Learning From Data
Lecture 6: Deep Neural Networks

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TBSI

October 29, 2021

Today's Lecture

Q&A Is canonical function the same as hypothesis in GLM?

$$\eta \xrightarrow[g^{-1} \text{ canonical link}]{g \text{ canonical response}} E[T(y)|x] \quad \mu$$

$\mu = g(\eta) = \frac{1}{1+e^{-\eta}}$. sigmoid.

$\eta \triangleq \theta^T x \Rightarrow h_\theta(x) = g(\theta^T x) = \frac{1}{1+e^{-\theta^T x}}$

$\eta = g^{-1}(\mu) = \underbrace{\log \frac{\mu}{1-\mu}}_{\text{logit}}$.

ANN

- Introduction to neural networks
  - Biological motivations
  - A case study
- Training a deep feedforward neural network
  - Forward pass
  - Backward propagation

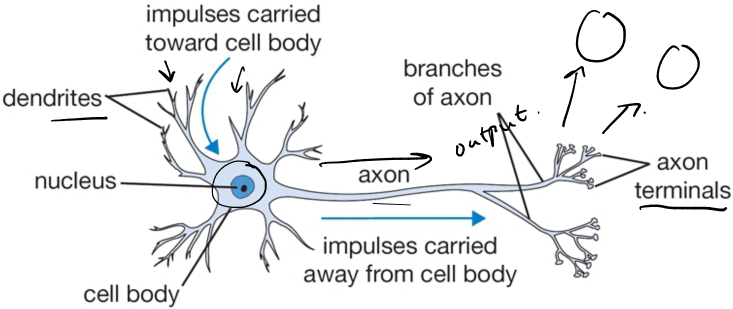
Introduction

- Biological motivation
- The XOR example

Biological motivation

connectionism

Schematic of a single neuron:



Each neuron takes information from other neurons, processes them, and then produces an output.

Biological motivation

How does a neuron process its input? (a *coarse* model)

- Takes the weighted average of I inputs, e.g. $z = \sum_{i=0}^{I} w_i(x_i)$
- Neuron fires if z is above some threshold

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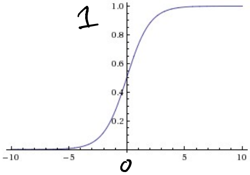
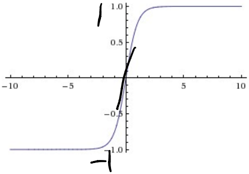
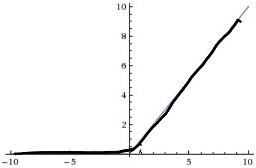
We call the threshold function **activation function**.



$sigmoid(z) = \frac{1}{1+e^{-z}}$



$tanh(z) = \frac{e^{z}-e^{-z}}{e^{z}+e^{-z}}$
$= 2(sigmoid(2z)) - 1$

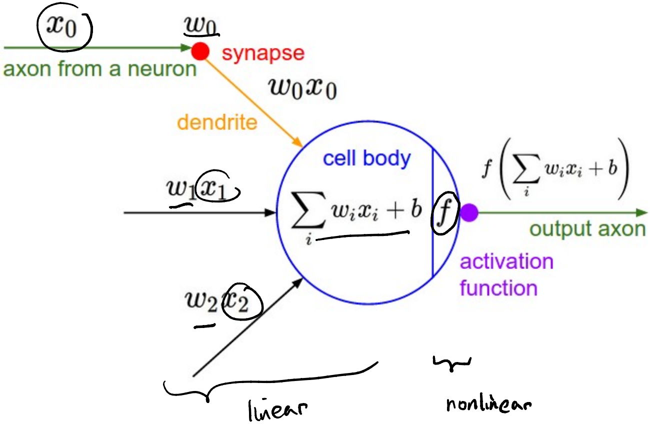


$ReLu(z) = max\{0, z\}$

Rectifying linear unit

Biological motivation

An artificial neuron with inputs x_1, x_2 and activation function f



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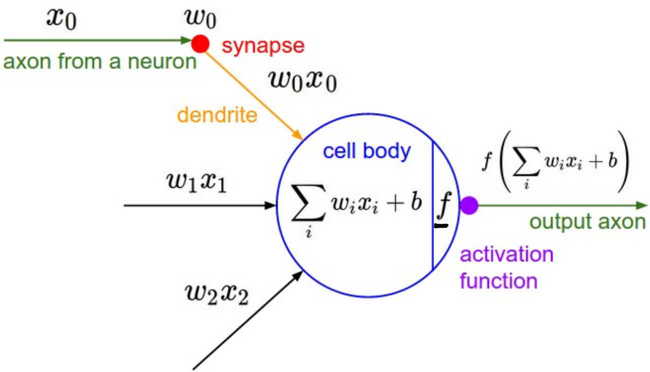

A single neuron is a (linear) binary classifier:

- When f is the sigmoid function, equivalent to binary softmax
- When f is the sign function, equivalent to the perceptron

$\text{sign}\left(\sum_i w_i x_i + b\right)$,

Neural networks

- The goal of a neural network is to approximate some function f^* such that $y = f^*(x)$.
- The neural network defines a mapping $y = f(x; \theta)$ and learns the value of parameters θ through training.

