Using neural nets to recognize hand-written digits

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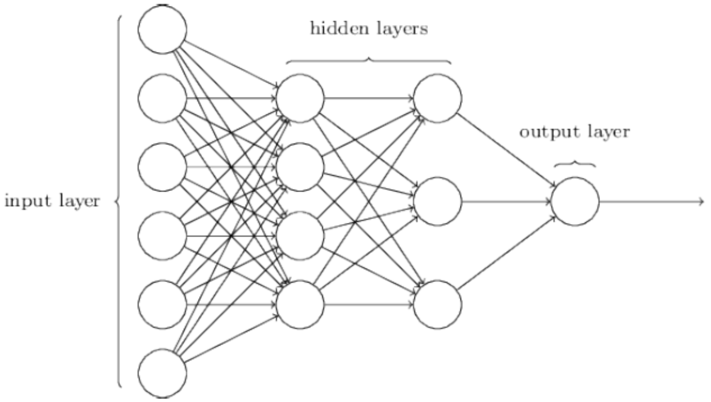
Reference

Most of the slides are taken from the first chapter of the online book by Michael Nielson:

- neuralnetworksanddeeplearning.com

Introduction

- Deep learning allows computational models that are composed of multiple layers to learn representations of data.
- Significantly improved state-of-the-art results in speech recognition, visual object recognition, object detection, drug discovery and genomics.



"deep" comes from having multiple layers of non-linearity

[Source: Yann LeCun, Yoshua Bengio, and Geoffrey Hinton, Deep Learning, Nature 2015]

Introduction

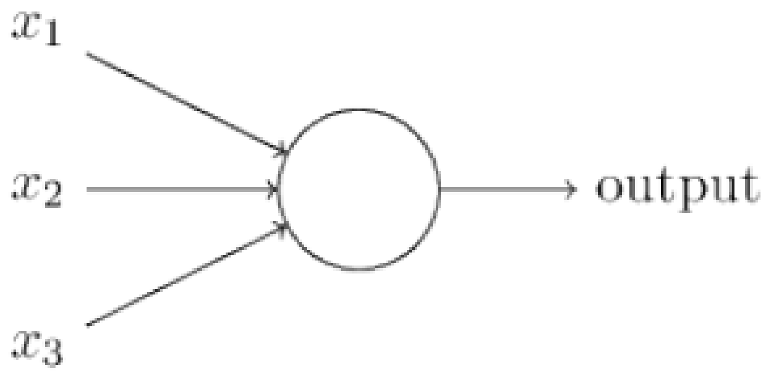
- “neural” is used because it is loosely inspired by neuroscience.

- The goal is generally to approximate some function f^*, e.g., consider a classifier $y = f^*(x)$:

  We define a mapping $y = f(\theta, x)$ and learn the value of the parameters θ that result in the best function approximation.

- Feedforward network is a specific type of deep neural network where information flows through the function being evaluated from input x through the intermediate computations used to define f, and finally to the output y.

Perceptron



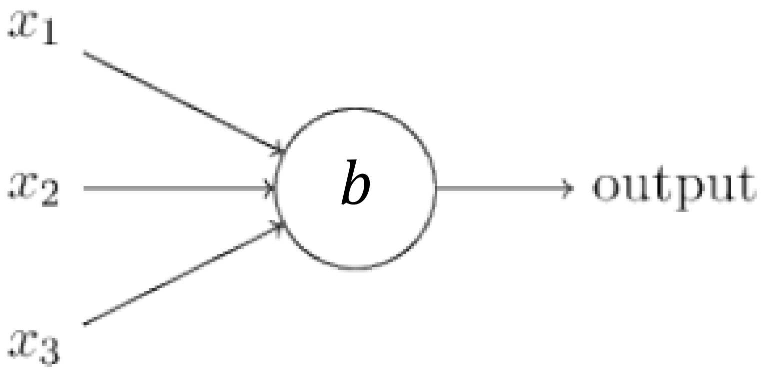
- A perceptron takes several Boolean inputs (x_1, x_2, x_3) and returns a Boolean output.

$$\text{output} = \begin{cases} 0 & \text{if } \sum_j w_j x_j \leq \text{ threshold} \\ 1 & \text{if } \sum_j w_j x_j > \text{ threshold} \end{cases}$$

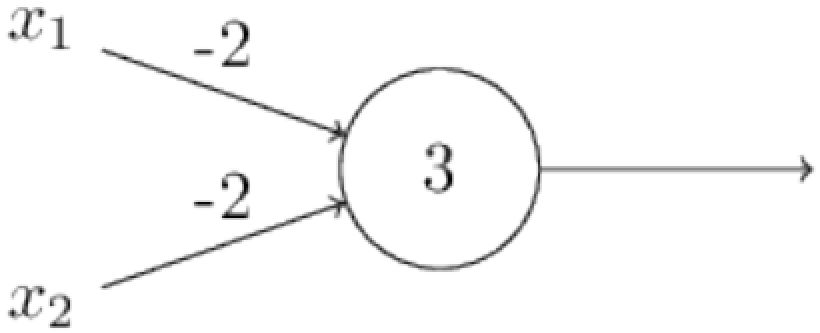
- The weights (w_1, w_2, w_3) and the threshold are real numbers.

Simplification (Threshold -> Bias)

$$\text{output} = \begin{cases} 0 & \text{if } w \cdot x + b \le 0 \\ 1 & \text{if } w \cdot x + b > 0 \end{cases}$$



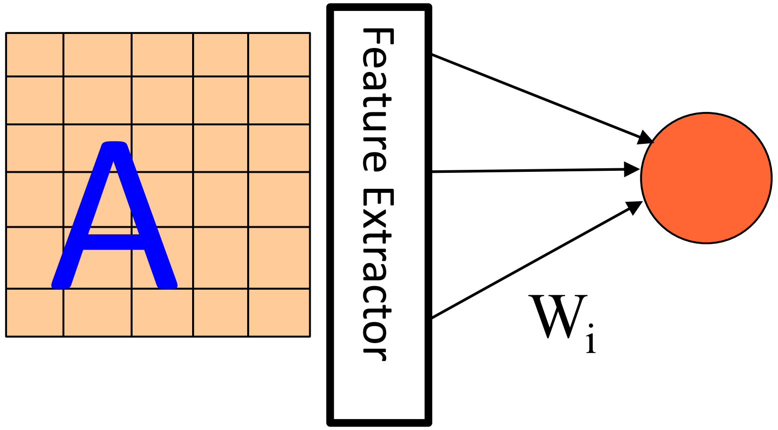
NAND gate using a perceptron



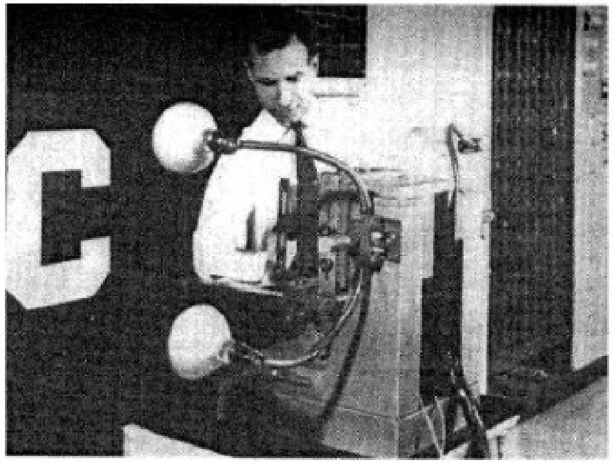
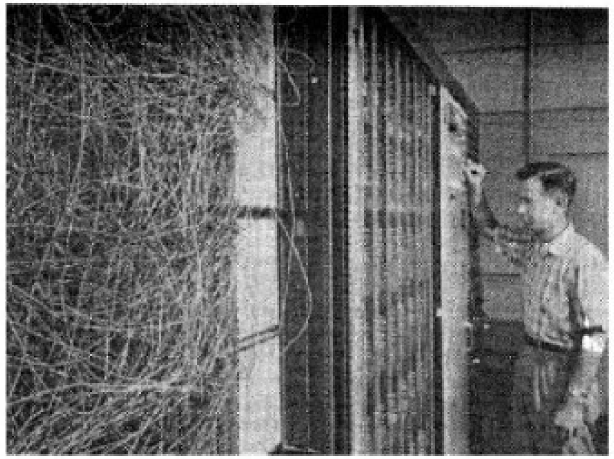
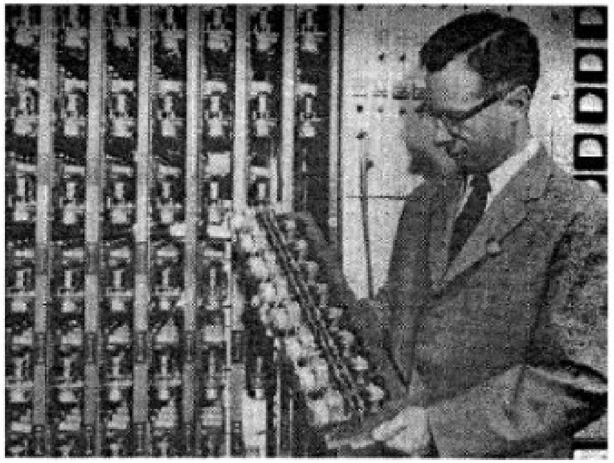
- NAND is equivalent to NOT AND

It’s an old paradigm

- The first learning machine: the Perceptron
  - Built at Cornell in 1960
- The Perceptron was a linear classifier on top of a simple feature extractor
- The vast majority of practical applications of ML today use glorified linear classifiers or glorified template matching.
- Designing a feature extractor requires considerable efforts by experts.



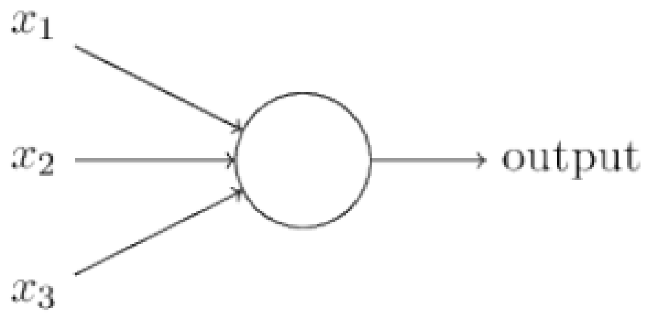
$$y = sign\left(\sum_{i=1}^{N} W_i F_i(X) + b\right)$$

Slide Credit: Marc'Aurelio Ranzato, Yann LeCun

Design the weights and thresholds for the following truth table

When all the three Boolean variables are 1s, we output 1, otherwise we output 0.

