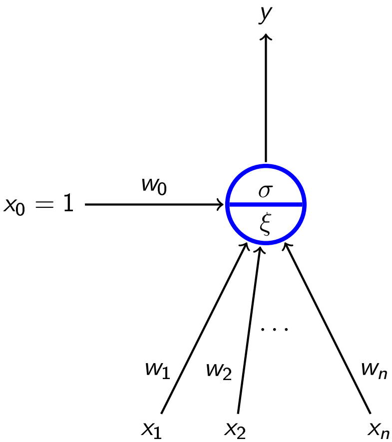

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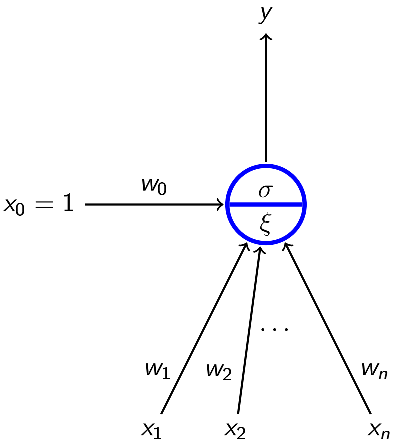

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  In general, other potentials are considered (e.g. Gaussian), more on this in PV021.

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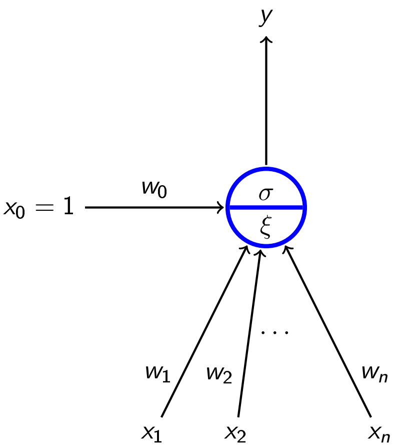

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- y *output* defined by $y = \sigma(\xi)$ where σ is an *activation function*.
  We consider several activation functions.

  e.g. *linear threshold function*

$$\sigma(\xi) = sgn(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

Formal Neuron vs Linear Models

Both linear classifier and linear (affine) function are special cases of the formal neuron.

- If σ is a linear threshold function

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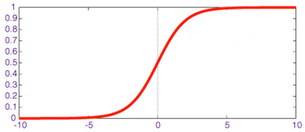
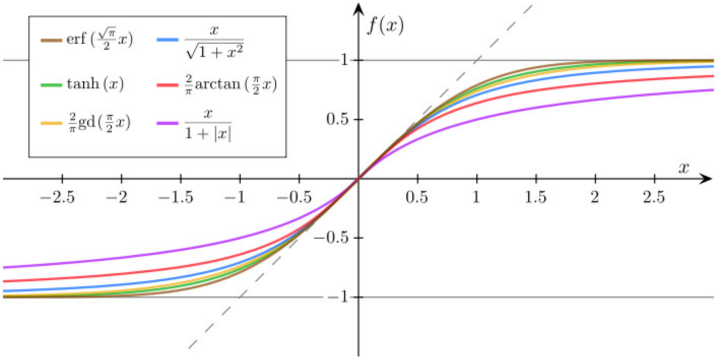
Many more activation functions are used in neural networks!

Sigmoid Functions

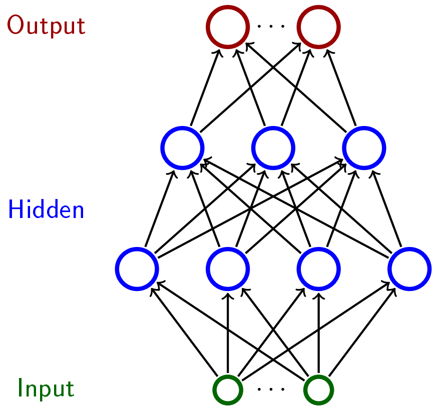
Logistic sigmoid $\sigma(\xi) = \dfrac{1}{1 + e^{-\xi}}$



Others ...



Multilayer Perceptron (MLP)



- Neurons are organized in *layers* (input layer, output layer, possibly several hidden layers)
- Layers are numbered from 0; the input is 0-th
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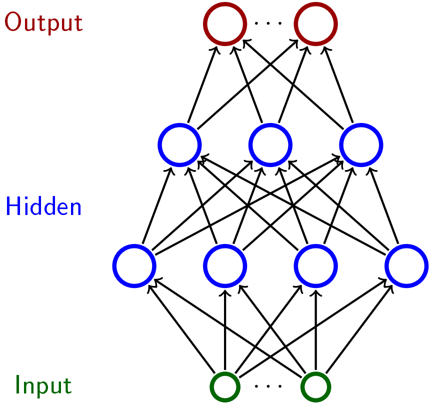

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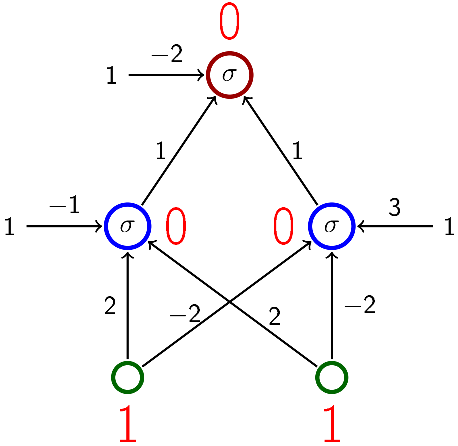
Intuition: The network computes a function as follows: Assign input values to the input neurons and 0 to the rest. Proceed upwards through the layers, one layer per step. In the ℓ-th step consider output values of neurons in $\ell-1$-th layer as inputs to neurons of the ℓ-th layer. Compute output values of neurons in the ℓ-th layer.

