Artificial Neural Networks II

COMPCSI 361

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Adapted from: Meng-Fen Chiang

WEEK 11

OUTLINE

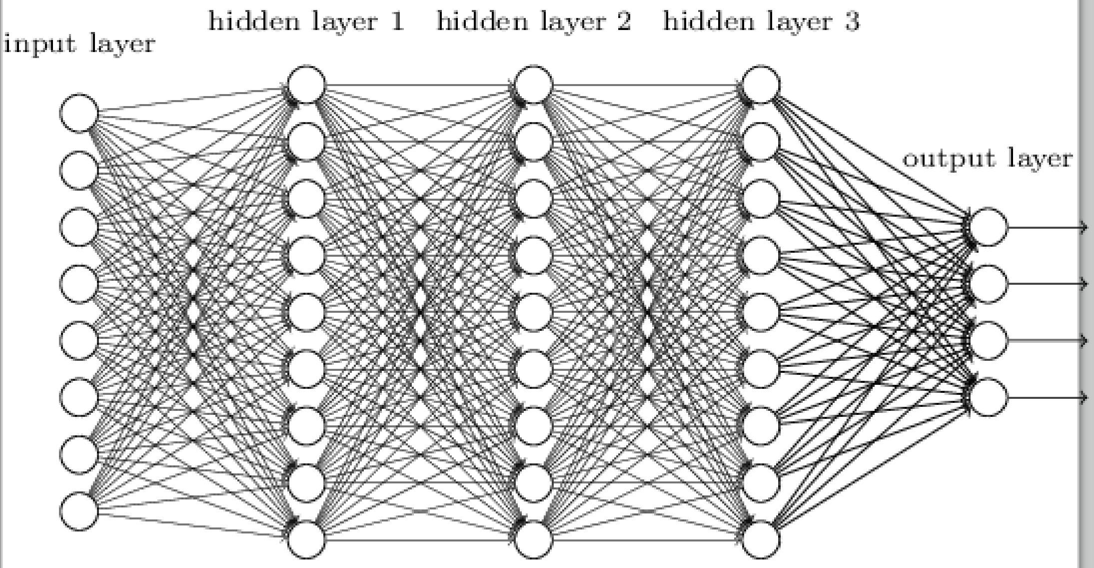
Introduction

Artificial Neural Networks (ANN)

- Single Unit: Architecture of Perceptron (NN1)
- Connection to Shallow Machine Learning (NN1)
- Multi-Layer Feed-Forward Neural Network (NN2)

Design Issues (NN3)

Deep Learning / Large Language Models (NN4)

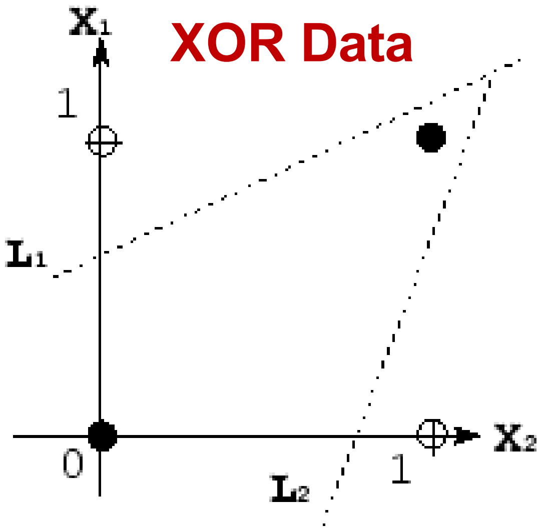


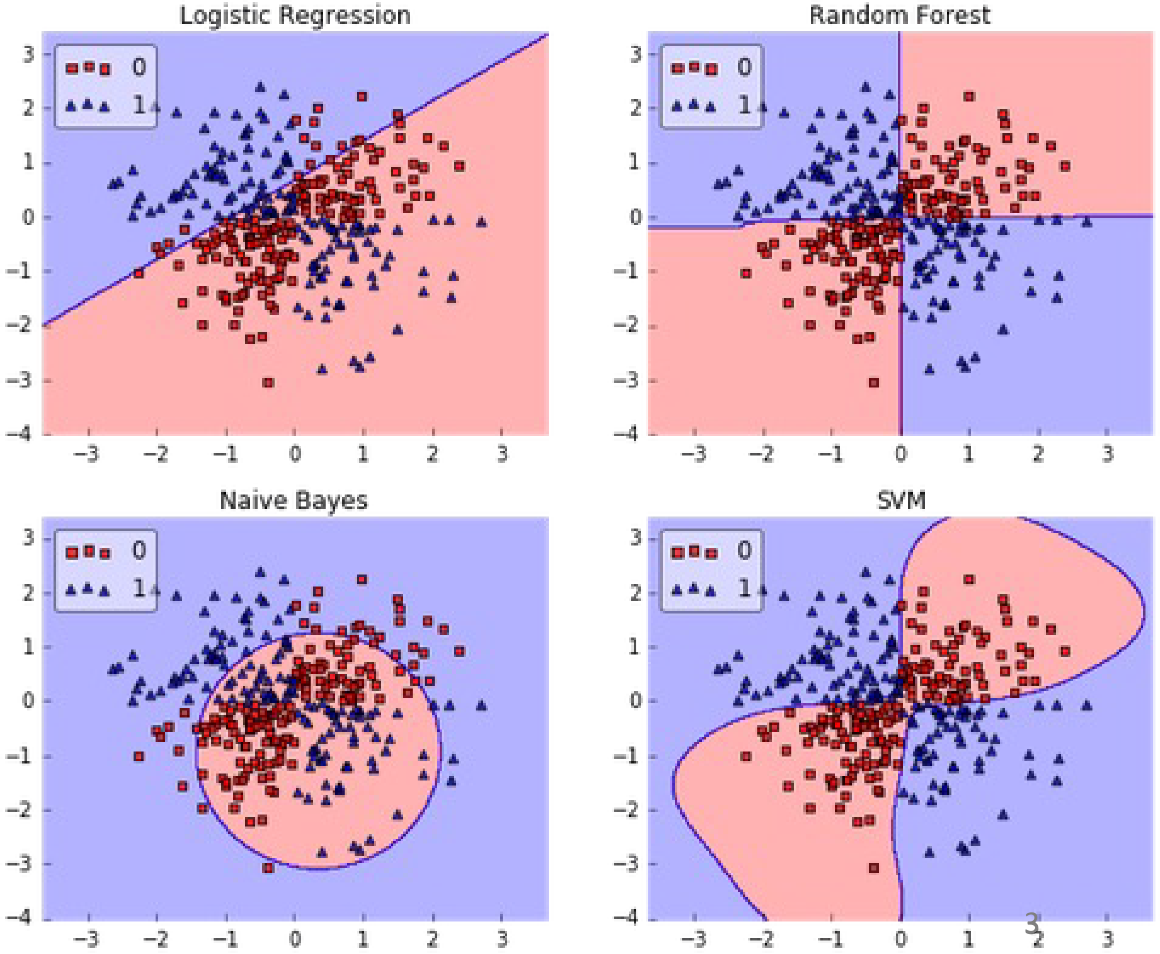
Non-Linearly Separable Data (XOR Data)

