Tufts

Class #19:
Neural Networks

Machine Learning (COMP 135): M. Allen, 30 March 20

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Neural Learning Methods

- An obvious source of biological inspiration for learning research: ***the brain***
- The work of McCulloch and Pitts on the perceptron (1943) started as research into how we could precisely model the ***neuron*** and the ***network of connections*** that allow animals (like us) to learn
- These networks are used as ***classifiers***: given an input, they label that input with a classification, or a distribution over possible classifications

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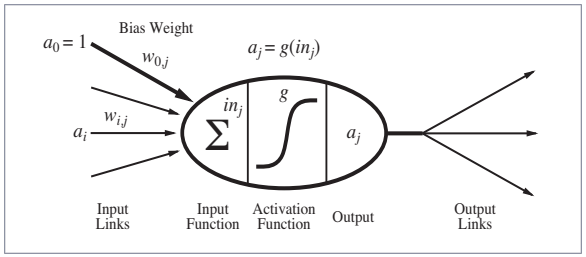
The Basic Neuron Model

Source: Russel & Norvig, *AI: A Modern Approach* (Prentice Hal, 2010)



- Neuron gets input from a set of other neurons, or from the problem input, and computes the function g
- Output a_j is either passed along to another set of neurons, or is used as final output for learning problem itself

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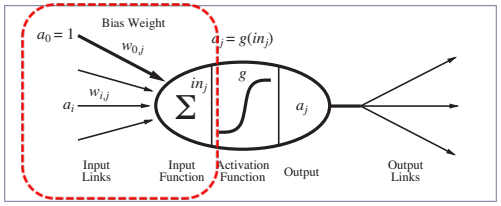
Input Bias Weights



- Each input a_i to neuron j is given a weight $w_{i,j}$
- Each neuron is treated as having a fixed dummy input, $a_0 = 1$
- The input function is then the weighted linear sum:

$$in_j = \sum_{i=0}^{n} w_{i,j}\, a_i = w_{0,j}\, a_0 + w_{1,j}\, a_1 + w_{2,j}\, a_2 + \cdots + w_{n,j}\, a_n$$

$$= w_{0,j} + w_{1,j}\, a_1 + w_{2,j}\, a_2 + \cdots + w_{n,j}\, a_n$$

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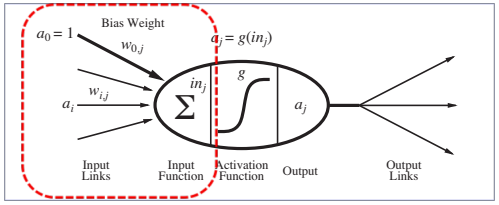
We've Seen This Before!



- The weighted linear sum of inputs, with dummy, $a_0 = 1$, is just a form of the cross-product that our classifiers have been using all along
  - Remember that the "neuron" here is just another way of looking at the perceptron idea we already discussed

$$in_j = \sum_{i=0}^{n} w_{i,j}\, a_i = w_{0,j} + w_{1,j}\, a_1, + w_{2,j}\, a_2 + \cdots + w_{n,j}\, a_n$$

$$= \mathbf{w}_j \cdot \mathbf{a}$$

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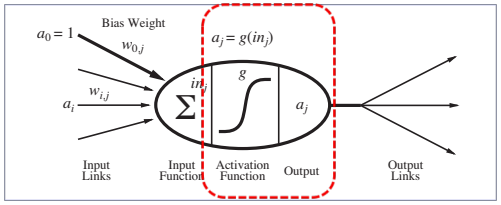
Neuron Output Functions



- While the ***inputs*** to any neuron are treated in a linear fashion, the ***output*** function g ***need not*** be linear
- The power of neural nets comes from fact that we can combine large numbers of neurons together to compute any function (linear or not) that we choose

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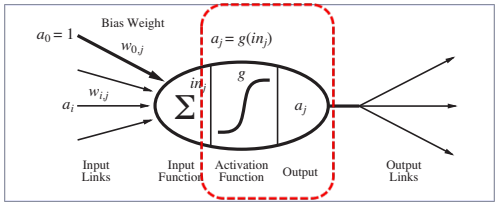
The Perceptron Threshold Function



- One possible function is the binary threshold, which is suitable for "firm" classification problems, and causes the neuron to activate based on a simple binary function:

$$g(in_j) = \begin{cases} 1 & \text{if } in_j \geq 0 \\ 0 & \text{else} \end{cases}$$

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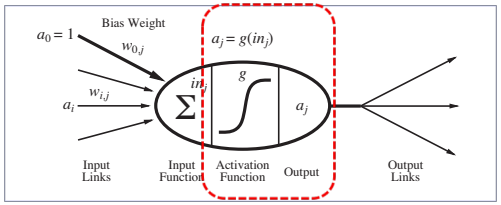
The Sigmoid Activation Function