Example



- Activation function: linear threshold

$$\sigma(\xi) = \begin{cases} 1 & \xi \geq 0\,; \\ 0 & \xi < 0. \end{cases}$$

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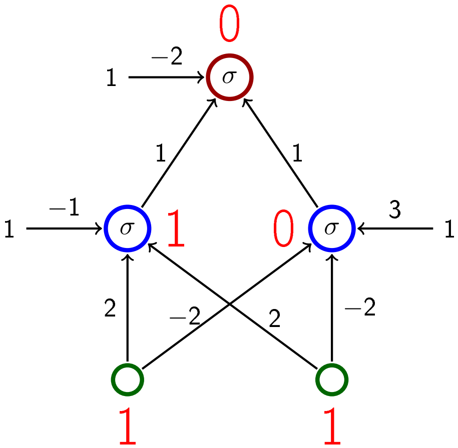

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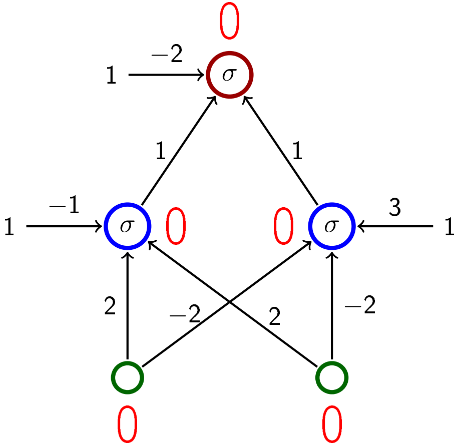

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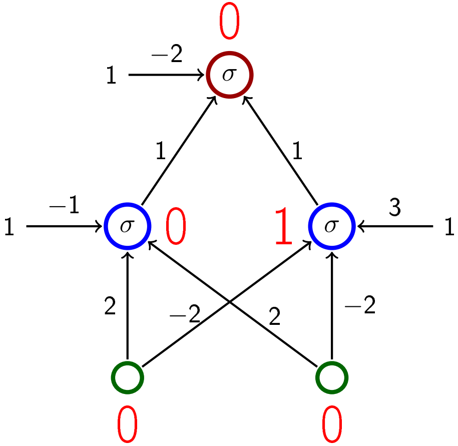

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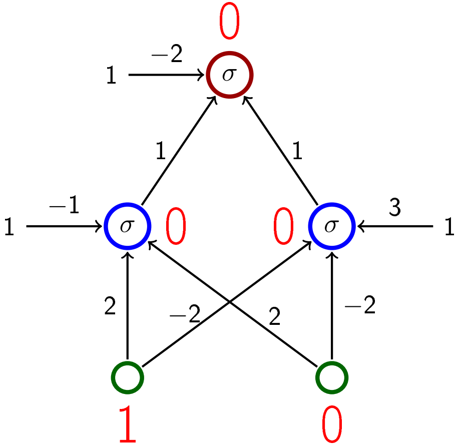

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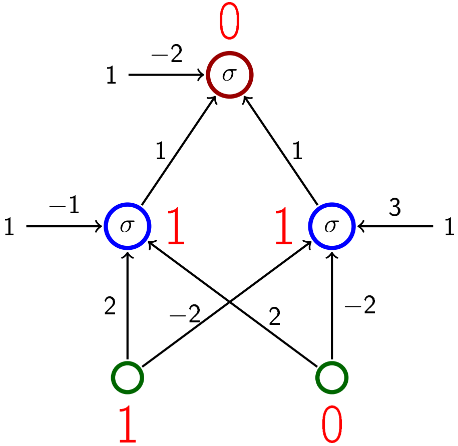

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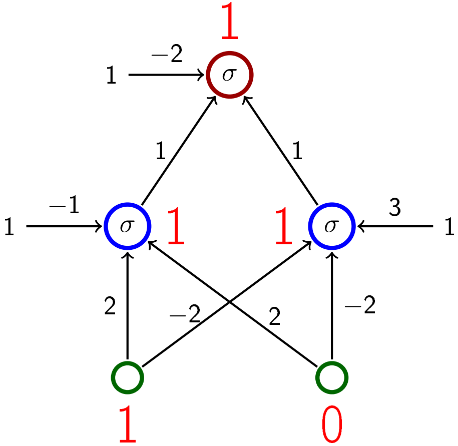

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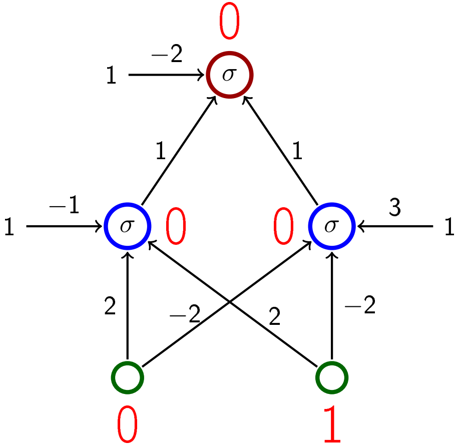