- Perceptron learning algorithm will fail because no linear hyperplane can separate the data perfectly

X_1	X_2	Y
0	0	0
0	1	1
1	0	1
1	1	0

$$Y = X_1 \oplus X_2$$





Source: https://sebastianraschka.com/faq/docs/clf-behavior-data.html

Multi-Layer Feed-Forward Neural Network (FFN)

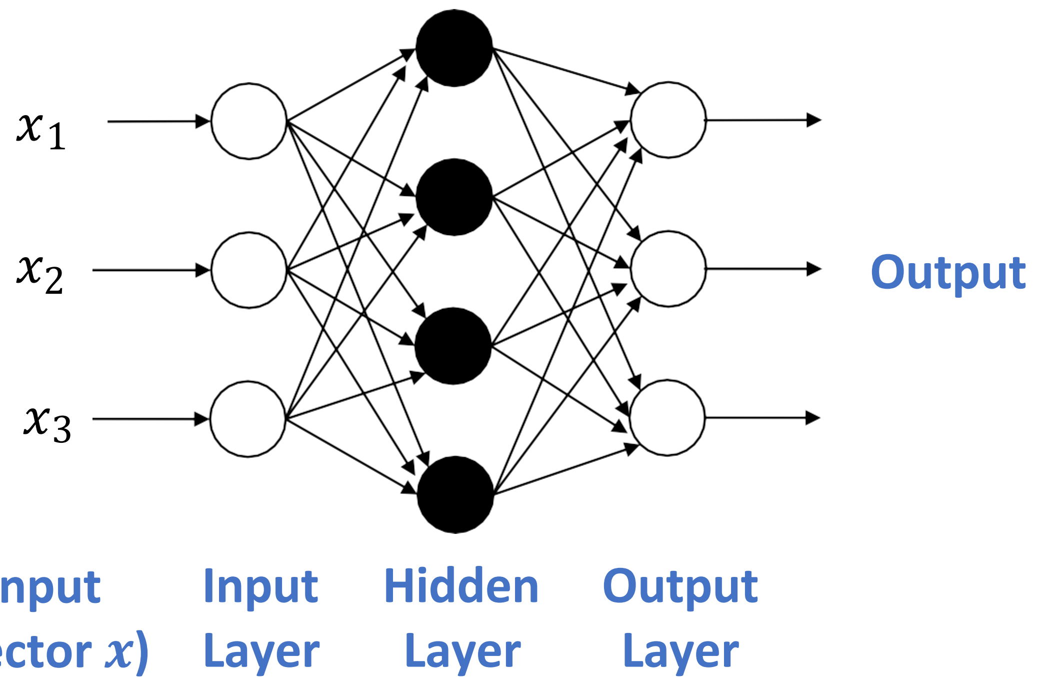
Architecture: A **two-layer** network

Activation Function:

- g : Nonlinear transformation
- e.g. sigmoid transformation

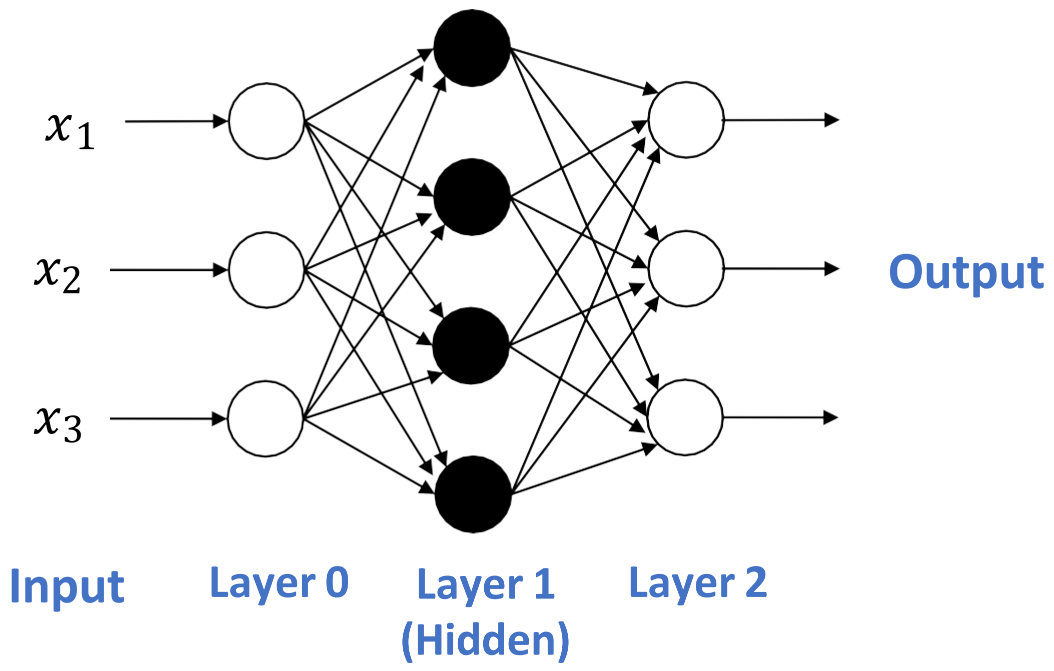
Hidden Layer: $\boldsymbol{h} = \mathrm{g}(W^{(1)}x + b^{(1)})$