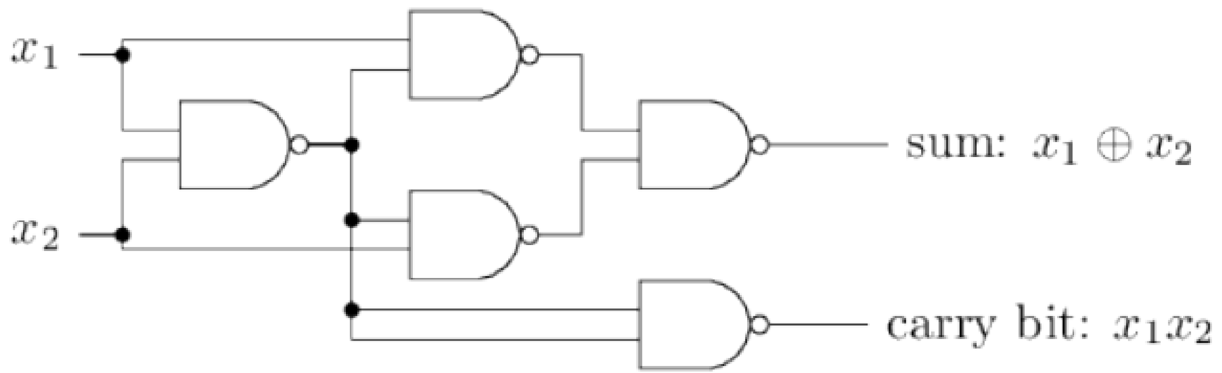


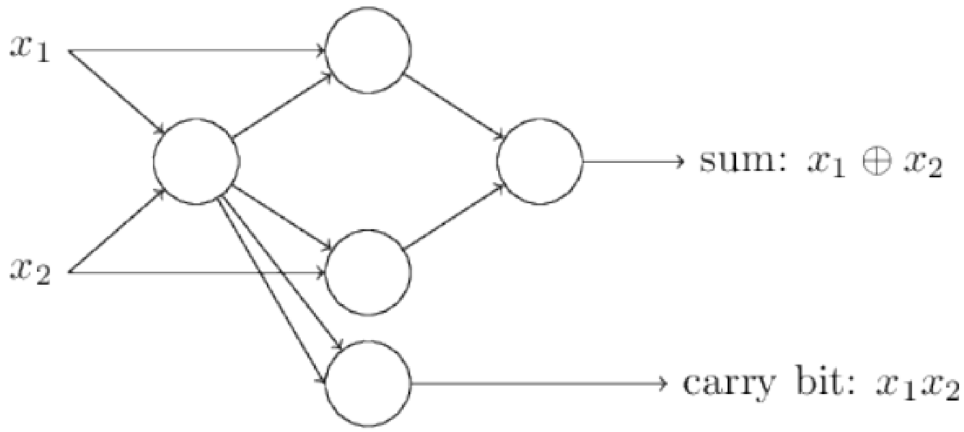
When all the three Boolean variables are 0s, we output 1, otherwise we output 0.

When two of the three Boolean variables are 1s, we output 1, otherwise we output 0.

NAND is universal for computation

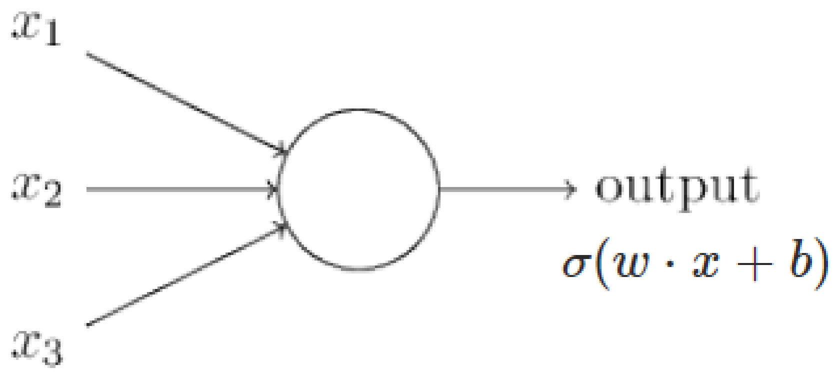
- XOR gate and AND gate





OR gate using perceptrons?

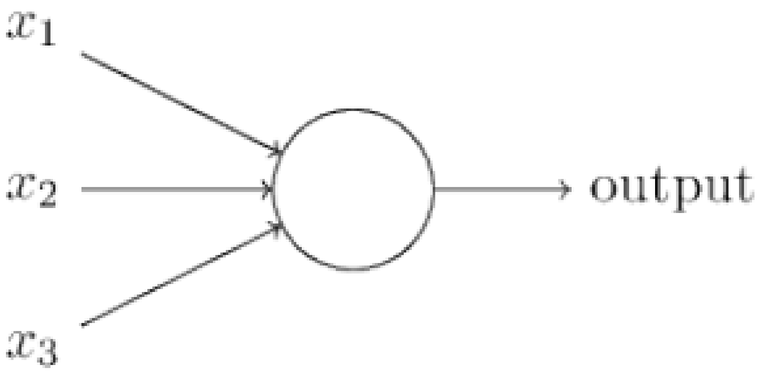
Sigmoid neuron



- A sigmoid neuron can take real numbers (x_1, x_2, x_3) within 0 to 1 and returns a number within 0 to 1. The weights (w_1, w_2, w_3) and the bias term b are real numbers.

Sigmoid function $\sigma(z) \equiv \frac{1}{1 + e^{-z}}$

Sigmoid neuron

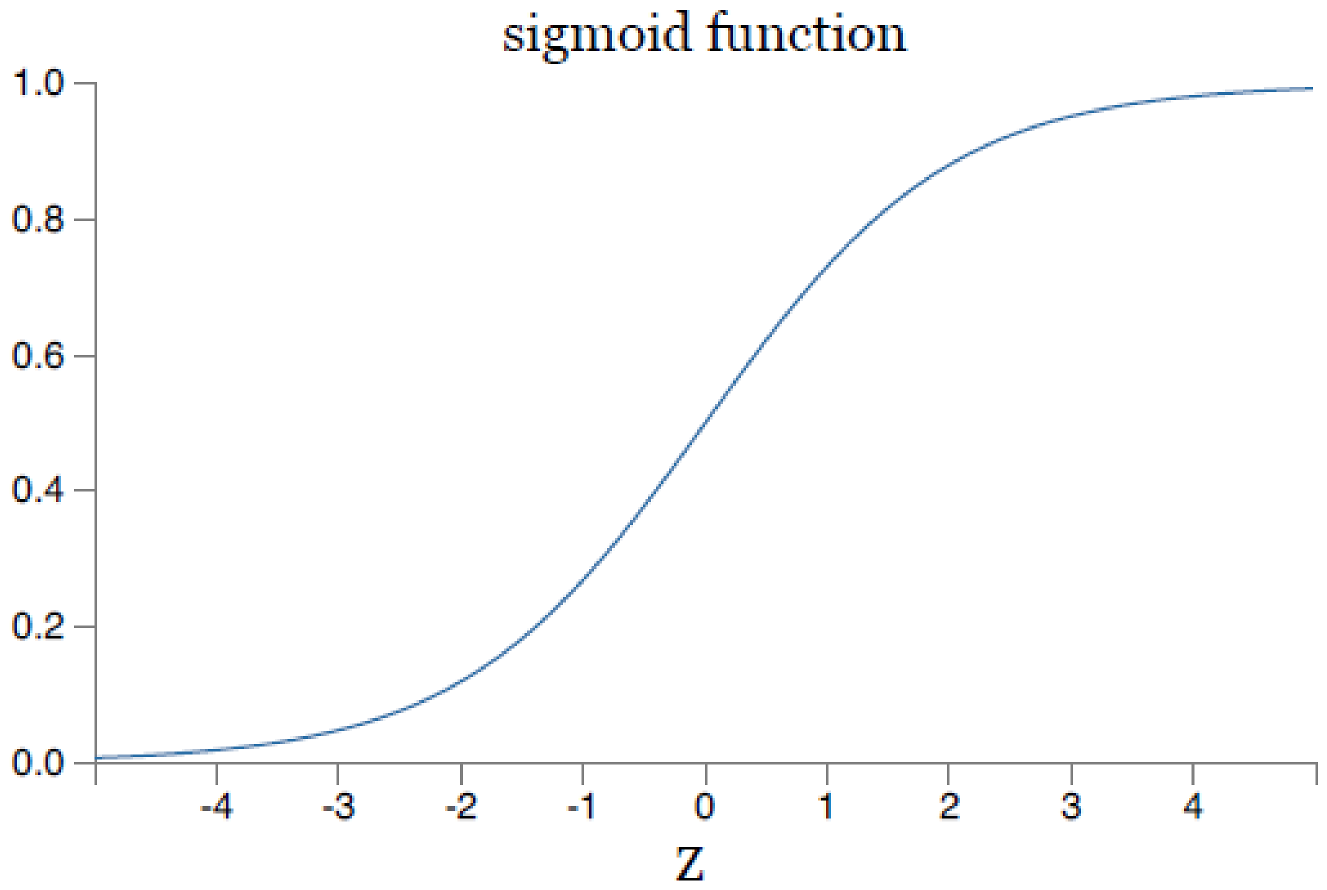


$$\frac{1}{1+\exp(-\sum_j w_j x_j - b)}$$

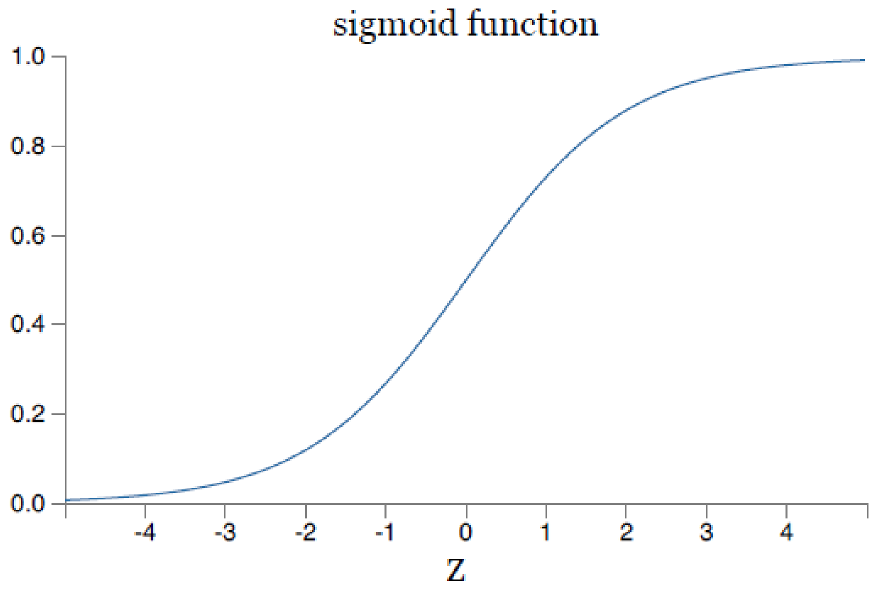
- A sigmoid neuron can take real numbers (x_1, x_2, x_3) within 0 to 1 and returns a number within 0 to 1. The weights (w_1, w_2, w_3) and the bias term b are real numbers.