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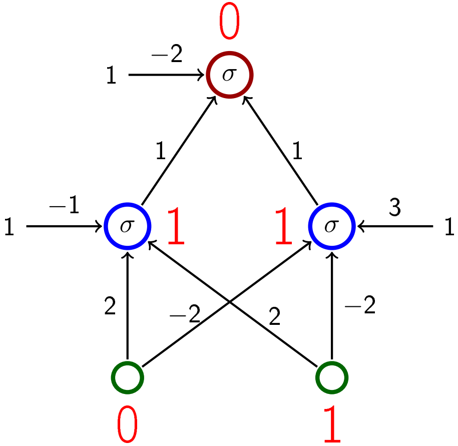

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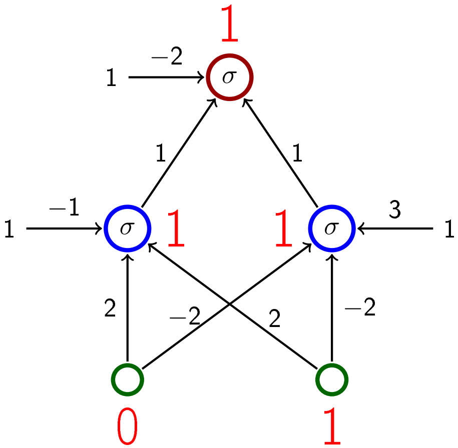

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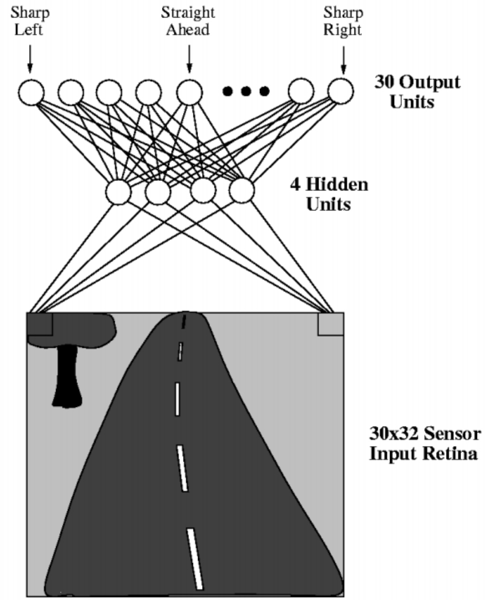
Classical Example – ALVINN



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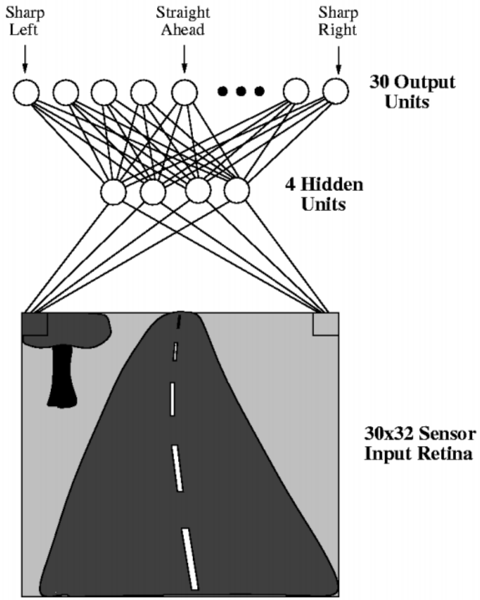

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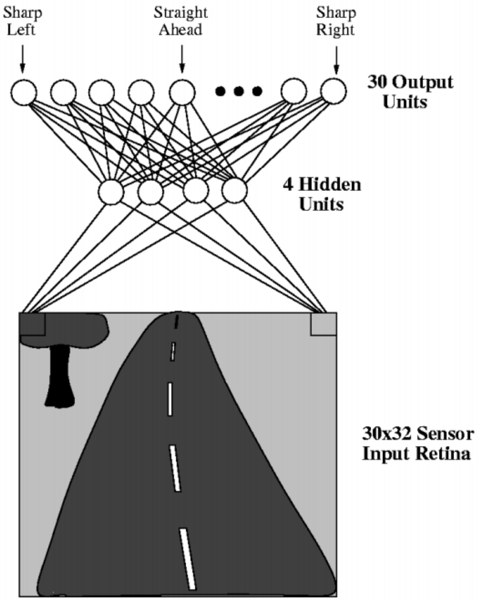

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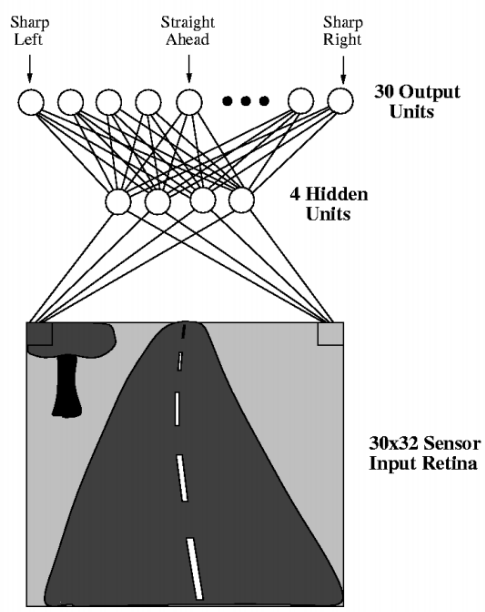

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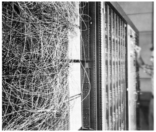
- The value of each input captures the shade of gray of the corresponding pixel.
- Output neurons indicate where to turn (to the center of gravity).