Output Layer: $\boldsymbol{o} = \mathrm{g}(\underbrace{W^{(2)}}_{\text{Weight Matrix}}\boldsymbol{h} + \underbrace{b^{(2)}}_{\text{Bias Term}})$



Multi-Layer (FF) Neural Network

- The **inputs** to the network correspond to the attributes measured for each training tuple
- Inputs are then weighted and fed simultaneously to a hidden layer
- The number of hidden layers is arbitrary
- The network is **feed-forward**: None of the weight cycles back to an input unit or to an output unit of a previous layer



Multi-Layer Neural Network

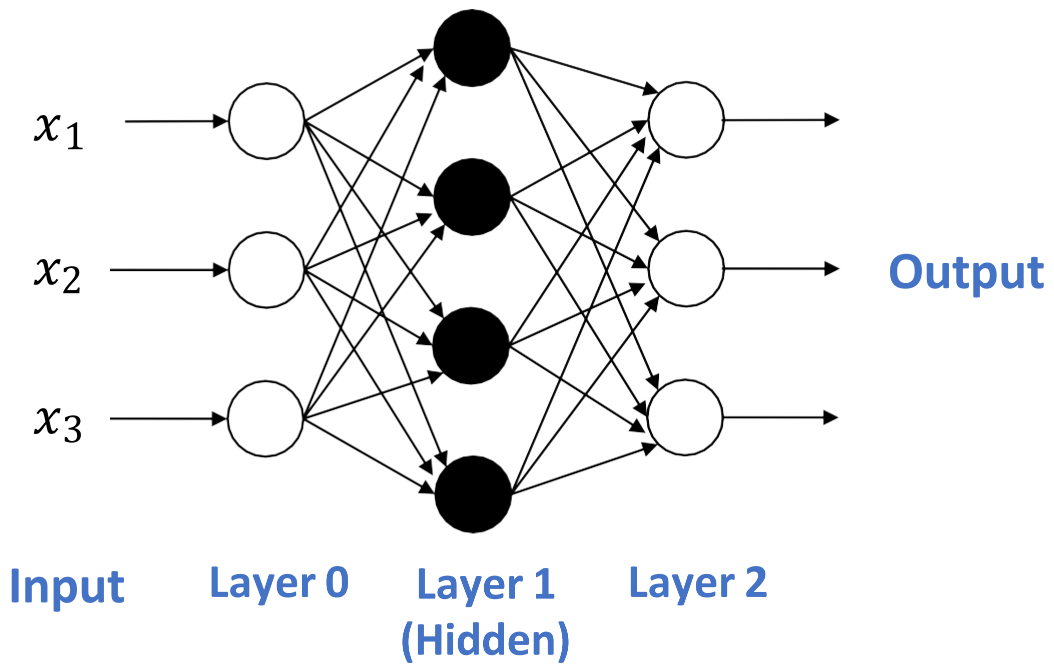
- Every node in a **hidden layer** operates on activations from preceding layer and transmits activations forward to nodes of next layer

$$\boldsymbol{h} = \mathrm{g}(\underbrace{W^{(1)}\,x + b^{(1)}}_{\text{Linear Predictor}})$$

Activation Value

Activation Function

- Networks perform **non-linear regression**: Given enough hidden units and enough training samples, they can closely approximate any continuous function