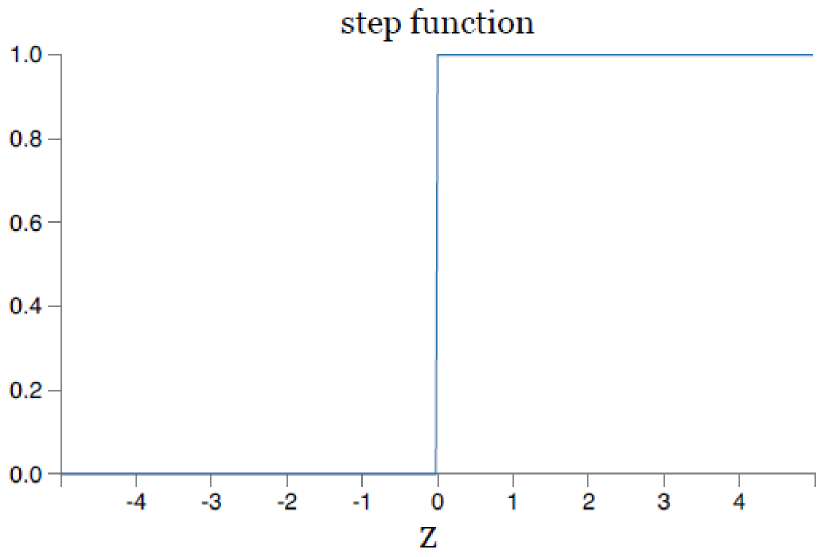
Sigmoid function

$$\sigma(z) \equiv \frac{1}{1+e^{-z}}$$



Sigmoid function can be seen as smoothed step function



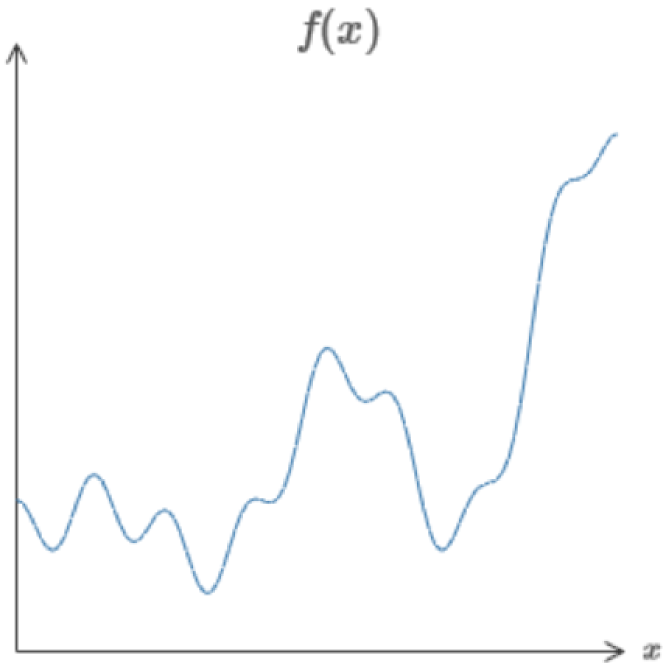


Reference for function approximation

Many of the slides are prepared using the following resources:

- http://neuralnetworksanddeeplearning.com/chap4.html

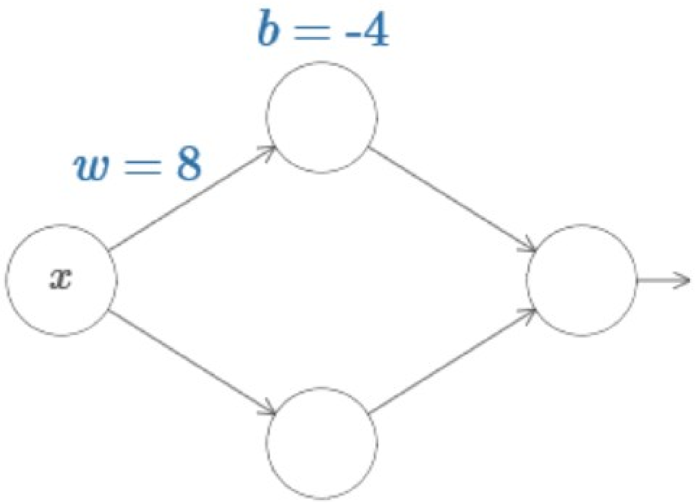
A simple function with one input and one output

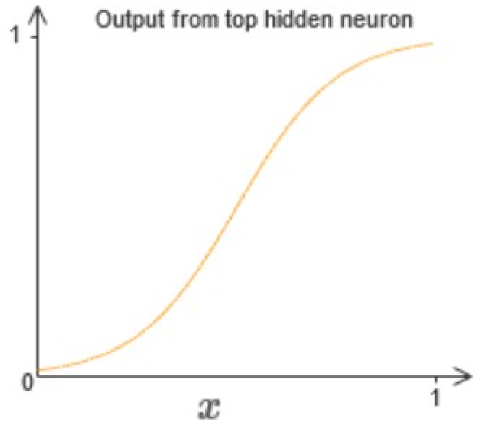


Goal: Show that such functions can be approximated using sigmoid units in a deep neural network.

The slides show a constructive argument to simulate any function.

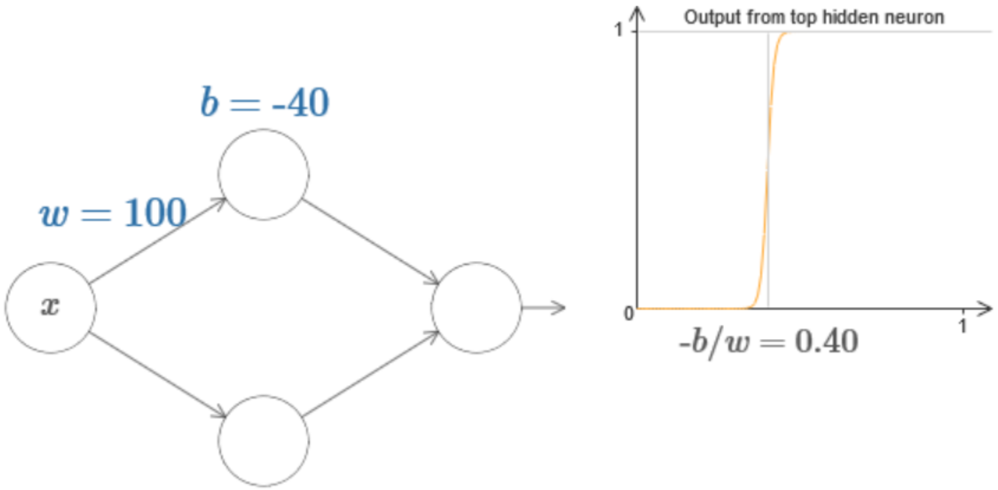
Approximating a step function using Sigmoid unit





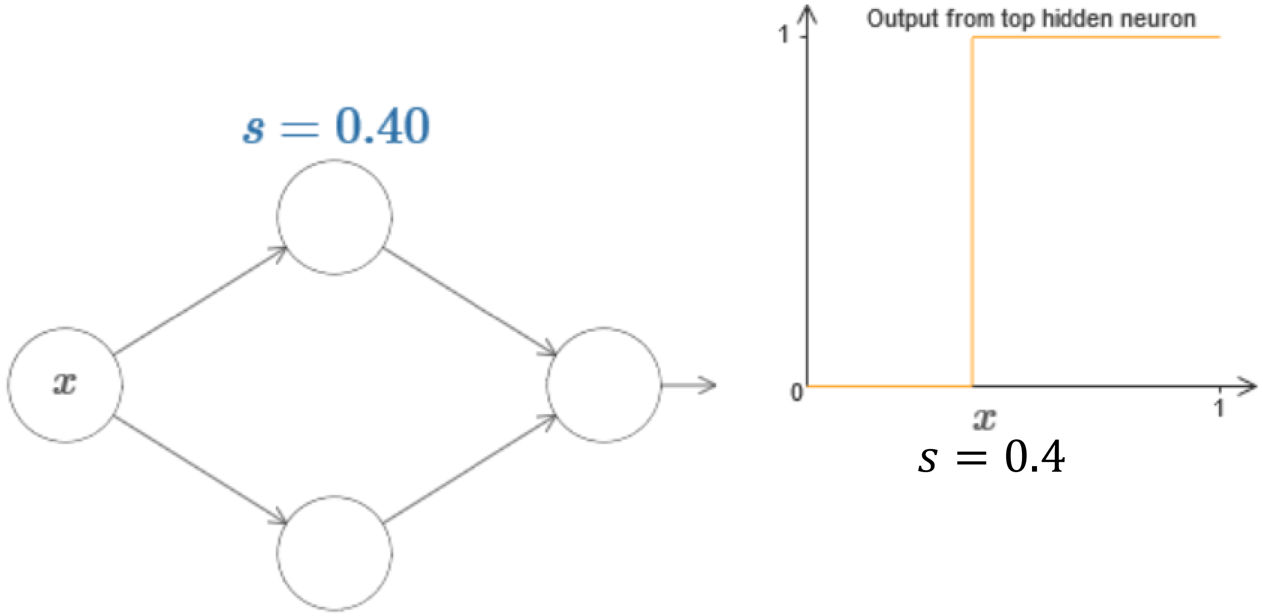
- Small weight and bias terms – coarse approximation of a step function

Approximating a step function using Sigmoid unit



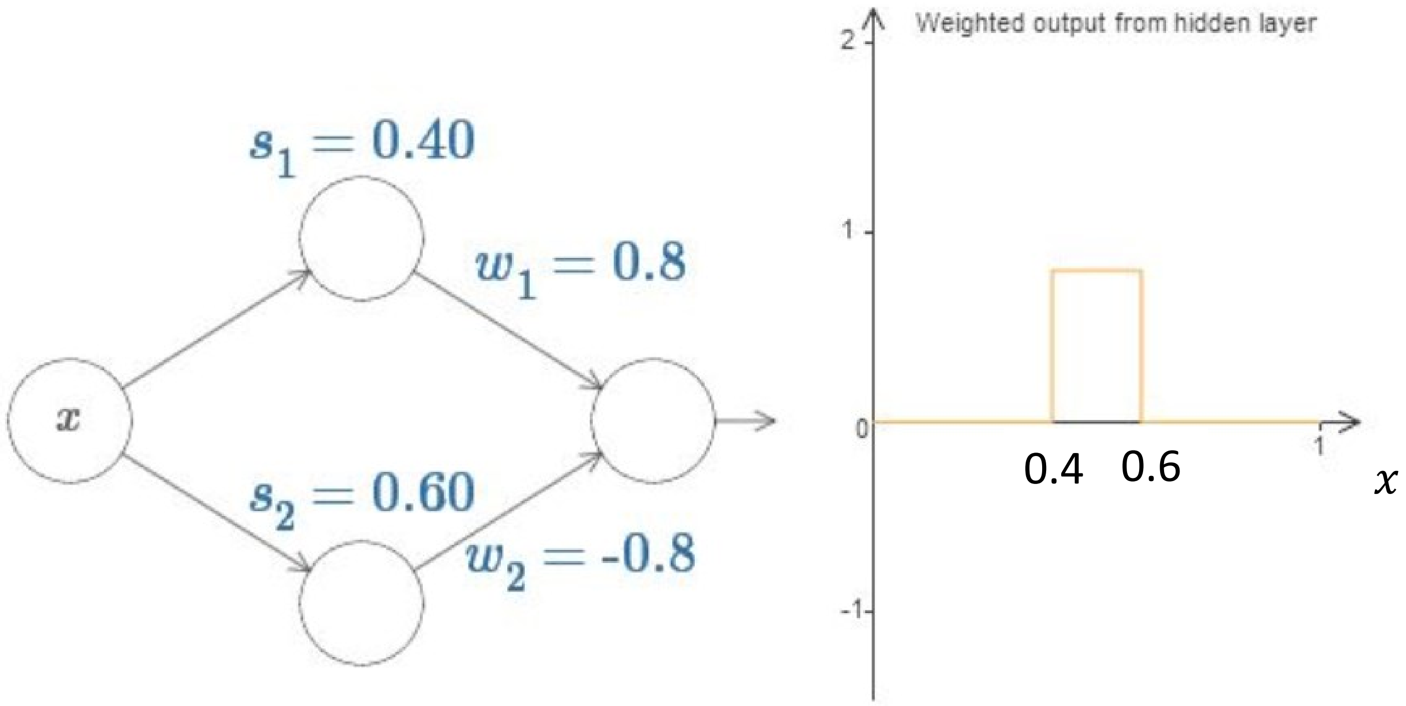
- Larger weight and bias terms – better approximation of a step function

Approximating a step function using Sigmoid unit



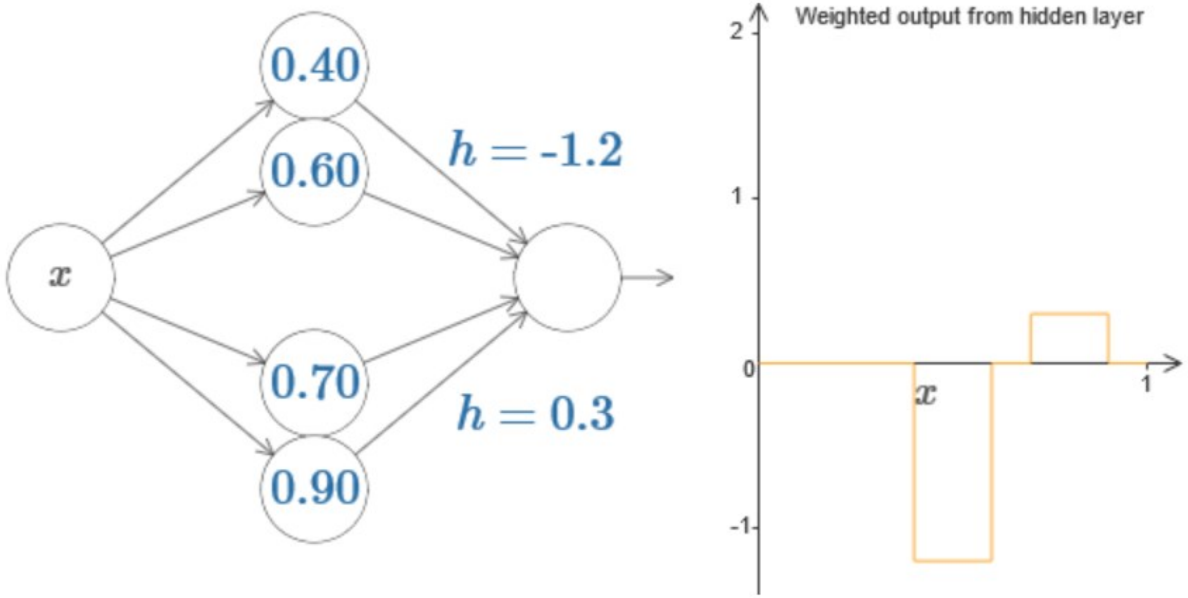
- Assume that a very large weight is used for all neurons. In that case, we can change the bias term to get different values for $s = -\frac{b}{w}$, the point where the step function starts.