Source: `http://jmvidal.cse.sc.edu/talks/ann/alvin.html`

A Bit of History

- Perceptron (Rosenblatt et al, 1957)



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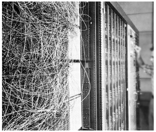

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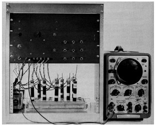
- Adaline (Widrow & Hof, 1960)



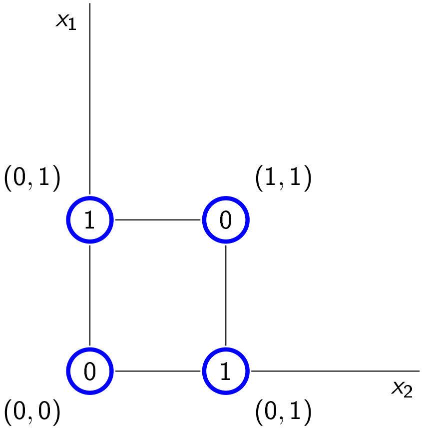
  - Single layer, the activation function *identity*

    (i.e., a bit more linear function)
  - Online version of the gradient descent
  - Used a new circuitry element called *memristor* which was able to "remember"history of current in form of resistance

In both cases, the expressive power is rather limited – can express only linear decision boundaries and linear (affine) functions.

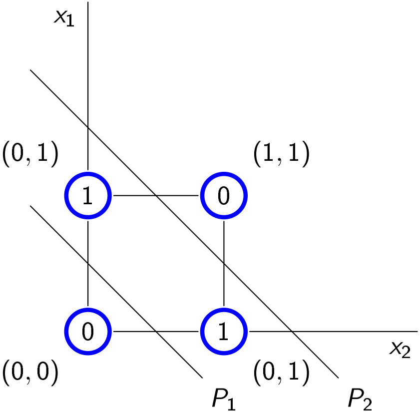
A Bit of History

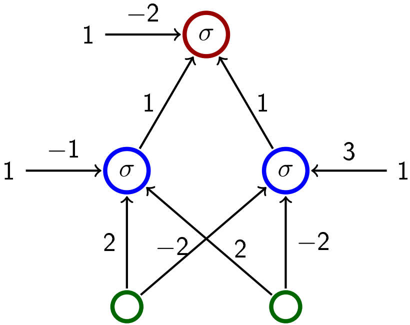
One of the famous (counter)-examples: XOR



No perceptron can distinguish between ones and zeros.

XOR vs Multilayer Perceptron





(Here σ is a linear threshold function.)

$P_1 : -1 + 2x_1 + 2x_2 = 0$ $\qquad$ $P_2 : 3 - 2x_1 - 2x_2 = 0$

The output neuron performs an intersection of half-spaces.

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... then the **backpropagation** appeared in 1986!

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- A value of a non-input neuron $j \in Z \setminus X$ when the computation is finished is $y_j = \sigma(\xi_j)$

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- Fixing weights of all neurons, the network computes a function $F[\vec{w}] : \mathbb{R}^{|X|} \to \mathbb{R}^{|Y|}$ as follows: Assign values of a given vector $\vec{x} \in \mathbb{R}^{|X|}$ to the input neurons, evaluate the network, then $F[\vec{w}](\vec{x})$ is the vector of values of the output neurons.

  Here we implicitly assume a fixed orderings on input and output vectors.

MLP – Learning

- Given a set D of training examples:

$$D = \left\{ \left(\vec{x}_k, \vec{d}_k\right) \quad \middle| \quad k = 1, \ldots, p \right\}$$

Here $\vec{x}_k \in \mathbb{R}^{|X|}$ and $\vec{d}_k \in \mathbb{R}^{|Y|}$. We write d_{kj} to denote the value in $\vec{d}_k$ corresponding to the output neuron j.

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- **Least Squares Error Function:** Let $\vec{w}$ be a vector of all weights in the network.

$$E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$$

where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} (y_j[\vec{w}](\vec{x}_k) - d_{kj})^2$$

MLP – Learning Algorithm

Batch Learning – Gradient Descent:

The algorithm computes a sequence of weights $\vec{w}^{(0)}, \vec{w}^{(1)}, \ldots$.

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- weights $\vec{w}^{(0)}$ are initialized randomly close to 0
- in the step $t+1$ (here $t = 0, 1, 2\ldots$) is $\vec{w}^{(t+1)}$ computed as follows:

$$w_{ji}^{(t+1)} = w_{ji}^{(t)} + \Delta w_{ji}^{(t)}$$

MLP – Learning Algorithm

Batch Learning – Gradient Descent:

The algorithm computes a sequence of weights $\vec{w}^{(0)}, \vec{w}^{(1)}, \ldots$.

- weights $\vec{w}^{(0)}$ are initialized randomly close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$) is $\vec{w}^{(t+1)}$ computed as follows:

  $$w_{ji}^{(t+1)} = w_{ji}^{(t)} + \Delta w_{ji}^{(t)}$$

  where

  $$\Delta w_{ji}^{(t)} = -\varepsilon(t) \cdot \frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t)})$$

  is the weight change w_{ji} and $0 < \varepsilon(t) \leq 1$ is the learning speed in the step $t+1$.

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Note that $\frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t)})$ is a component of ∇E, i.e. the weight change in the step $t+1$ can be written as follows: $\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon(t) \cdot \nabla E(\vec{w}^{(t)})$.