- A function that has been more often used in neural networks is the logistic (also known as the Sigmoid), as seen before
- This gives us a "soft" value, which we can often interpret as the ***probability*** of belonging to some output class

$$g(in_j) = \frac{1}{1 + e^{-in_j}}$$

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Power of Perceptron Networks

- A single-layer network combines a *linear* function of input weights with the *non-linear* output function
  - If we threshold output, we have a boolean (1/0) function
  - This is sufficient to compute numerous linear functions

x_1 OR x_2

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	1

x_1 AND x_2

x_1	x_2	y
0	0	0
0	1	0
1	0	0
1	1	1

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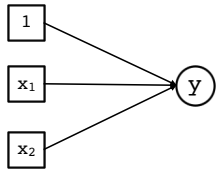
Power of Perceptron Networks

- A single-layer network with inputs for variables (x_1, x_2), and bias term (x_0 == 1), can compute OR of inputs
  - Threshold: (y == 1) if weighted sum (S >= 0); else (y == 0)

x_1 OR x_2

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	1



- *What* weights can we apply to the three inputs to produce OR?
  - One answer: $-0.5 + x_1 + x_2$

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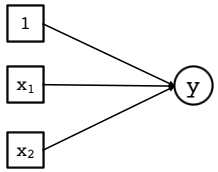
Power of Perceptron Networks

x_1 AND x_2

x_1	x_2	y
0	0	0
0	1	0
1	0	0
1	1	1



- What about the AND function instead?
  - One answer: $-1.5 + x_1 + x_2$

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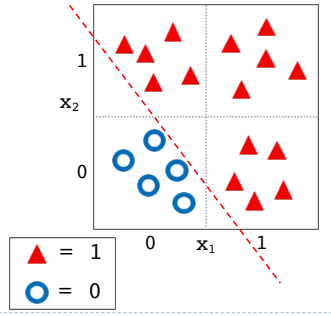
Linear Separation with Perceptron Networks

- We can think of binary functions as dividing (x1, x2) plane
- The ability to express such a function is *analogous* to the ability to linearly separate data in such regions

x_1 OR x_2

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	1



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Linear Separation with Perceptron Networks

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x_1 AND x_2

x_1	x_2	y
0	0	0
0	1	0
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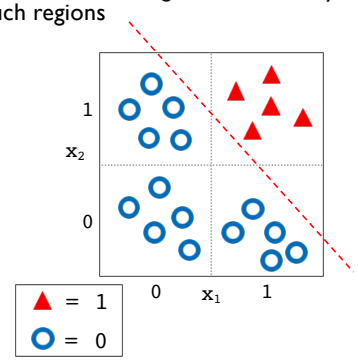

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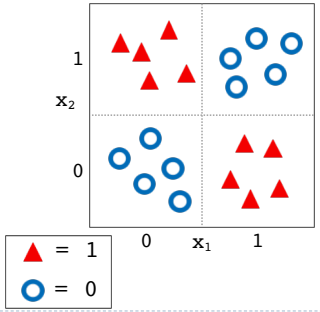
Functions with Non-Linear Boundaries

- There are some functions that cannot be expressed using a single layer of linear weighted inputs, and a non-linear output
- Again, this is analogous to the *inability* to linearly separate data in some cases

x_1 XOR x_2

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0



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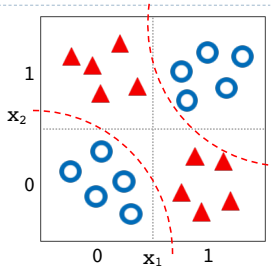
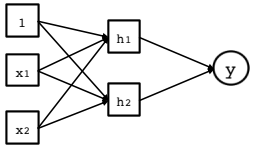
MLP's for Non-Linear Boundaries

- Neural networks gain expressive power because they can have *more than* one layer
- A multi-layer perceptron has one or more hidden layers between input and output
- Each hidden node applies a non-linear activation function, producing output that it sends along to the next layer
  - In such cases, much more complex functions are possible, corresponding to non-linear decision boundaries (as in current homework assignment)





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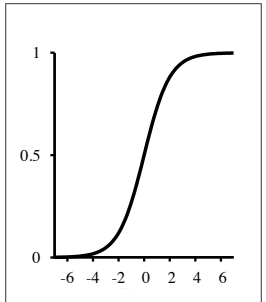
Review: Properties of the Sigmoid Function



$$g(in_j) = \frac{1}{1 + e^{-in_j}}$$

- The Sigmoid takes its name from the shape of its plot
- It always has a value in range:
  $0 \leq x \leq 1$
- The function is everywhere differentiable, and has a ***derivative*** that is easy to calculate, which turns out to be useful for learning:

$$g'(in_j) = g(in_j)(1 - g(in_j))$$

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Do We Always Use the Logistic Sigmoid?