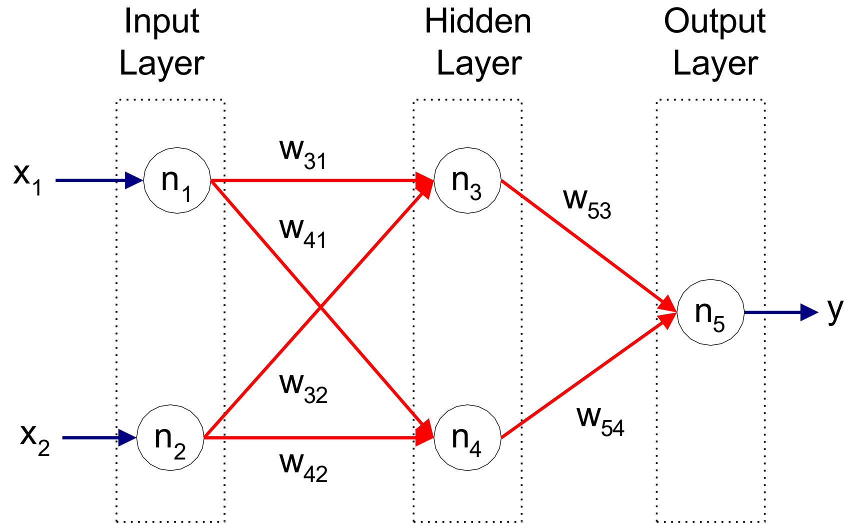


Multiple Layer Neural Network

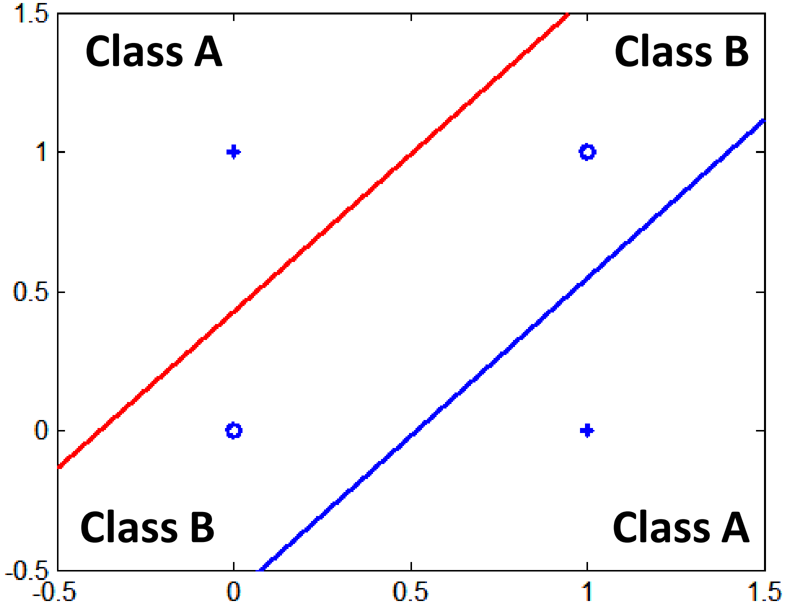
- Given a set of training data $S = ((x^{(1)}, y^{(1)}), \dots, (x^{(\mathrm{n})}, y^{(\mathrm{n})}))$
- $y^{(\mathrm{i})}$ is categorical: classification task (multi-class or binary)
- $y^{(\mathrm{i})}$ is continuous: regression task
- Goal: Find $\boldsymbol{w}$, such that minimize the empirical risk is minimized
- Solution: Stochastic gradient descent (SGD) + chain rule = Backpropagation

Example: XOR Problem

- With at least one hidden layer + non-linear activation function, multi-layer FFN can solve classification task involving nonlinear decision surfaces



Decision Surface: node n_3



Decision Surface: node n_4

Universal Function Approximation Theorem

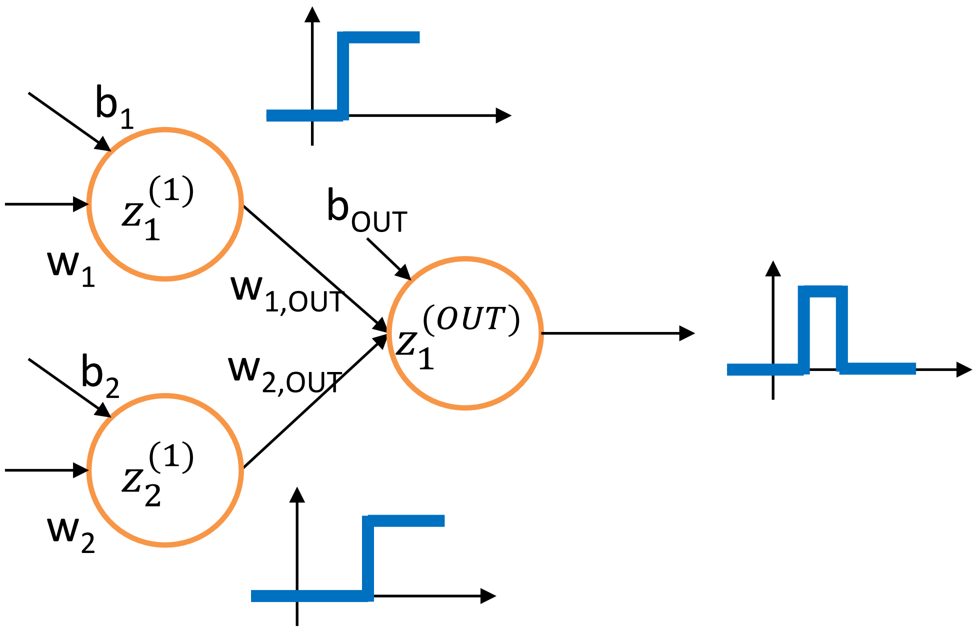
Hornik theorem 1: Whenever the activation function is *bounded and nonconstant*, then, for any finite measure μ, standard multilayer feedforward networks can approximate any function in $L^p(\mu)$ (the space of all functions on R^k such that $\int_{R^k} |f(x)|^p d\mu(x) < \infty$) arbitrarily well, provided that sufficiently many hidden units are available.

Hornik theorem 2: Whenever the activation function is *continuous, bounded and nonconstant*, then, for arbitrary compact subsets $X \subseteq R^k$, standard multilayer feedforward networks can approximate any continuous function on X arbitrarily well with respect to uniform distance, provided that sufficiently many hidden units are available.