MLP – Gradient Computation

For every weight w_{ji} we have (obviously)

$$\frac{\partial E}{\partial w_{ji}} = \sum_{k=1}^{p} \frac{\partial E_k}{\partial w_{ji}}$$

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It holds that

$$\frac{\partial E_k}{\partial w_{ji}} = \delta_j \cdot y_j(1 - y_j) \cdot y_i$$

where

$$\delta_j = y_j - d_{kj} \qquad \text{pro } j \in Y$$

$$\delta_j = \sum_{r \in j^{\rightarrow}} \delta_r \cdot y_r(1 - y_r) \cdot w_{rj} \qquad \text{pro } j \in Z \smallsetminus (Y \cup X)$$

(Here $y_r = y[\vec{w}](\vec{x}_k)$ where $\vec{w}$ are the current weights and $\vec{x}_k$ is the input of the k-th training example.)

Multilayer Perceptron – Backpropagation

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  - Assign $\delta_j = y_j - d_{kj}$ for all $j \in Y$
  - In the layer ℓ, assuming that δ_r has been computed for all neurons r in the layer $\ell + 1$, compute

    $$\delta_j = \sum_{r \in j^{\rightarrow}} \delta_r \cdot y_r(1 - y_r) \cdot w_{rj}$$

    for all j from the ℓ-th layer.

Example

Assume $w_{30}^{(0)} = w_{50}^{(0)} = w_{41}^{(0)} = w_{42}^{(0)} = w_{54}^{(0)} = 1$ and $w_{40}^{(0)} = w_{31}^{(0)} = w_{32}^{(0)} = w_{53}^{(0)} = -1$. Consider a training set $\{((1,0),1)\}$.

Then

$y_1 = 1,$

$y_2 = 0,$

$y_3 = \sigma(w_{30} + w_{31}^{(0)} y_1 + w_{32}^{(0)} y_2) = 0.5,$

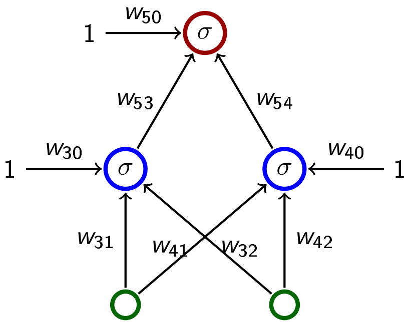
$y_4 = 0.5,$

$y_5 = 0.731058.$

$\delta_5 = y_5 - 1 = -0.268942,$

$\delta_4 = \delta_5 \cdot y_5 \cdot (1 - y_5) * w_{54}^{(0)} = -0.052877,$

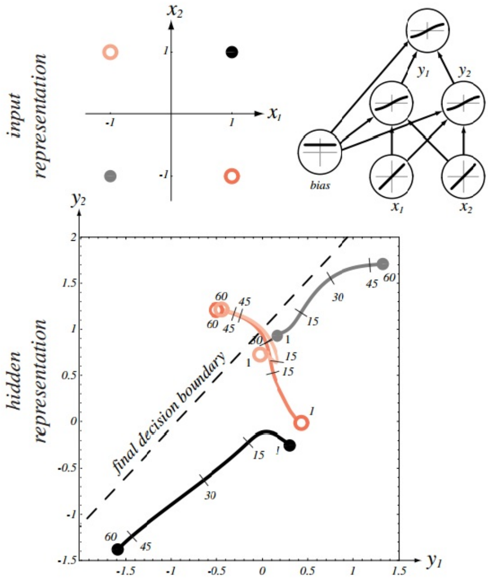
$\delta_3 = 0.052877.$



$$\frac{\partial E_1}{\partial w_{53}} = \delta_5 \cdot y_5 \cdot (1 - y_5) \cdot y_3 = -0.026438,$$
$$\frac{\partial E_1}{\partial w_{54}} = \delta_5 \cdot y_5 \cdot (1 - y_5) \cdot y_4 = -0.026438,$$
$$\frac{\partial E_1}{\partial w_{30}} = \delta_3 \cdot y_3 \cdot (1 - y_3) \cdot 1 = 0.01321925,$$

....

Illustration of Gradient Descent – XOR



Source: Pattern Classification (2nd Edition); Richard O. Duda, Peter E. Hart, David G. Stork

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- In practice, does converge to low error for many large networks on real data.
- Many epochs (thousands) may be required, hours or days of training for large networks.
- To avoid local-minima problems, run several trials starting with different random weights (random restarts).
  - Take results of trial with lowest training set error.
  - Build a committee of results from multiple trials (possibly weighting votes by training set accuracy).

There are many more issues concerning learning efficiency (data normalization, selection of activation functions, weight initialization, training speed, efficiency of the gradient descent itself etc.) – see PV021.

Hidden Neurons Representations

Trained hidden neurons can be seen as newly constructed features.
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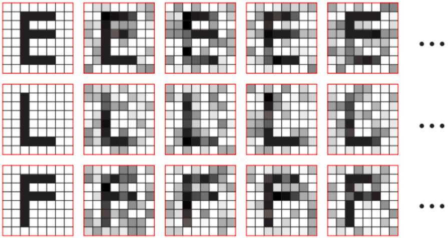
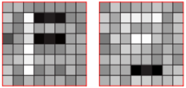
Consider a two-layer MLP, 64-2-3 for classification of letters (three output neurons, each corresponds to one of the letters).

sample training patterns

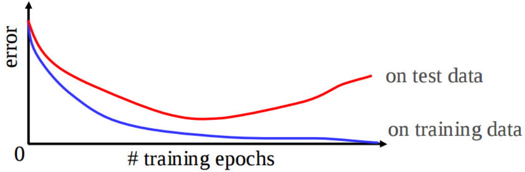




learned input-to-hidden weights

Overfitting

- Due to their expressive power, neural networks are quite sensitive to overfitting.