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- The neural network defines a mapping $y = f(x; \theta)$ and learns the value of parameters θ through training.
- Define **error function** that measures prediction error of f: e.g. a common error function used in classification is the **logarithmic loss** a.k.a. **cross-entropy loss**:

log-loss

Given P, Q. distributions of y

$$H(p,q) = \mathbb{E}_{y \sim p}(\log q(y)) = \sum_y p(y) \log(q(y))$$

$$L = y \log(\hat{y}) + (1 - y) \log(1 - \hat{y})$$

$p(y) \to$ real label probability

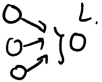
P

$q(y) \to$ predicted label probability

$\hat{y} \sim Q$

  - $\hat{y} = f(x; \theta)$ is the predicted output
  - y is the true output

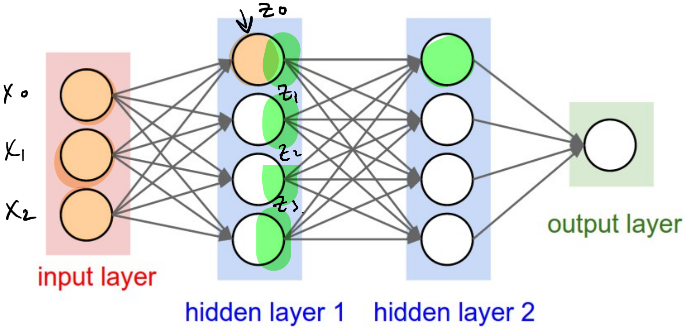
A single layer of neurons are unable to approximate complex functions.



A feed forward neural network

In a **feed-forward neural network** (a.k.a. **multi-layer perceptron**), all units of one layer is connected to all of the next layer. fully connected network

$$f = f^{(3)}(f^{(2)}(f^{(1)}(x)))$$



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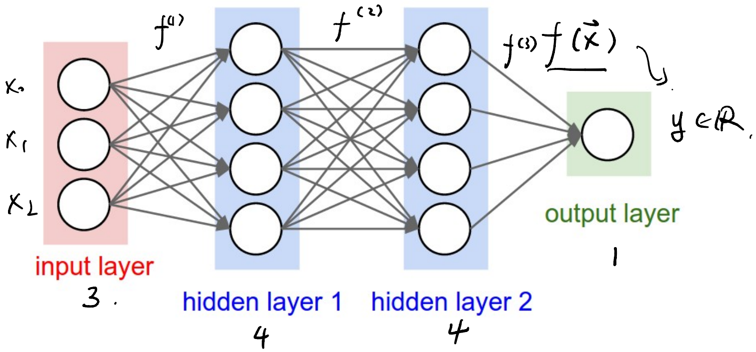


- number of layers are called **depth** of the neural network
- number of units in a layer is called **width** of a layer

The XOR problem

training data

XOR : the exclusive or

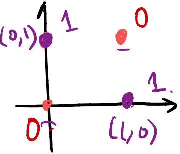
i	x_1	x_2	$y = x_1 \oplus x_2$
1	0	0	0
2	0	1	1
3	1	0	1
4	1	1	0

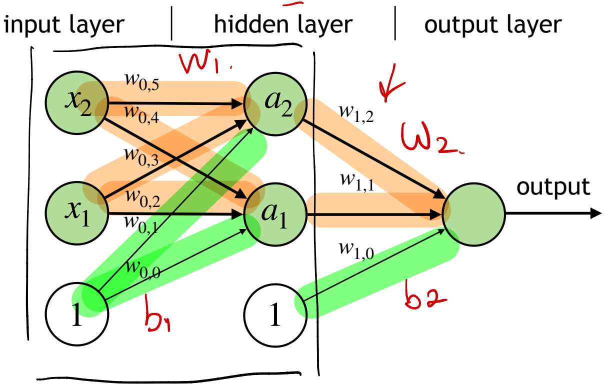
$$h(x) = f_2(w_2^T f_1(W_1 x + b_1) + b_2)$$

activition function: $f_1(\mathbf{z}), f_2(z)$

network weights: $W_1 = \begin{bmatrix} w_{0,2} & w_{0,4} \\ w_{0,3} & w_{0,5} \end{bmatrix}$,

$$b_1 = \begin{bmatrix} w_{0,0} \\ w_{0,1} \end{bmatrix}, w_2 = \begin{bmatrix} w_{1,2} \\ w_{1,1} \end{bmatrix}, b_2 = w_{1,0}$$