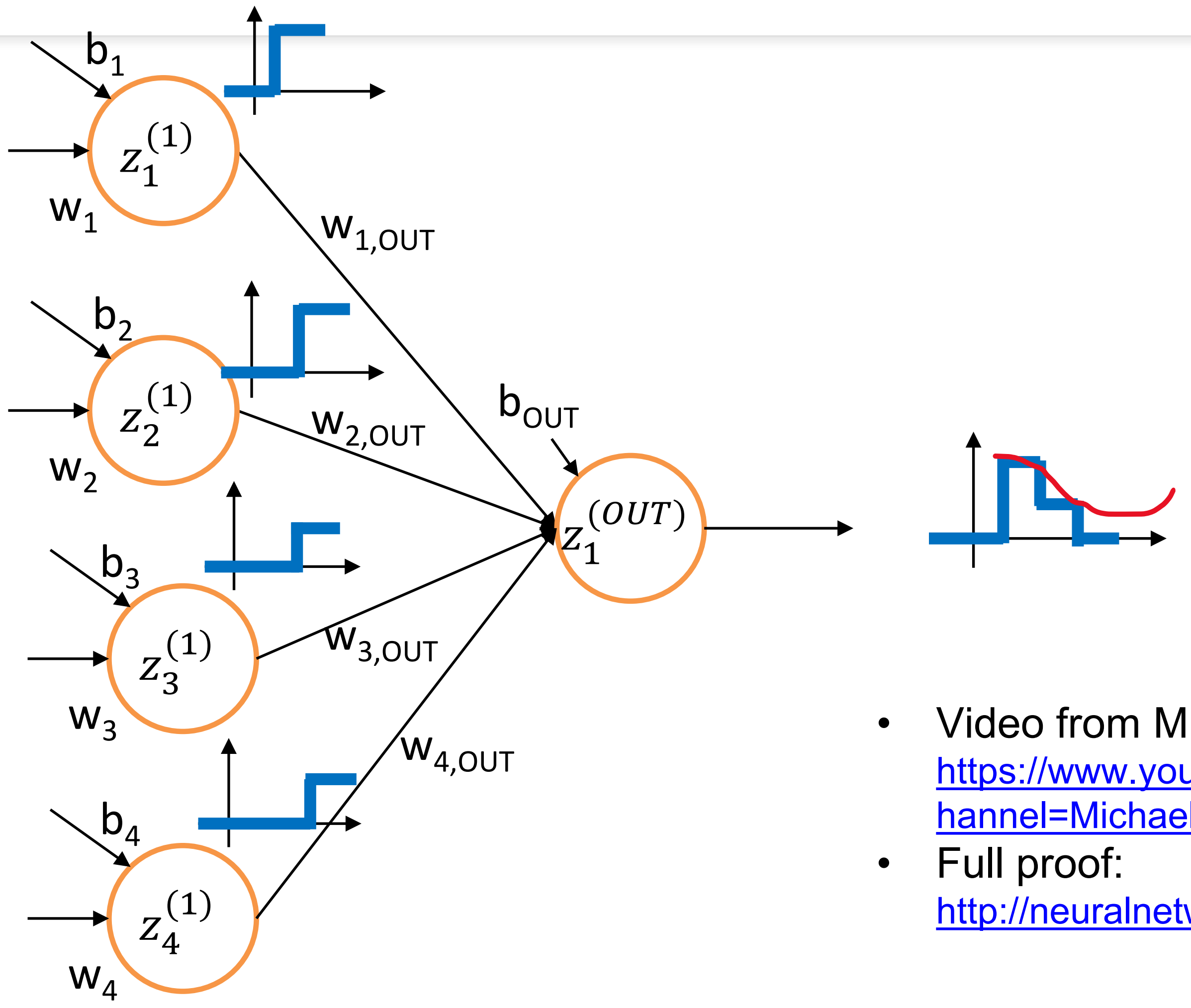
<u>In summary:</u> Given any continuous function f(x), if a 2-layer neural network has enough hidden units, then there is a choice of weights that allow it to closely approximate f(x).

Cybenko (1989) "Approximations by superpositions of sigmoidal functions"
Hornik (1991) "Approximation Capabilities of Multilayer Feedforward Networks"
Leshno and Schocken (1991) "Multilayer Feedforward Networks with Non-Polynomial Activation Functions Can Approximate Any Function"