Approximating a bump function



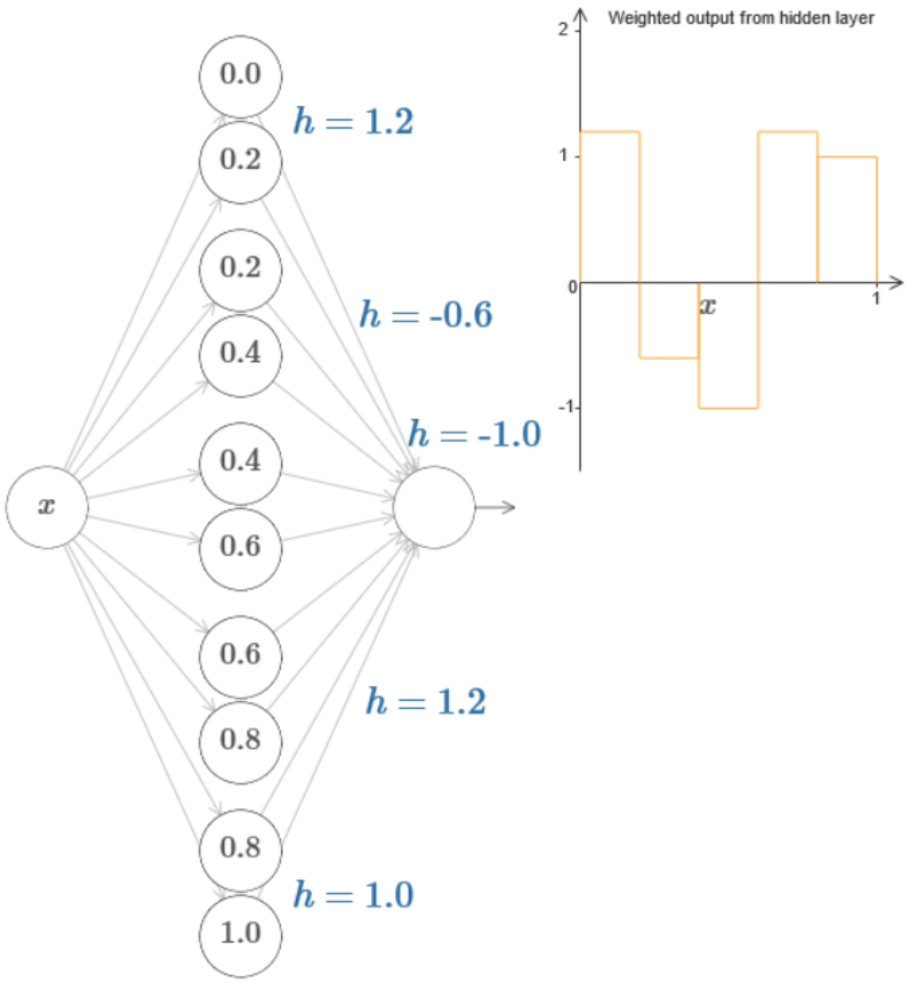
- You can simulate a simple bump function using two neurons with different “s” values to indicate the start and end points for the bump function.
- The weights are designed such a manner that $w_1 = -w_2$, depending on whether the bump function is above or below “x” axis.

Approximating two bumps

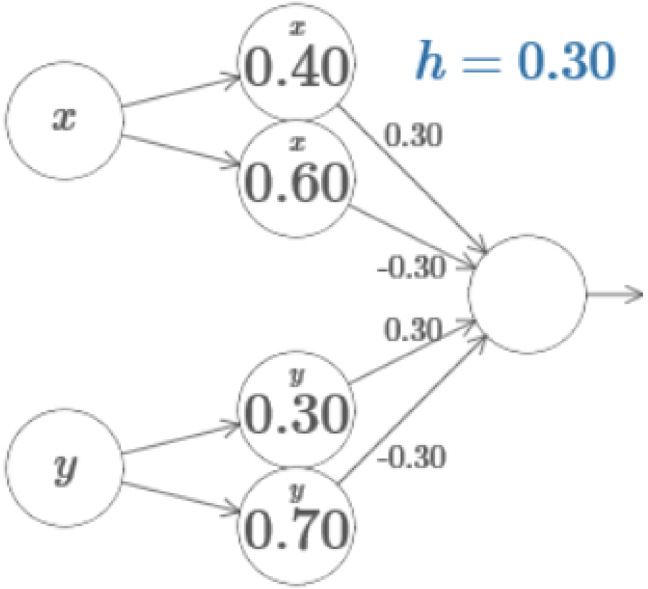


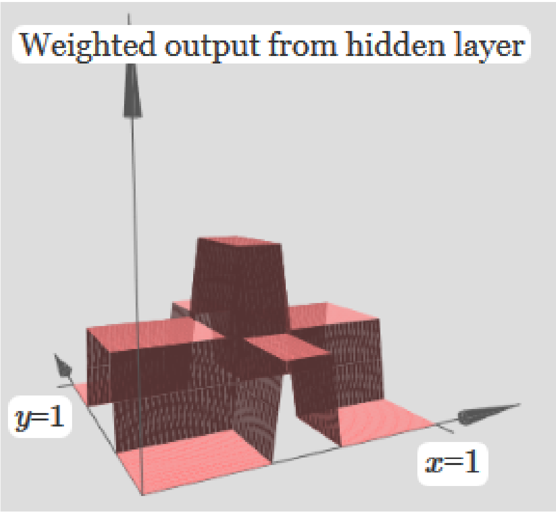
- The first bump is from s=0.4 to 0.6 and the second bump is from s=0.7 to 0.9.

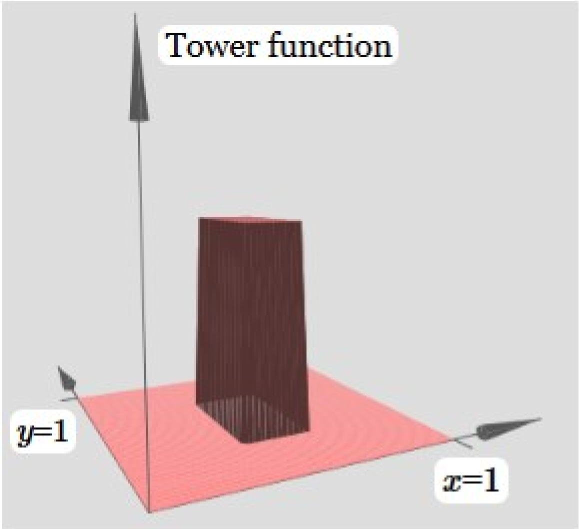
Approximating multiple bumps



Functions with multiple inputs



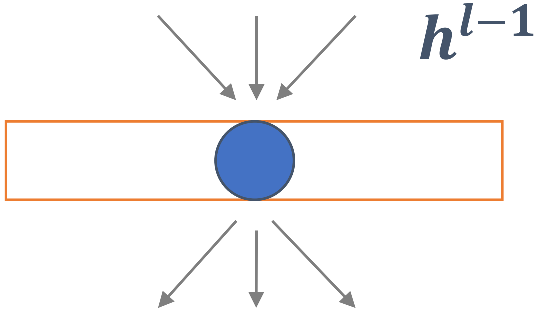




- It is not hard to see that the entire approach can be extended for cases with multiple inputs.

Other Activation functions

One activation unit in
an intermediate layer



1. Rectifier Linear Unit (ReLU):

$$h_i^l = max\,\{\,\underbrace{0}_{\text{Inactive}},\, \underbrace{W_i^l h^{l-1} + b_i^l}_{\text{Active (>0)}}\,\}$$

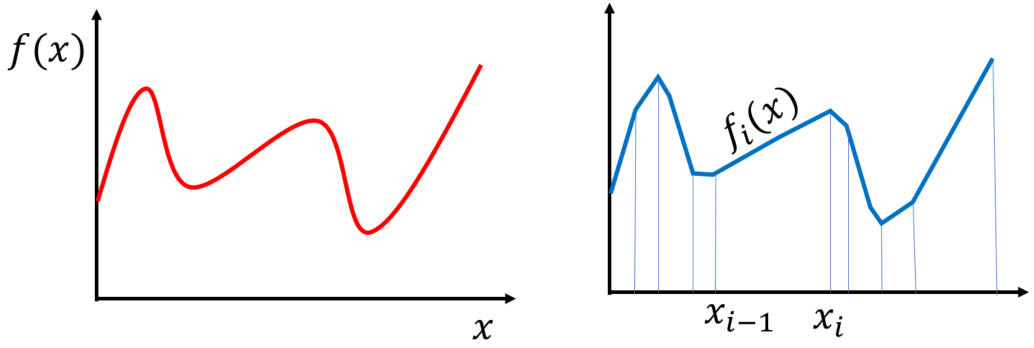
2. Maxout:

$$h_i^l = max\,\{\,W_i^{1\,l} h^{l-1} + b_i^{1\,l}, \ldots, W_i^{k\,l} h^{l-1} + b_i^{k\,l}\,\}$$

In both cases, the DNN is a piecewise linear function.

Background – Piecewise linear functions

- Networks that use activation functions such as ReLU or maxout are piece-wise linear functions.



Piece-wise linear functions in 1D – We have linear functions for small pieces or regions

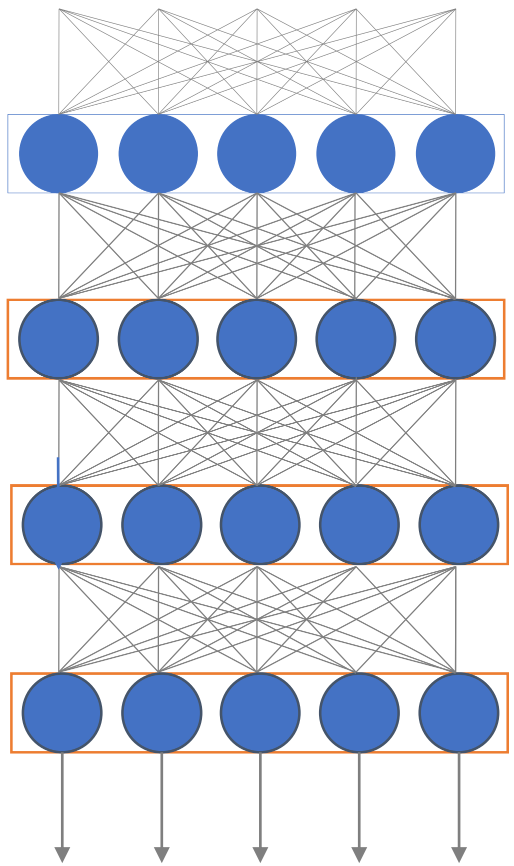
Piece-wise linear function in 2D – the depths can be obtained from different linear functions for different triangles (Carolinska institute, Sweden)

- The # of linear regions ↔ Expressiveness or representability of piece-wise linear networks.