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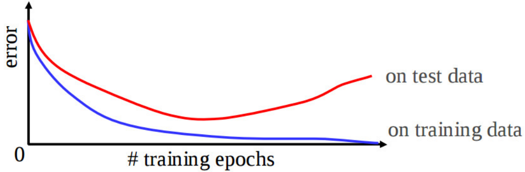
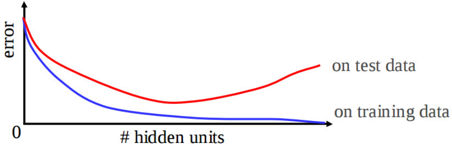


- Keep a hold-out validation set and test accuracy on it after every epoch. Stop training when additional epochs actually increase the validation error.

Overfitting – The Number of Hidden Neurons

- Too few hidden neurons prevent the network from adequately fitting the data.
- Too many hidden units can result in overfitting.
  (There are advanced methods that prevent overfitting even for rich models, such as regularization, where the error function penalizes overfitting – see PV021.)



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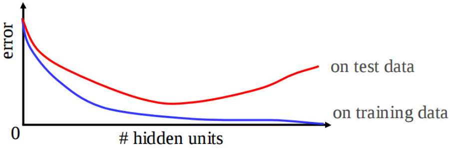


- Use cross-validation to empirically determine an optimal number of hidden units.

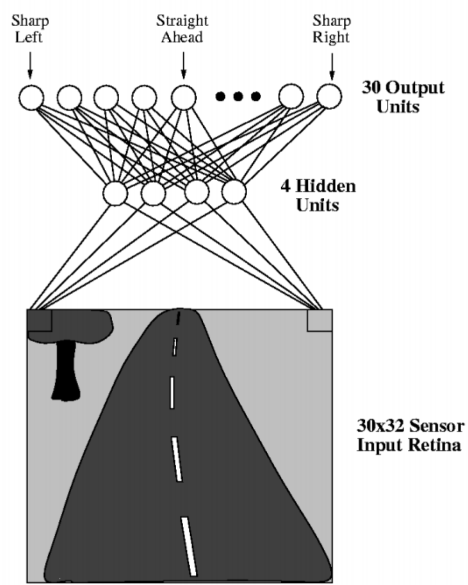
  There are methods that automatically construct the structure of the network based on data, they are not much used though.

Applications

- Text to Speech and vice versa
- Fraud detection
- finance & business predictions
- Game playing (backgammon is a classical example, AlphaGo is the modern one)
- Image recognition

  This is the main area in which the current state-of-the-art deep networks excel.
- (artificial brain and intelligence)
- ...

ALVINN


Sharp Left
Straight Ahead
Sharp Right
30 Output Units
4 Hidden Units
30x32 Sensor Input Retina

ALVINN

- Two layer MLP, $960 - 4 - 30$ (sometimes $960 - 5 - 30$)

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- Direction corresponds to the center of gravity.

  I.e., output neurons are considered as points of mass evenly distributed along a line. Weight of each neuron corresponds to its value.

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  - $\vec{d}_k \approx$ corresponding direction of the steering wheel set by the driver
- the values $\vec{d}_k$ computed using Gaussian distribution:

$$d_{ki} = e^{-D_i^2/10}$$

where D_i is the distance between the i-th output from the one that corresponds to the real direction of the steering wheel.

(This is better than the binary output because similar road directions induce similar reaction of the driver.)

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Naive approach: just take images from the camera.

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  - let the driver go crazy! (a bit dangerous, expensive, unreliable)
- Images are very similar (the network basically sees the road from the right lane), may be overtrained.

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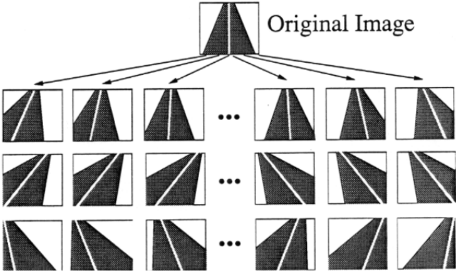

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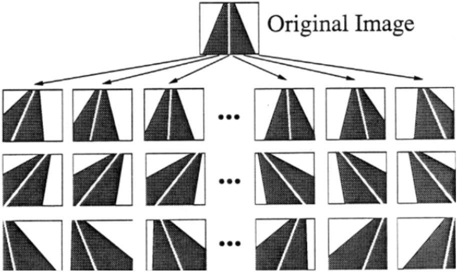

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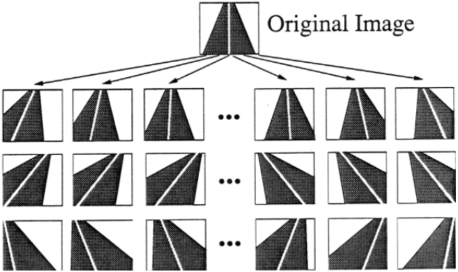

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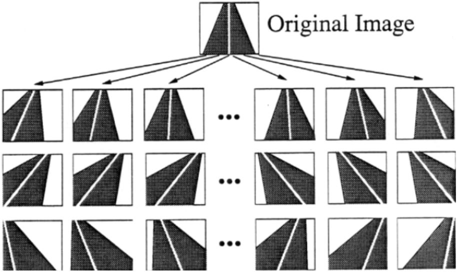