Intuition for the theorem



Intuition for the theorem

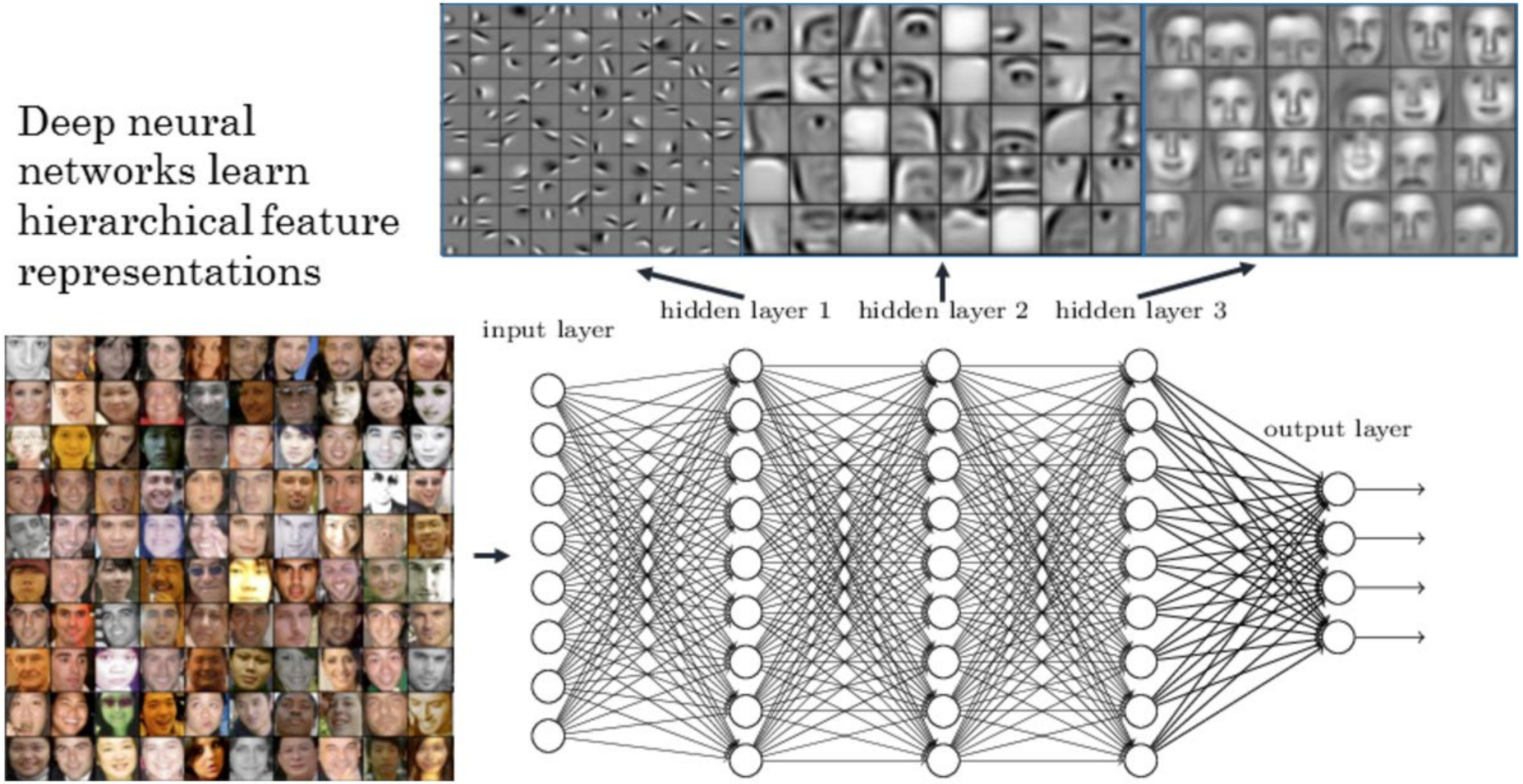


- Video from Michael Nielsen: https://www.youtube.com/watch?v=Ijqkc7OLenI&ab_channel=MichaelNielsen
- Full proof: http://neuralnetworksanddeeplearning.com/chap4.html

Multiple Hidden Layers

- Activations at hidden layers can be viewed as features extracted as functions of inputs
- Every **hidden** layer represents a level of abstraction
  - Complex features are compositions of simpler features
- Number of layers is the depth of ANN → Deeper networks express complex hierarchy of features

Multiple Hidden Layers



Le Cun et al. (2015)
Raphael et al. (2019)

Capability of Neural Network

- M_1: 0 hidden layer + linear activation function → linear surface
- M_2: 0 hidden layer + non-linear activation function → linear surface (LR)
- M_3: 1 hidden layer + linear activation function → combination of linear surface
- M_4: 1 hidden layer + non-linear activation function → non-linear surface (MLP)

Training: Backpropagation

- Iteratively process a set of training tuples & compare the network's prediction with the actual known target value

- **Loss Function.** For each training tuple, the **weights** are modified to **minimize the loss** between the network's prediction and the actual target value, say mean squared error

- Stochastic gradient descent + chain rule = Backpropagation
  - Modifications are made in the “backwards” direction
  - From the **output layer**, through each **hidden layer** down to the **first hidden layer**, hence “backpropagation”

RECAP: (1) Chain Rule (2) Gradient Descent

- **The Chain Rule**: if f and g are both differentiable and $F(x) = f \circ g$ is the composite function defined by $F(\ x)= f(g(x))$, then F is differentiable and F' is given by the product:

$$F'(x) = f'(g(\mathrm{x}))\, g'(\mathrm{x})$$

In Leibniz notation, if $y = f(u)$ and $u = g(x)$ are both differentiable functions, then

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$

- **Gradient descent**: Update parameters in the direction of "maximum descent" in the loss function across all points
- **Stochastic gradient descent (SGD):** update the weight for every instance
- **Mini-batch SGD**: update over min-batches of instances

Source: https://en.wikipedia.org/wiki/Chain_rule

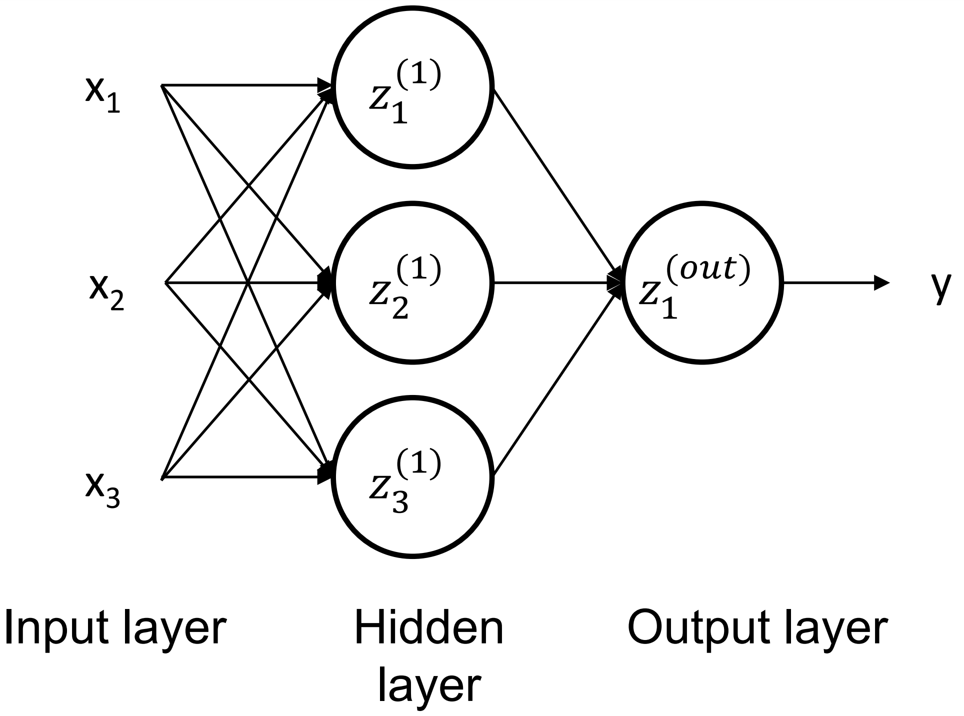
Training: Backpropagation

- For each training instance:

   1. **Make a prediction (forward pass/propagation)**
   2. Measure the error/loss
   3. **Go through each layer in reverse to measure the error contribution from each connection (backward pass/propagation)**
   4. Slightly tweak the connection weights to reduce the error (SGD step)