Notation for deep neural network (DNN)

Notation:

- Input: $\boldsymbol{x}$
- Output: $\boldsymbol{y}$
- Number of layers: $\boldsymbol{L}$
- Width of layer $\boldsymbol{l}$: $\boldsymbol{n_l}$
- Output of layer $\boldsymbol{l}$: $\boldsymbol{h^l} \in \mathbb{R}^{\boldsymbol{n_l}}$



$\boldsymbol{x} \quad (\boldsymbol{h^0}) - \boldsymbol{Input}$

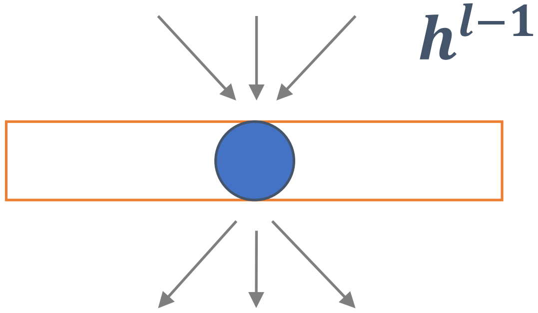
$\boldsymbol{h^1}$

$\boldsymbol{h^{L-1}}$

$\boldsymbol{y} \quad (\boldsymbol{h^L}) - \boldsymbol{Output}$

Activation functions

One activation unit in
an intermediate layer



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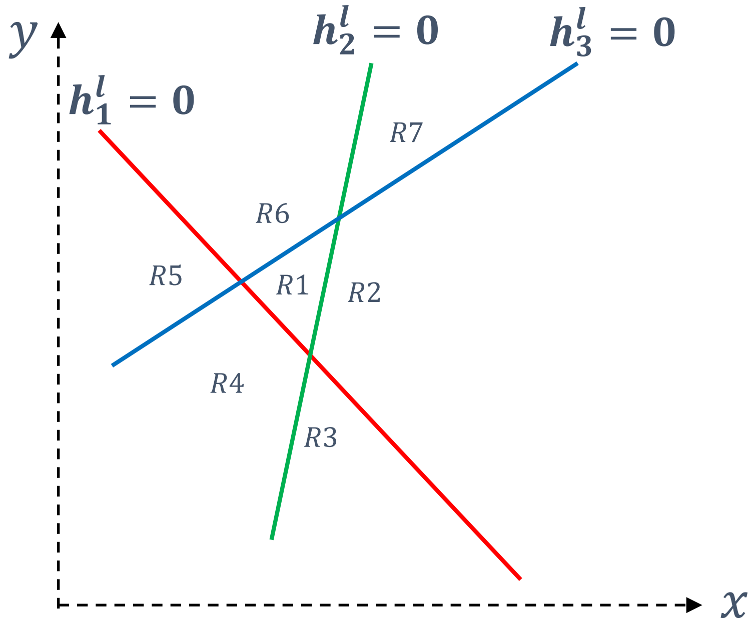
In both cases, the DNN is a piecewise linear function.

The number of regions in one layer using ReLUs

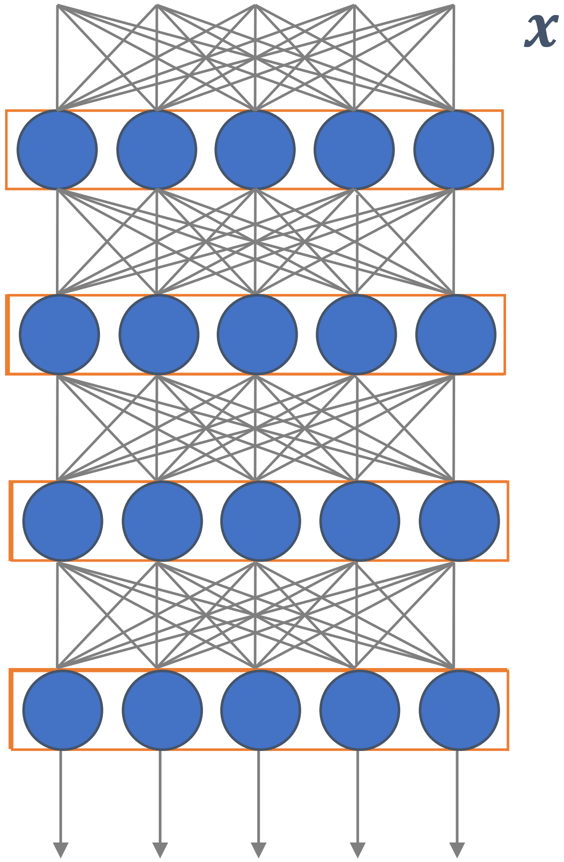


- $h_i^l = 0$ *is nothing but a hyperplane*
- 3 *hyperplanes partition the 2D space into 7 regions*

Activation Patterns and Linear Regions

For ReLUs, we characterize these regions using the concept of activation patterns (Montufar, 2017):

- For a given input $\boldsymbol{x}$



Activation Patterns and Linear Regions

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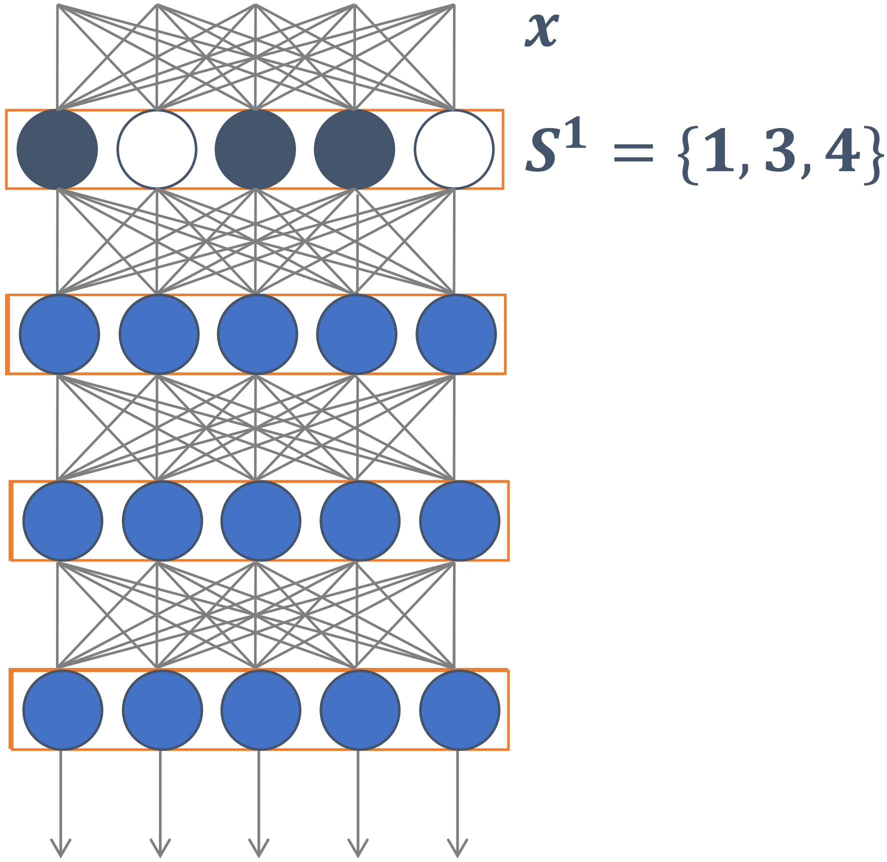
- For a given input $\boldsymbol{x}$
- There is an activation set $\boldsymbol{S^l} \subseteq \{\mathbf{1}, \mathbf{2}, \dots, \boldsymbol{n^l}\}$ for each layer l such that $\boldsymbol{i} \in \boldsymbol{S^l}$ iff $\mathbf{h_i^l} > \mathbf{0}$



Activation Patterns and Linear Regions

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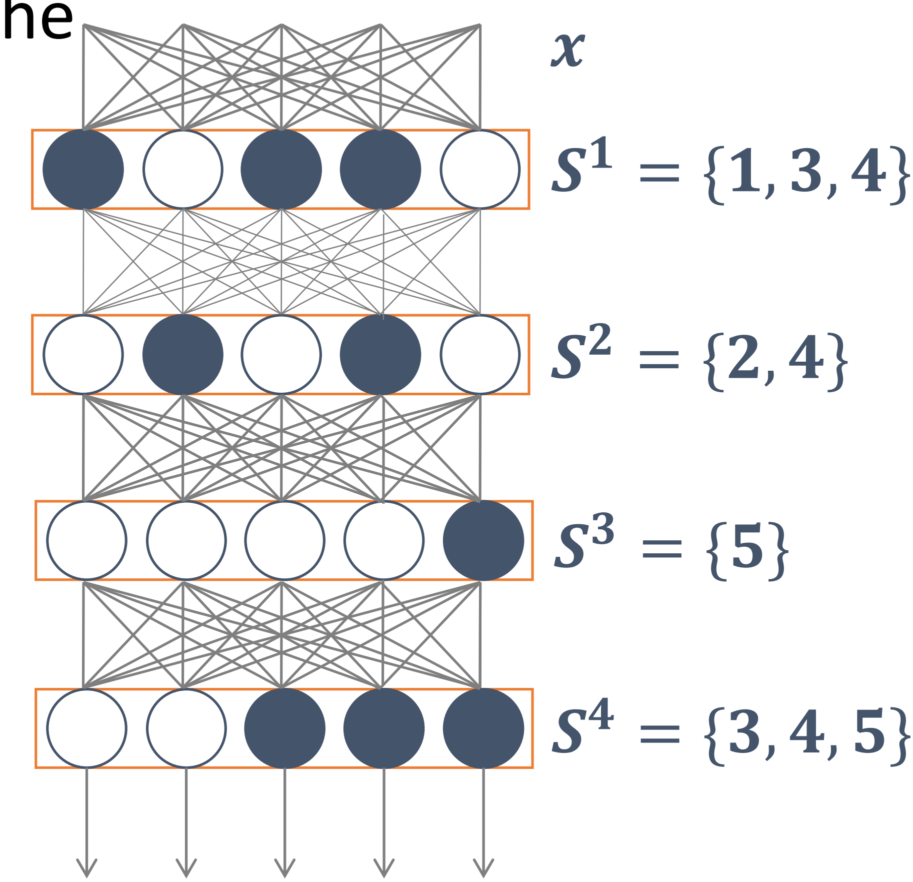
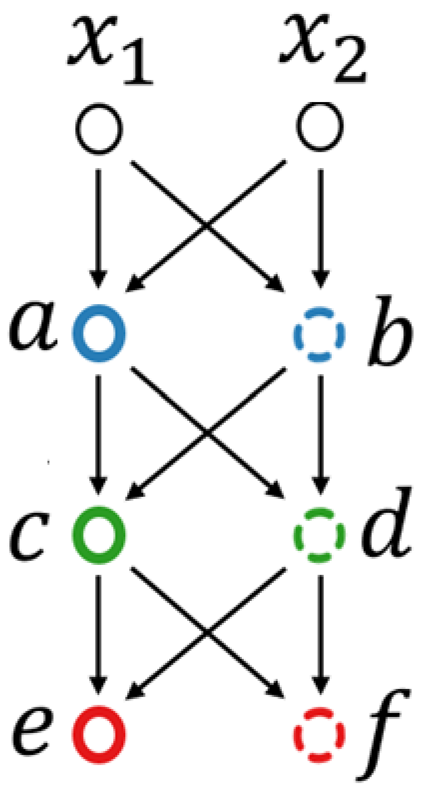
- For a given input $\boldsymbol{x}$
- There is an activation set $\boldsymbol{S}^{l} \subseteq \{\mathbf{1}, \mathbf{2}, \dots, \boldsymbol{n}^{l}\}$ for each layer l such that $\boldsymbol{i} \in \boldsymbol{S}^{l}$ iff $\mathbf{h}_{\mathrm{i}}^{\mathrm{l}} > \mathbf{0}$
- The activation pattern of $\boldsymbol{x}$ is $\boldsymbol{\mathcal{S}} = (\boldsymbol{S}^{1}, \dots, \boldsymbol{S}^{l})$