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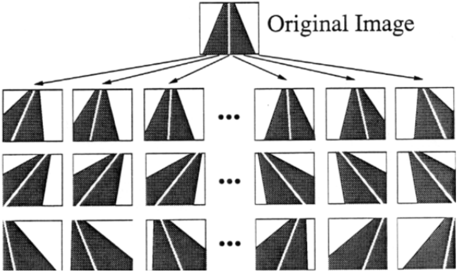

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Výsledek:

- Training took 5 minutes, the speed was 4 miles per hour
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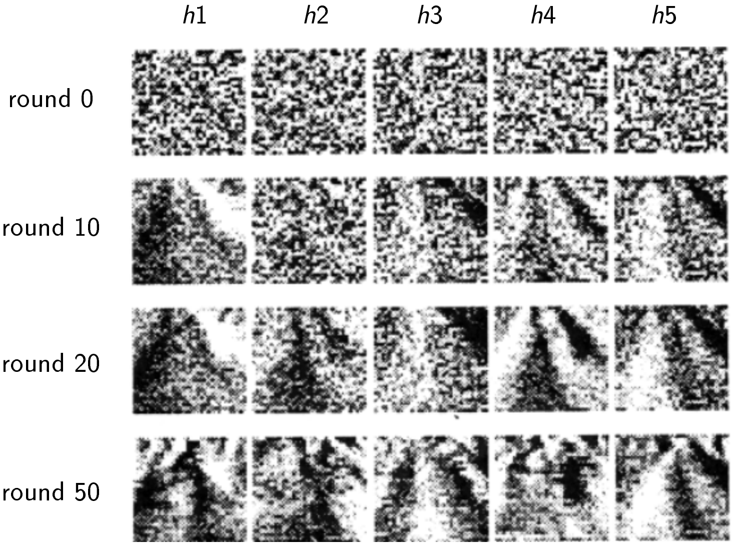
- ALVINN was able to go through roads it never "seen" and in different weather

ALVINN – Weight Learning



Here $h1, \ldots, h5$ are values of hidden neurons.

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- Unsupervised learning – Self-Organizing Maps
- Reinforcement learning
  - learning to make decisions, or play games, sequentially
  - neural networks have been used – temporal difference learning

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- In 2006 a solution was found by Hinton et al:
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    More precisely: The lowest hidden layer learns patterns in data, second lowest learns patterns in data transformed through the first layer, and so on.

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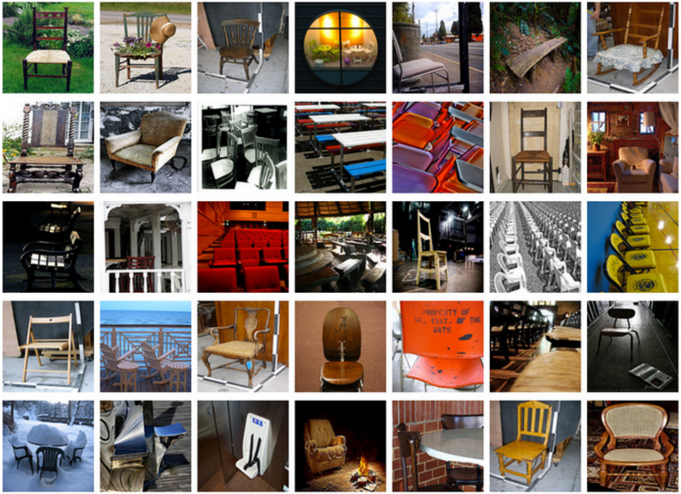
    More precisely: The lowest hidden layer learns patterns in data, second lowest learns patterns in data transformed through the first layer, and so on.
  - Then use a supervised learning algorithm to only *fine tune* the weights to the desired input-output behavior.

A rather heavy machinery is needed to develop this, but you will be rewarded by insight into a *very* modern and expensive technology.

ImageNet Large-Scale Visual Recognition Challenge (ILSVRC)

ImageNet database (16,000,000 color images, 20,000 categories)



ImageNet Large-Scale Visual Recognition Challenge (ILSVRC)

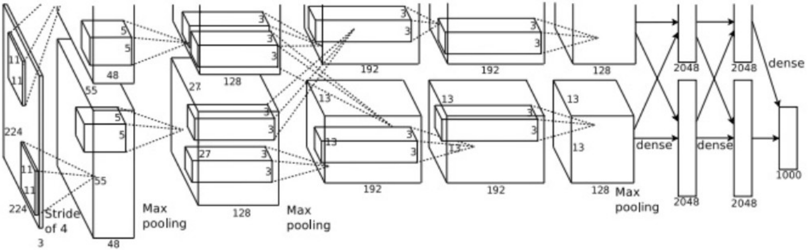
Competition in classification over a subset of images from ImageNet.

In 2012: Training se 1,200,000 images, 1000 categories. Validation set 50,000, Test set 150,000.

Many images contain several objects $\rightarrow$ typical rule is top-5 highest probability assigned by the net.

KSH síť

ImageNet classification with deep convolutional neural networks, by Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton (2012).