The XOR problem

$a_1 = f_1(z_1)$
$a_2 = f_1(z_2)$

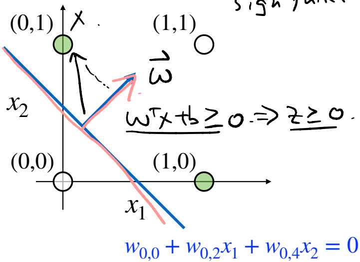
$z = (W_1 x + b_1) = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$

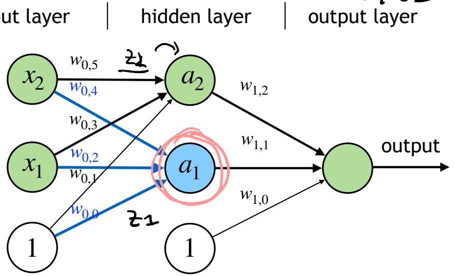
$$h(x; W_1, b_1, w_2, b_2) = f_2(w_2^T f_1(W_1 x + b_1) + b_2)$$

$a = \text{sign}(z) = \begin{cases} 1 & z \geq 0 \\ 0 & \text{o.w.} \end{cases} = 1\{z \geq 0\}$

Suppose $f_1(\mathbf{z}) = \begin{bmatrix} \mathbf{1}\{z_1 \geq 0\} \\ \mathbf{1}\{z_2 \geq 0\} \end{bmatrix}$, $f_2(z) = \mathbf{1}\{z \geq 0\}$. One solution:

sign function





x_1	x_2	a_1
0	0	**0**
0	1	**1**
1	0	**1**
1	1	**1**

or

The XOR problem

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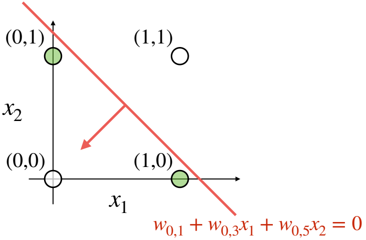

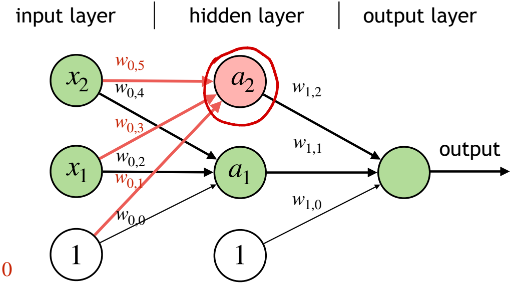

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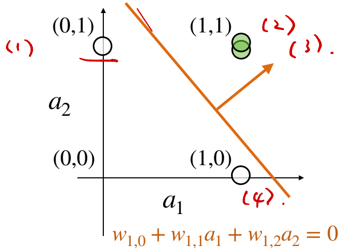

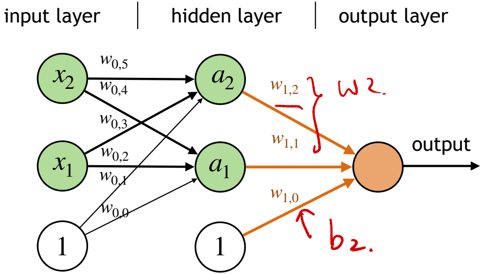

hidden layer
feature extractor

	x_1	x_2	a_1	a_2	y
(1)	0	0	0	1	**0**
(2)	0	1	1	1	**1**
(3)	1	0	1	1	**1**
(4).	1	1	1	0	**0**

XOR.

Universal approximation theorem

Universal approximation theorem (Cybenko,1989; Hornik et al., 1991) A feed-forward network with a single hidden layer containing a finite number of neurons can approximate any continuous functions on compact subsets of $\mathbb{R}^n$, under mild assumptions on the activation function.