A linear region is the set of all points with a same activation pattern

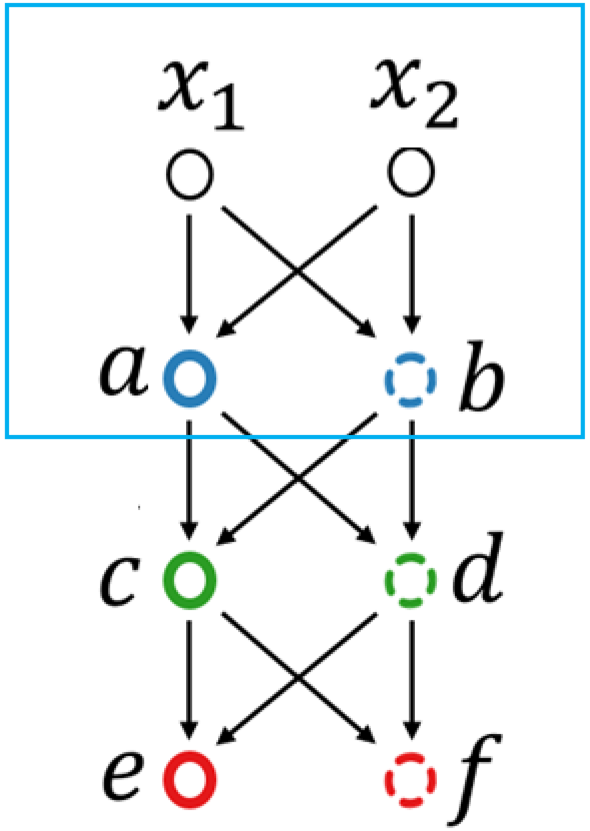


Linear regions in the case of multiple layers



A simple network
with 3 hidden layers

Linear regions in the case of multiple layers



A simple network
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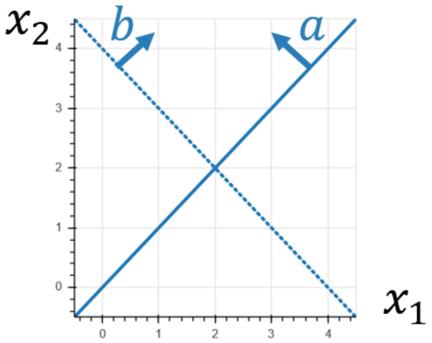
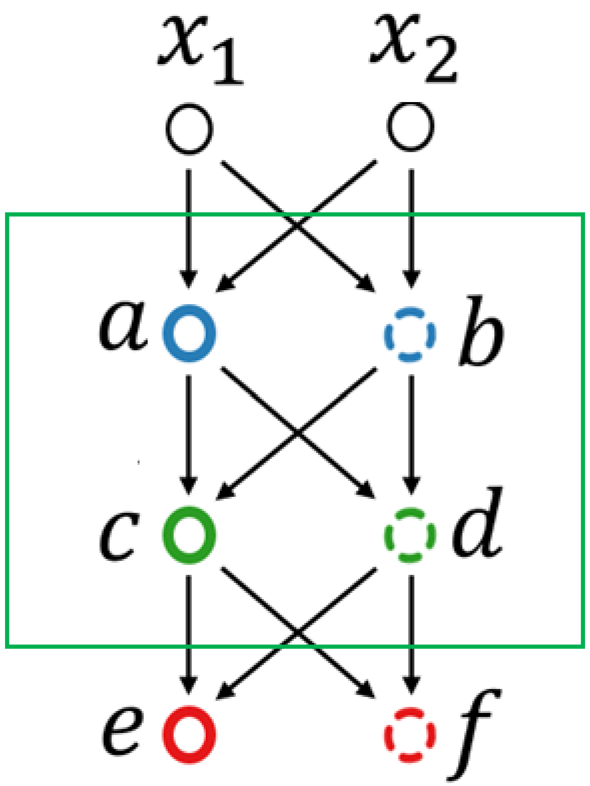


Hyperplanes partitioning the
regions of previous layers

Linear regions in the case of multiple layers



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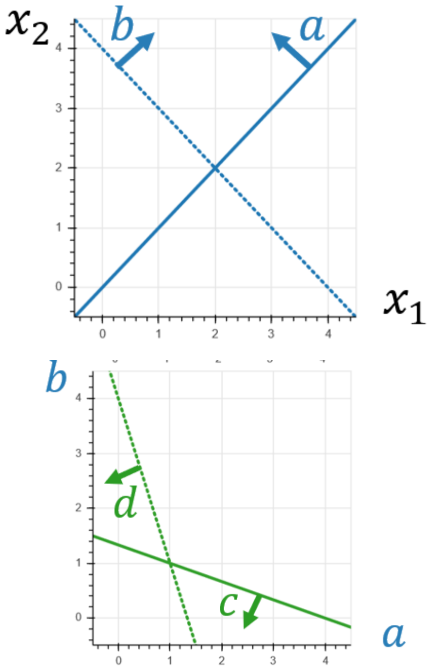

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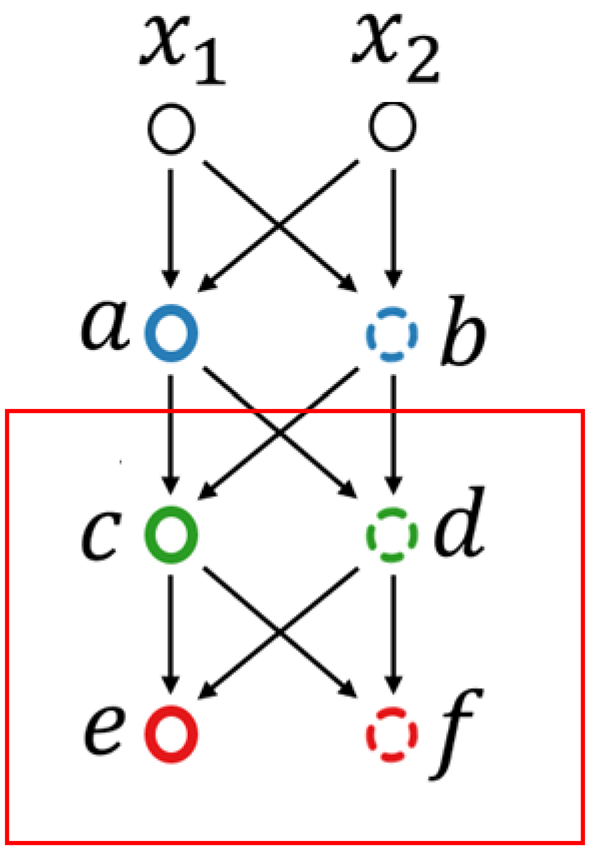

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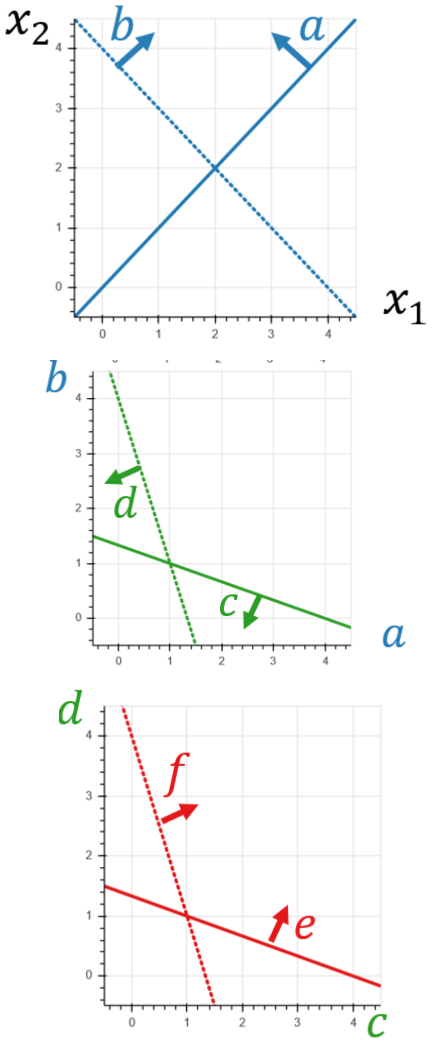

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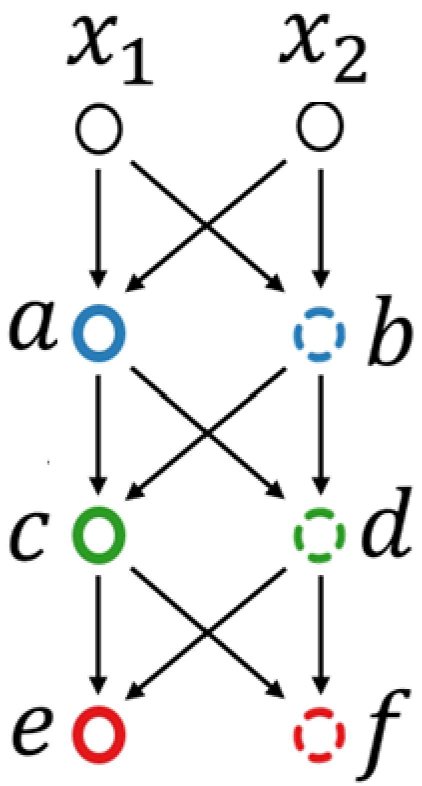