Trained on two GPUs (NVIDIA GeForce GTX 580)

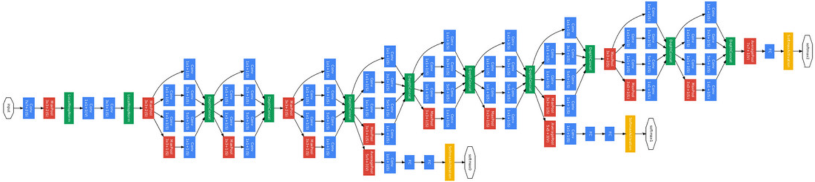
Results:

- Accuracy 84.7% in top-5 (second best alg. at the time: 73.8%)
- 63.3% in "perfect" classification (top-1)

ILSVRC 2014

The same set of images as in 2012, top-5 criterium.

GoogLeNet: deep convolutional net, 22 layers



Results:

- 93.33% in top-5

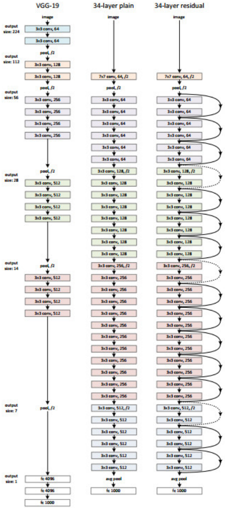
Superhuman power?

Superhuman GoogLeNet?!

Andrej Karpathy: ...the task of labeling images with 5 out of 1000 categories quickly turned out to be extremely challenging, even for some friends in the lab who have been working on ILSVRC and its classes for a while. First we thought we would put it up on [Amazon Mechanical Turk]. Then we thought we could recruit paid undergrads. Then I organized a labeling party of intense labeling effort only among the (expert labelers) in our lab. Then I developed a modified interface that used GoogLeNet predictions to prune the number of categories from 1000 to only about 100. It was still too hard - people kept missing categories and getting up to ranges of 13-15% error rates. In the end I realized that to get anywhere competitively close to GoogLeNet, it was most efficient if I sat down and went through the painfully long training process and the subsequent careful annotation process myself... The labeling happened at a rate of about 1 per minute, but this decreased over time... Some images are easily recognized, while some images (such as those of fine-grained breeds of dogs, birds, or monkeys) can require multiple minutes of concentrated effort. I became very good at identifying breeds of dogs... Based on the sample of images I worked on, the GoogLeNet classification error turned out to be 6.8%... My own error in the end turned out to be 5.1%, approximately 1.7% better.

ILSVRC 2015

- Microsoft network ResNet: 152 layers, complex architecture
- Trained on 8 GPUs
- 96.43% **accuracy** in top-5



ILSVRC

ilsvrc.png

Deeper Insight into the Logistic Sigmoid

Consider a perceptron (that is a linear classifier):

$$\xi = w_0 + \sum_{i=1}^{n} w_i \cdot x_i$$

and $y = sgn(\xi) = \begin{cases} 1 & \xi \geq 0 \\ 0 & \xi < 0 \end{cases}$

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Recall, that the *signed distance* from the decision boundary determined by $\xi = 0$ is (here $\vec{x} = (x_1, \ldots, x_n)$ and $\vec{w} = (w_1, \ldots, w_n)$)

$$\frac{w_0 + \sum_{i=1}^{n} w_i \cdot x_i}{\sqrt{\sum_{i=1}^{n} w_i^2}} = \frac{\xi}{\sqrt{\sum_{i=1}^{n} w_i^2}}$$

This value is positive for $\vec{x}$ on the side of $\vec{w}$ and negative on the opposite.

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This value is positive for $\vec{x}$ on the side of $\vec{w}$ and negative on the opposite.

For simplicity, assume that $\sqrt{\sum_{i=1}^{n} w_i^2} = 1$, and thus that the potential ξ is *equal to the signed distance of $\vec{x}$ from the boundary*.

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It is not unreasonable to assume that

- conditioned on $c = 1$, the signed distance ξ is normally distributed with the mean ξ^1 and variance (for simplicity) 1,
- conditioned on $c = 0$, the signed distance ξ is normally distributed with the mean ξ^0 and variance (for simplicity) 1.

(Notice that ξ may be negative, which means that such point is on the wrong side of the boundary (the same for $\xi > 0$).)

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Now, can we decide what is the probability of $c = 1$ given a distance?

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For simplicity, assume that $\xi^1 = -\xi^0 = 1/2$.

$$\begin{aligned} P(1 \mid \xi) &= \frac{p(\xi \mid 1)P(1)}{p(\xi \mid 1)P(1) + p(\xi \mid 0)P(0)} \\ &= \frac{LR}{LR + 1/clr} \end{aligned}$$

where

$$LR = \frac{p(\xi \mid 1)}{p(\xi \mid 0)} = \frac{\exp(-(\xi - 1/2)^2/2)}{\exp(-(\xi + 1/2)^2/2)} = \exp(\xi)$$

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So

$$P(1 \mid \xi) = \frac{\exp(\xi)}{\exp(\xi) + 1} = \frac{1}{1 + e^{-\xi}}$$

Thus the logistic sigmoid applied to $\xi = w_0 + \sum_{i=1}^{n} w_i \cdot x_i$ gives *the probability* of $c = 1$ given the input!

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So if we use the logistic sigmoid as an activation function,

and turn the neuron into a classifier as follows:

$$\text{classify a given input } \vec{x} \text{ as 1 iff } y \geq 1/2$$

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This is the basis of logistic regression.

Given training data, we may compute the weights $\vec{w}$ that maximize the likelihood of the training data (w.r.t. the probabilities returned by the neuron).

An extremely interesting observation is that such $\vec{w}$ maximizing the likelihood coincides with the minimum of least squares for the corresponding linear function (that is the same neuron but with identity as the activation function).