- While historically popular, the logistic function is ***not*** always used in modern neural network research
  - There are many other functions that can be, and are, used
  - Some models even use combinations of different functions on different layers of the network
  - Often, the logistic is used at the final layer only, where it is sometimes called a ***softmax*** (probability) function
  - In our presentation, we will assume the logistic, but the overall details of the key algorithm do not change if we use something else
- In general, we want a function that is
  1. Non-linear: allowing for more complex outputs.
  2. Differentiable: standard back-propagation algorithms for learning in the networks use gradient-based approaches, and require access to the derivative of the function

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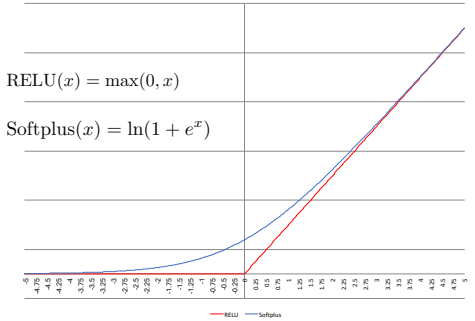
Other Popular Activation Functions



- The rectifier (or "ramp") function is popular for many modern applications
  - A network using the rectifier is known as a rectifier linear unit (ReLU)
- The Softplus function is a smooth approximation to the rectifier

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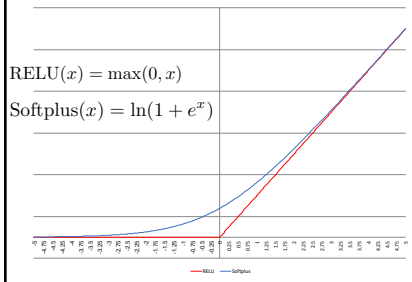
Other Popular Activation Functions



- The ReLU function has derivative:

$$\frac{\delta \,\mathrm{ReLU}}{\delta x}(x) = \begin{cases} 0 & \text{if input } x < 0 \\ 1 & \text{if input } x > 0 \\ undef & \text{if input } x = 0 \end{cases}$$

- For many purposes, the undefined value of the derivative is simply set ***arbitrarily*** (say to 0.5)
- Alternatively, if using Softplus approximation, we have a well-defined derivative everywhere:

$$\frac{\delta \,\mathrm{Softplus}}{\delta x}(x) = \frac{1}{1+e^{-x}}$$

The derivative of Softplus is the Sigmoid Logistic!

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Activation Functions Everywhere!

Logistic	$f(x) = \frac{1}{1+e^{-x}}$	$\frac{\delta f}{\delta x}(x) = f(x)(1-f(x))$
ReLU	$f(x) = \max(0, x)$	$\frac{\delta f}{\delta x}(x) = \{0,\ undef,\ 1\}$
Softplus	$f(x) = \ln(1+e^{x})$	$\frac{\delta f}{\delta x}(x) = \frac{1}{1+e^{-x}}$
Hyperbolic Tangent	$f(x) = \frac{1-e^{-2x}}{1+e^{-2x}}$	$\frac{\delta f}{\delta x}(x) = 1 - f(x)^2$
Gaussian	$f(x) = e^{-\frac{x^2}{2}}$	$\frac{\delta f}{\delta x}(x) = -x\, f(x)$

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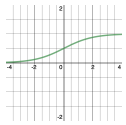
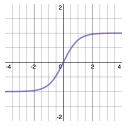
Choosing Activation Functions

- Functions have different pros and cons:

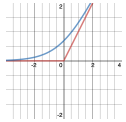
1. Sigmoid: historically popular, less so today
   - Susceptible to saturation: very large weights, tiny gradients
   - Not zero-centered, which is sometimes inconvenient
   - More popular as an *output probability* function (softmax)



2. Hyperbolic tangent
   - Can saturate like the sigmoid, but *is* zero-centered



3. ReLU/Softplus: most popular function in modern uses
   - ReLU is susceptible to "dying" neurons (these do not contribute to output in any real way)
   - Sensitive to learning rate
   - Softplus sometimes preferred, due to its smoothness



This Week & Next

- **Topics**: Neural Networks
- **Homework 04 (last one!)**
  - Out Monday, 30 March
  - Due Monday, 13 April, 5:00 PM Eastern
- **Office Hours**:
  - Virtual office hours with Zoom links can be found on the class Piazza and Canvas sites