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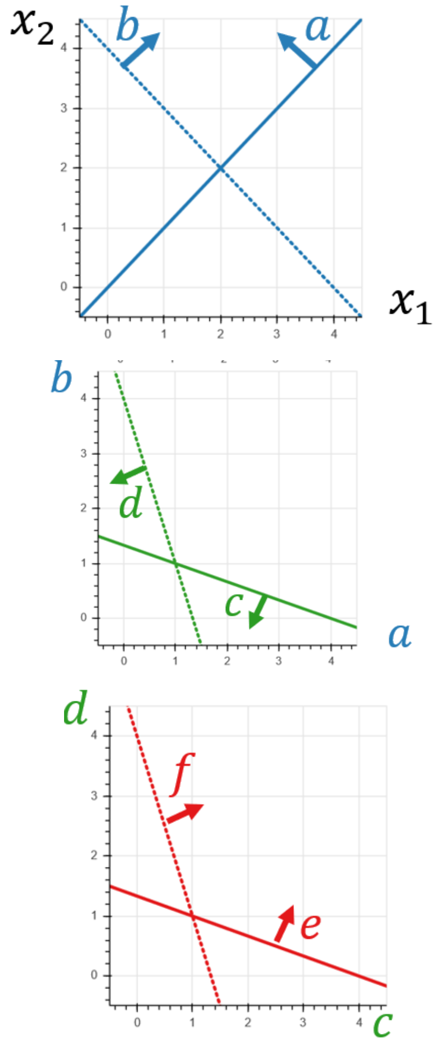
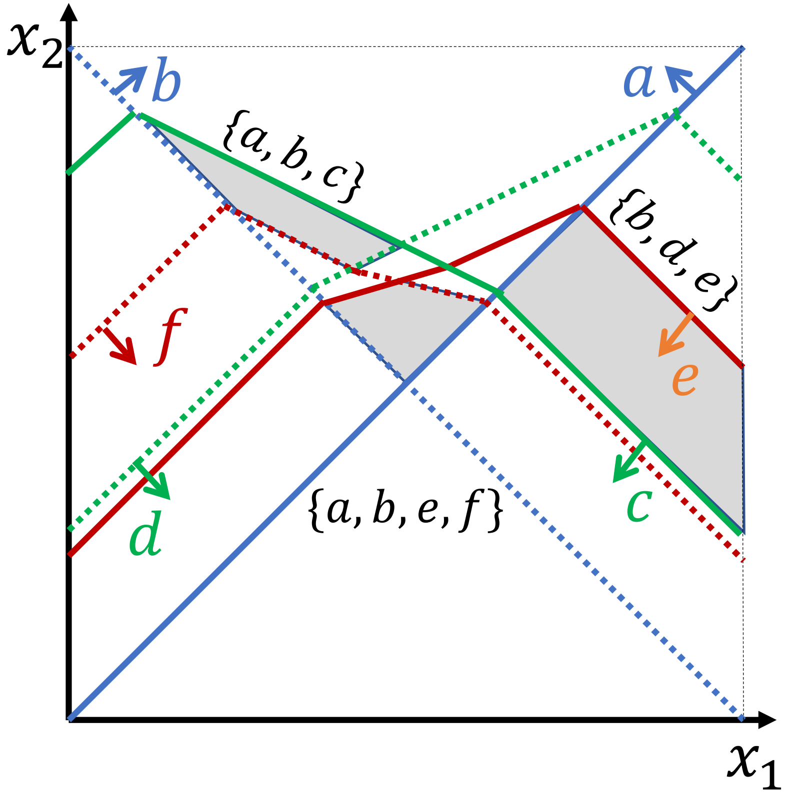


Hyperplanes partitioning the regions of previous layers



Linear regions on the original input space

Small changes in parameters produce small changes in output for sigmoid neurons

(small change in parameters)

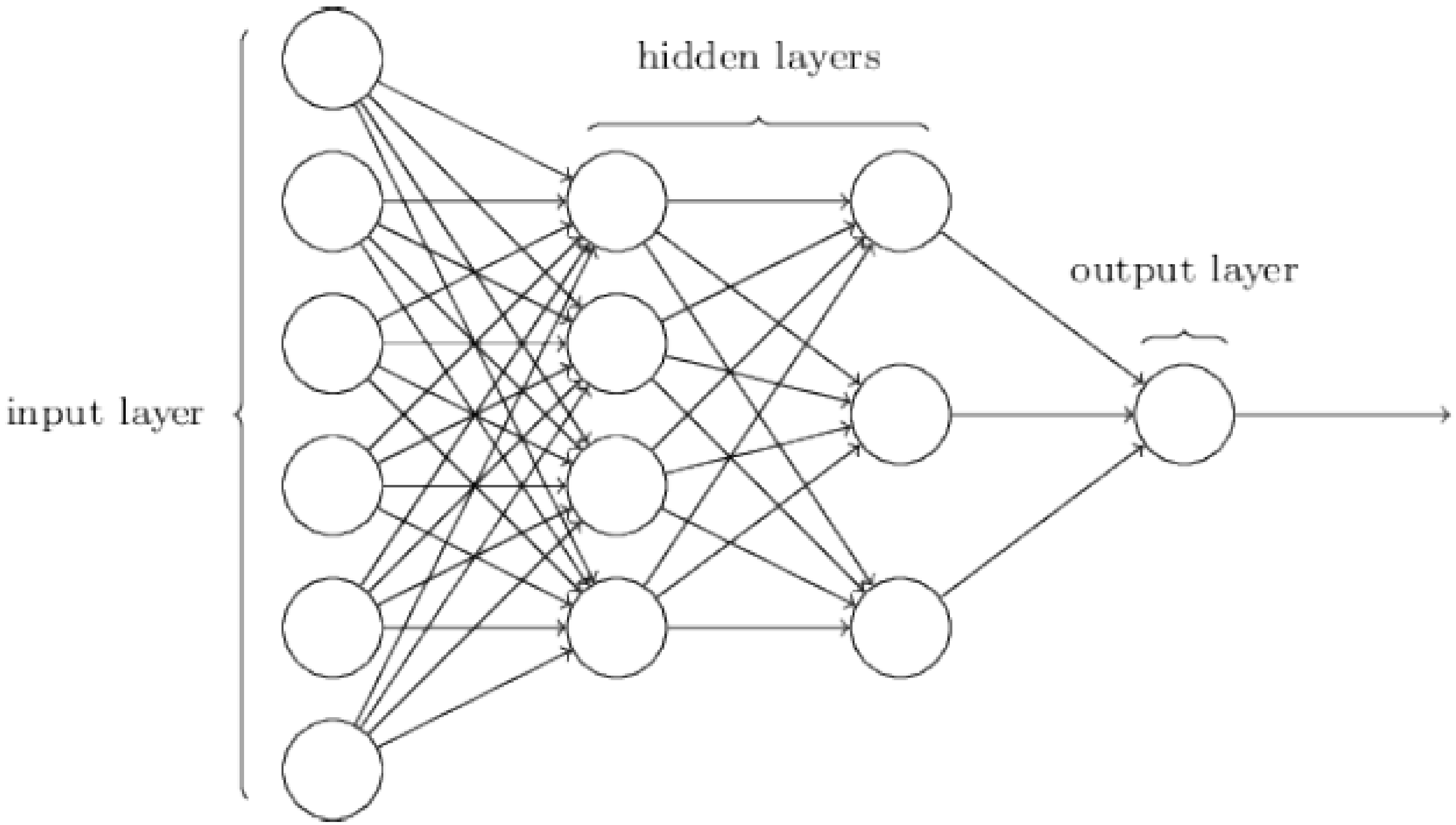
$$\Delta \text{output} \approx \sum_j \frac{\partial \, \text{output}}{\partial w_j} \Delta w_j + \frac{\partial \, \text{output}}{\partial b} \Delta b$$

(small change in output)

(partial derivatives)

- $\Delta output$ is approx. a linear function in small changes in weights and bias terms.
- Not for perceptrons!
    - The outputs flip from 0 to 1 or vice versa for small change in inputs.

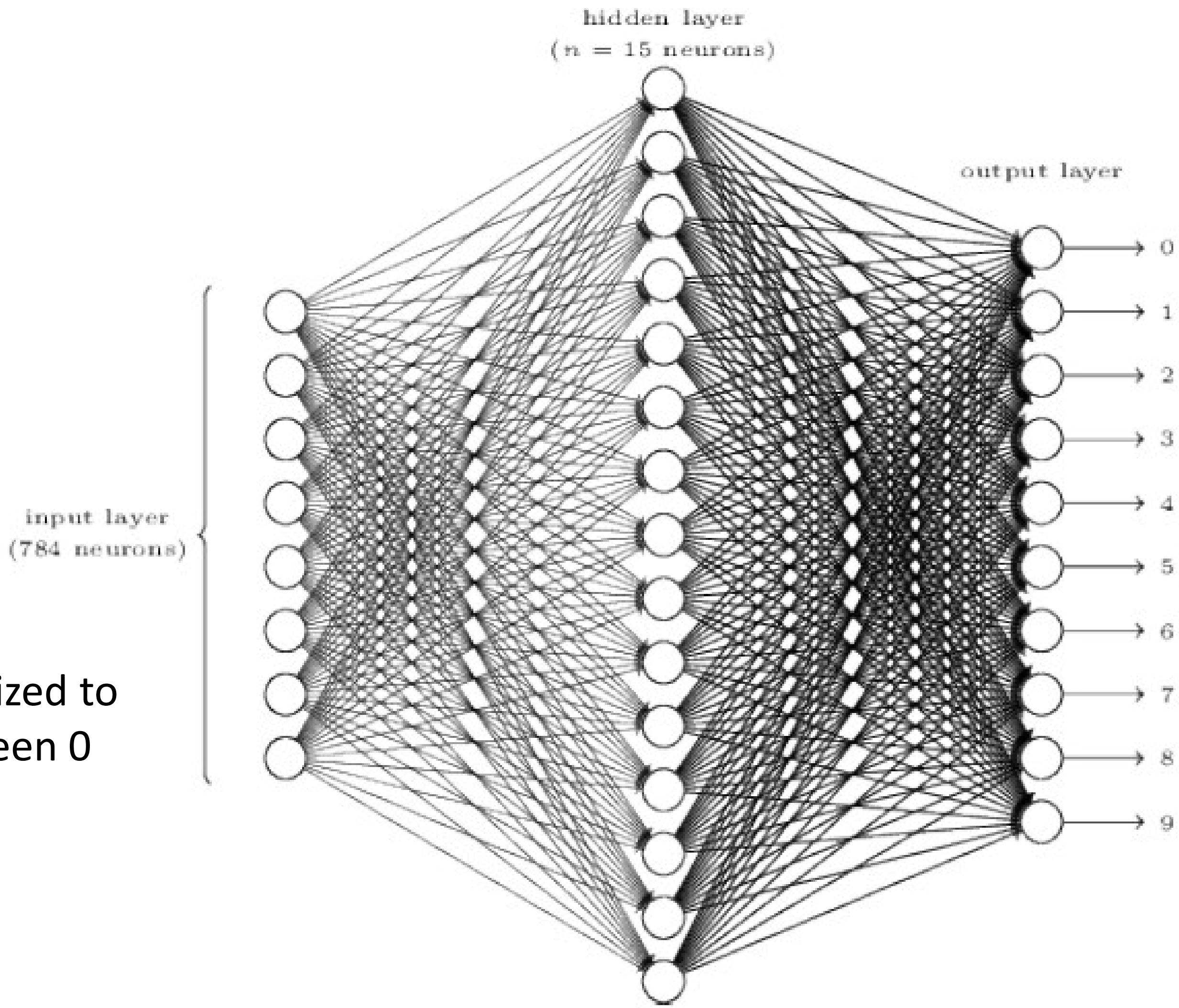
The architecture of neural networks



MNIST data

- Each grayscale image is of size 28x28.
- 60,000 training images and 10,000 test images
- 10 possible labels (0,1,2,3,4,5,6,7,8,9)