Until stopping criterion is reached

Backpropagation example step by step



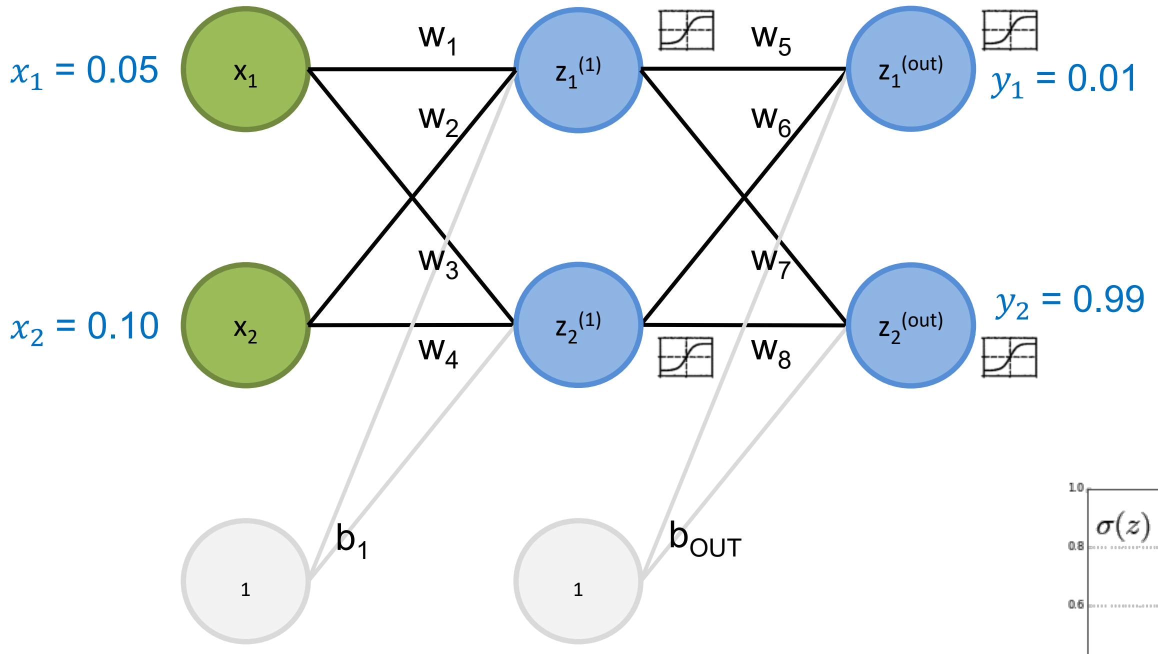
$$out\_z_i^{(k)} = \mathrm{g}\left(in\_z_i^{(k)}\right)$$

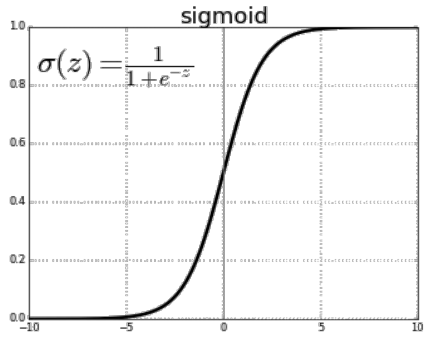
$$in\_z_i^{(k)} = \sum_j w_{i,j}^{(k-1,k)} out\_z_j^{(k-1)}$$

$in\_z_i^{(k)}$ is the input of neuron i in layer k (after input function)

$out\_z_i^{(k)}$ is the output of neuron i in layer k (after activation)

Backpropagation example step by step

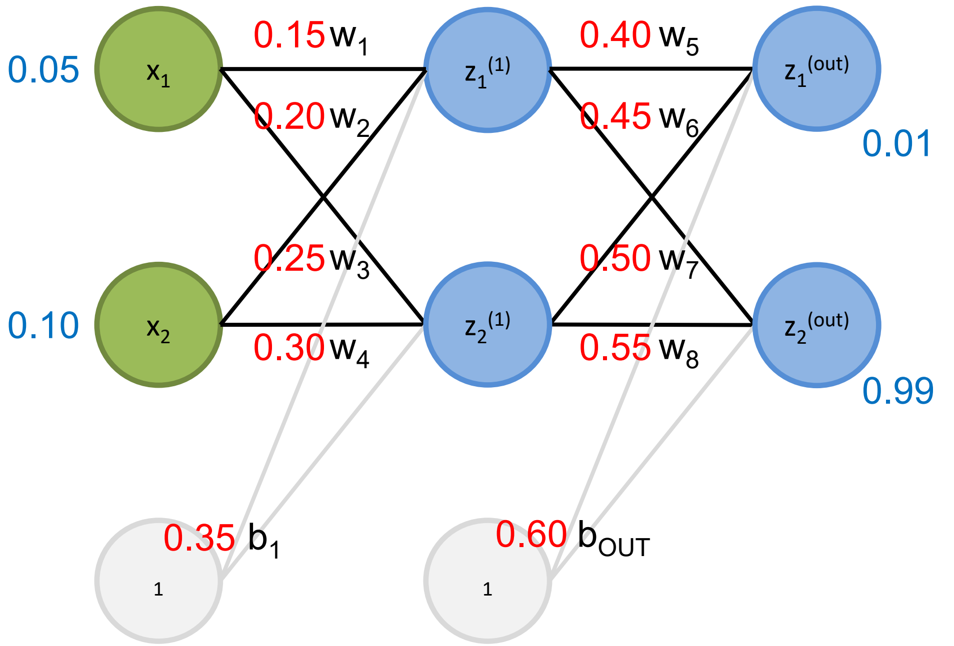




https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Backpropagation example step by step