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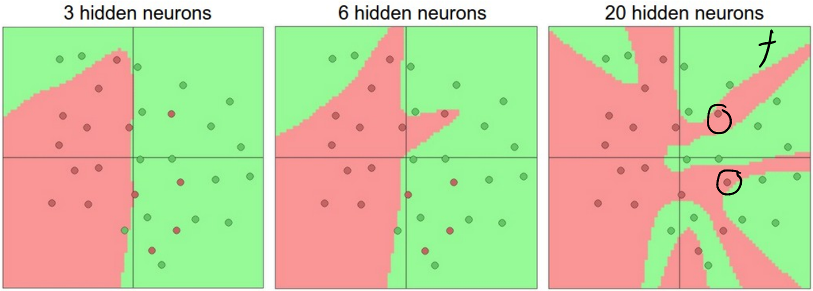
- First proved by George Cybenko in 1989 for sigmoid activation function;
- With one hidden layer, layer width of an *universal approximator* has to be exponentially large $\leftarrow$ *More effective to increase the* ***depth*** *of neural networks*
- ReLU networks with width n+1 is sufficient to approximate any continuous function of n-dimensional input variables if depth is allowed to grow. (Lu et. al, 2017; Hanin 2018)

width $\leftrightarrow$ depth. deeper.

Overfitting

Increase the size and number of layers in a neural network,

- the **capacity** , i.e. representation power of the network increases.
- but overfitting can occur: fits the noise in the data instead of the (assumed) underlying relationship.



Regularization

One way to control overfitting in training neural networks
A common regularization approach is **parameter norm penalties**

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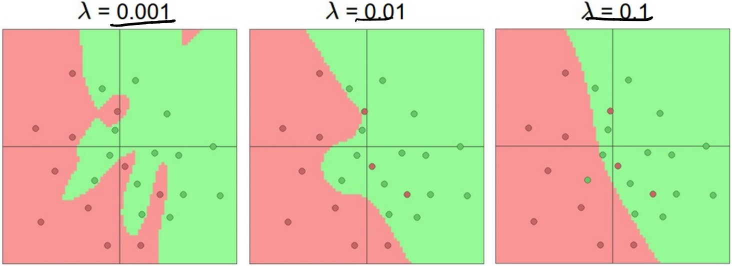
$$\underline{\tilde{L}(w; X, y)} = L(w; X, y) + \underline{\lambda \Omega(w)} \downarrow$$

- L2 parameter regularization: $\underline{\Omega(w) = \frac{1}{2}||w||_2^2 = \frac{1}{2}w^T w}$ drives the weights closer to the origin



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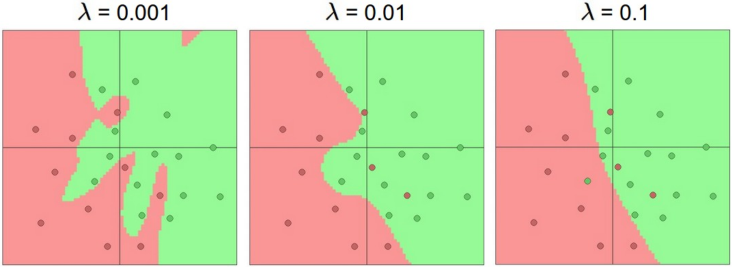


- L1 parameter regularization: $\Omega(w) = \underline{||w||_1 = \sum_{i=1}^{k} |w_i|}$ drives solutions more sparse.

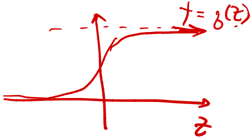
Training a Deep Feedforward Network

Forward pass and Backpropagation

Forward pass and Backpropagation

See Powerpoint slides.

Practical issues

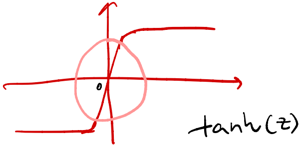


$\nabla f(z) \approx 0$ when z is very large or very small.

Which activation function to use?

- *sigmoid* function $\sigma(z)$: gradient $\nabla f(z)$ **saturates** when z is highly positive or highly negative. Not suitable for hidden unit activation.

Practical issues



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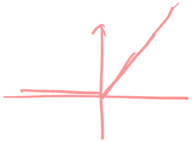
Practical issues



$\max(0, x)$ $\begin{cases} 1. & x \geq 0 \\ 0. & x < 0 \end{cases}$

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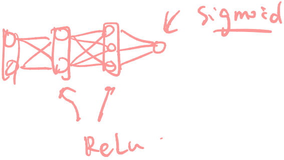
- $ReLu(z)$: easy to optimize (6 times faster than sigmoid), often used with affine transformation $g(W^T x + b)$



Additional resources

Deep neural network is a relative young field with lots of empirical results. Read more on the practical things to do for building and training neural networks:

- Stanford Class on Convolutional Neural Networks: http://cs231n.github.io
- Ian Goodfellow, Yoshua Bengio and Aaron Courville, *Deep Learning*, MIT Press, 2016

Demos:

- http://vision.stanford.edu/teaching/cs231n-demos/linear-classify/
- https://playground.tensorflow.org/