Digit recognition using 3 layers

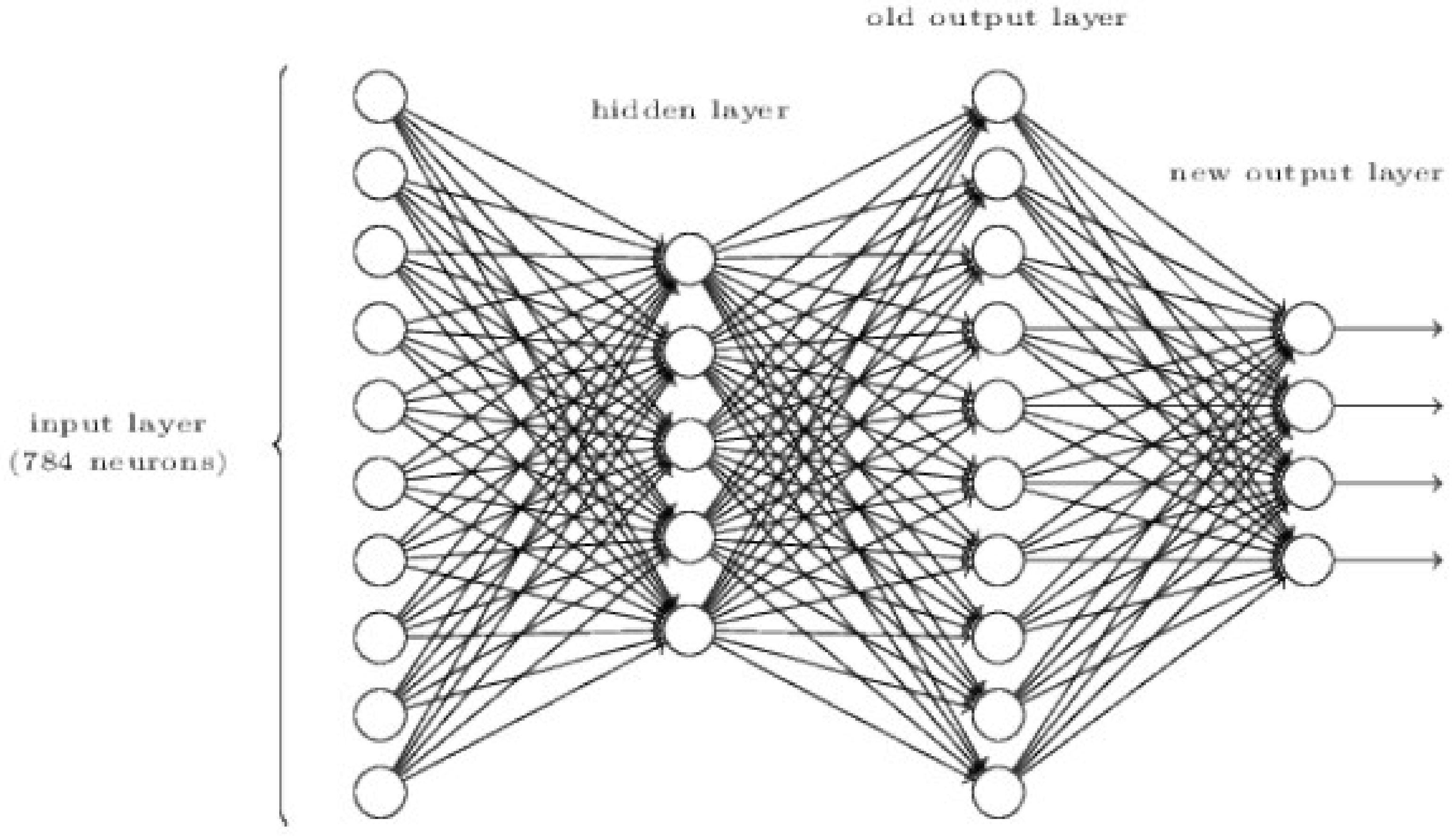


Input normalized to a value between 0 and 1.

Example outputs:

6 ->
[0 0 0 0 0 0 1 0 0 0]’

Compute the weights and biases for the last layer

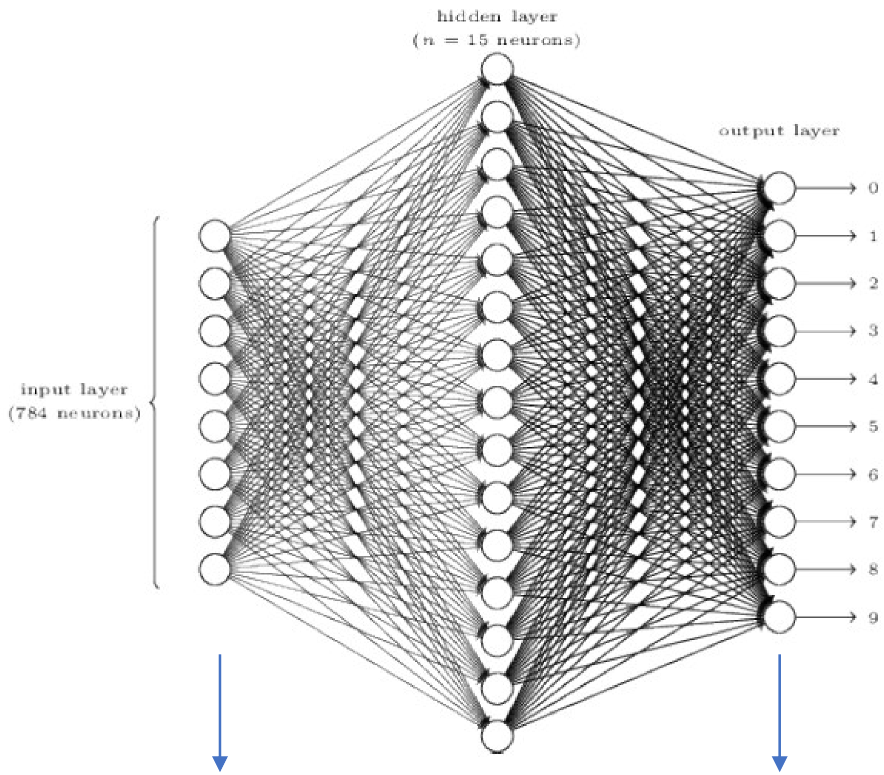


Cost function

$$C(w,b) \equiv \frac{1}{2n} \sum_x \|y(x) - a\|^2$$

parameters to compute

# of input samples



input -> x

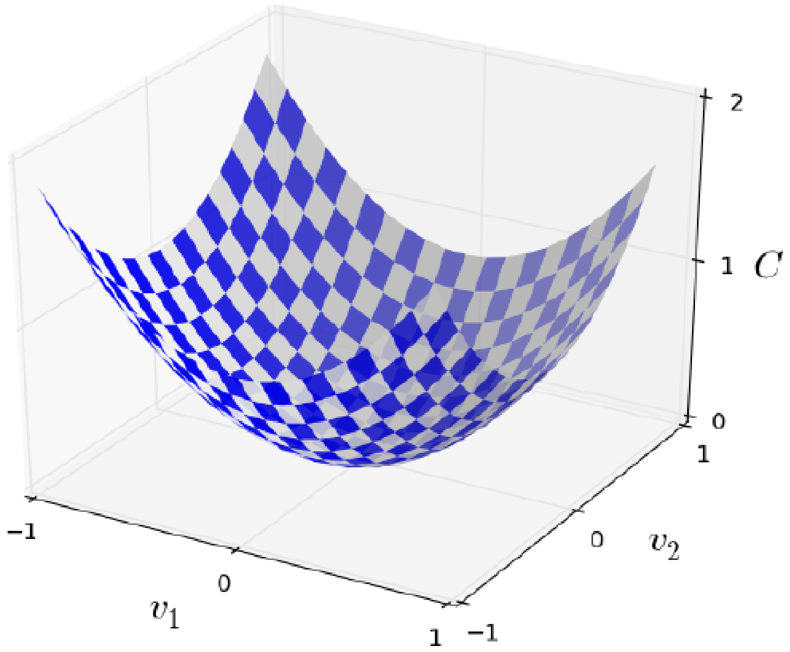
vector output -> a

- We assume that the network approximates a function $y(x)$ and outputs a.
- We use a quadratic cost function, i.e., mean squared error or MSE.

Cost function

- Can the cost function be negative in the above example?
- What does it mean when the cost is approximately equal to zero?

Gradient Descent



$$\Delta C \approx \frac{\partial C}{\partial v_1}\Delta v_1 + \frac{\partial C}{\partial v_2}\Delta v_2$$

Small changes in parameters to leads to small changes in output

$$\nabla C \equiv \left(\frac{\partial C}{\partial v_1}, \frac{\partial C}{\partial v_2}\right)^T$$

Gradient vector!

$$\Delta v = -\eta \nabla C$$

Change the parameter using learning rate (positive) and gradient vector!

$$v \rightarrow v' = v - \eta \nabla C$$

Update rule!

- Let us consider a cost function $C(v_1, v_2)$ that depends on two variables.
- The goal is to change the two variables to minimize the cost function.

Cost function from the network

$$C(w,b) \equiv \frac{1}{2n} \sum_x \|y(x) - a\|^2$$

parameters to compute

# of input samples

$$w_k \rightarrow w'_k = w_k - \eta \frac{\partial C}{\partial w_k}$$

$$b_l \rightarrow b'_l = b_l - \eta \frac{\partial C}{\partial b_l}$$

What are the challenges in gradient descent when you have a large number of training samples?

$\nabla C = \frac{1}{n} \sum_x \nabla C_x$ Gradient from a set of training samples.

Stochastic gradient descent

- The idea is to compute the gradient using a small set of randomly chosen training data.
- We assume that the average gradient obtained from the small set is close to the gradient obtained from the entire set.

Stochastic gradient descent

$$\frac{\sum_{j=1}^{m} \nabla C_{X_j}}{m} \approx \frac{\sum_x \nabla C_x}{n} = \nabla C$$

- Let us consider a mini-batch with m randomly chosen samples.

- Provided that the sample size is large enough, we expect the average gradient from the m samples is approximately equal to the average gradient from all the n samples.

Thank You

DERIVATIVE RULES

$$\frac{d}{dx}\left(x^n\right) = nx^{n-1}$$

$$\frac{d}{dx}\left(a^x\right) = \ln a \cdot a^x$$

$$\frac{d}{dx}\left(f(x)\cdot g(x)\right) = f(x)\cdot g'(x) + g(x)\cdot f'(x)$$

$$\frac{d}{dx}\left(\frac{f(x)}{g(x)}\right) = \frac{g(x)\cdot f'(x) - f(x)\cdot g'(x)}{\left(g(x)\right)^2}$$

$$\frac{d}{dx}\left(f(g(x))\right) = f'(g(x))\cdot g'(x)$$

$$\frac{d}{dx}\left(\ln x\right) = \frac{1}{x}$$

$$\frac{d}{dx}\left(\sin x\right) = \cos x$$

$$\frac{d}{dx}\left(\cos x\right) = -\sin x$$

$$\frac{d}{dx}\left(\tan x\right) = \sec^2 x$$

$$\frac{d}{dx}\left(\cot x\right) = -\csc^2 x$$

$$\frac{d}{dx}\left(\sec x\right) = \sec x \tan x$$

$$\frac{d}{dx}\left(\csc x\right) = -\csc x \cot x$$

$$\frac{d}{dx}\left(\arcsin x\right) = \frac{1}{\sqrt{1-x^2}}$$

$$\frac{d}{dx}\left(\arctan x\right) = \frac{1}{1+x^2}$$

$$\frac{d}{dx}\left(\operatorname{arc\,sec} x\right) = \frac{1}{x\sqrt{x^2-1}}$$

$$\frac{d}{dx}\left(\sinh x\right) = \cosh x$$

$$\frac{d}{dx}\left(\cosh x\right) = \sinh x$$

Source: http://math.arizona.edu/~calc/Rules.pdf

INTEGRAL RULES

$$\int x^n dx = \frac{1}{n+1} x^{n+1} + c, \quad n \neq -1$$

$$\int a^x dx = \frac{1}{\ln a} a^x + c$$

$$\int \frac{1}{x} dx = \ln|x| + c$$

$$\int \frac{dx}{\sqrt{1-x^2}} = \arcsin x + c$$

$$\int \frac{dx}{1+x^2} = \arctan x + c$$

$$\int \frac{dx}{x\sqrt{x^2-1}} = \operatorname{arc}\sec x + c$$

$$\int \sin x dx = -\cos x + c$$

$$\int \cos x dx = \sin x + c$$

$$\int \sec^2 x dx = \tan x + c$$

$$\int \sinh x dx = \cosh x + c$$

$$\int \csc^2 x dx = -\cot x + c$$

$$\int \sec x \tan x dx = \sec x + c$$

$$\int \csc x \cot x dx = -\csc x + c$$

$$\int \cosh x dx = \sinh x + c$$

Source: http://math.arizona.edu/~calc/Rules.pdf