- Initialisation of the weights



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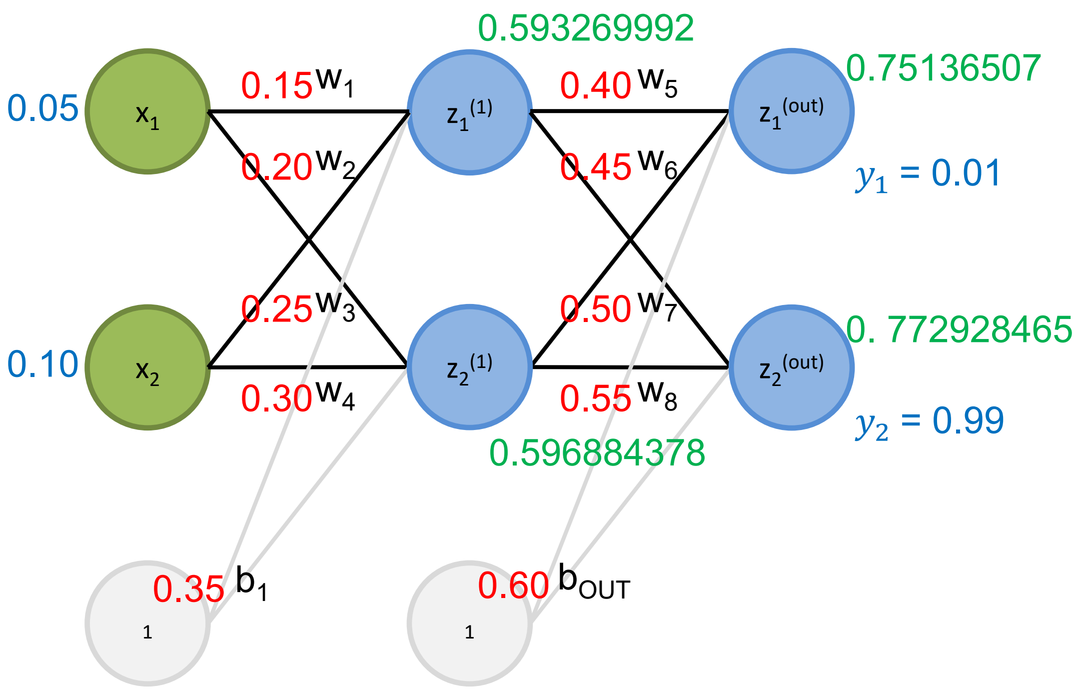
Backpropagation example step by step

- Forward propagation



$$out\_z_1^{(1)} = S(\underbrace{w_1 * x_1 + w_2 * x_2 + b_1 * 1}_{in\_z_1^{(1)}})$$
$$= S(0.15 * 0.05 + 0.20 * 0.10 + 0.35 * 1)$$
$$= S(0.3775)$$
$$= 0.593269992$$

$$out\_z_2^{(1)} = S(\underbrace{w_3 * x_1 + w_4 * x_2 + b_1 * 1}_{in\_z_2^{(2)}})$$
$$= S(0.25 * 0.05 + 0.30 * 0.10 + 0.35 * 1)$$
$$= 0.596884378$$

$$out\_z_1^{(out)} = S(\underbrace{w_5 * out\_z_1^{(1)} + w_6 * out\_z_2^{(1)} + b_{OUT} * 1}_{in\_z_1^{(out)}})$$
$$= 0.75136507$$

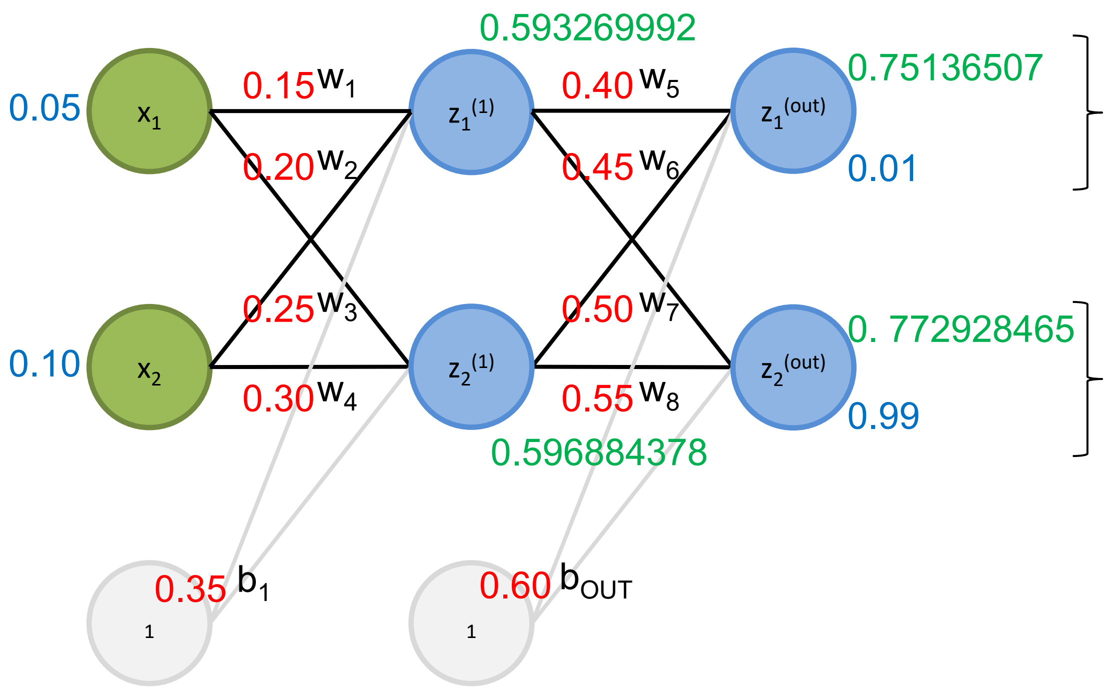
$$out\_z_1^{(out)} = S(\underbrace{w_7 * out\_z_1^{(1)} + w_8 * out\_z_2^{(1)} + b_{OUT} * 1}_{in\_z_2^{(out)}})$$
$$= 0.772928465$$

https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Backpropagation example step by step

- Calculating the total error

$$E(y,\hat{y}) = \frac{1}{2}||y-\hat{y}||^2$$



$$E_{z_1^{(out)}} = \frac{1}{2}(0.01 - 0.75136507)^2 = 0.274811083$$

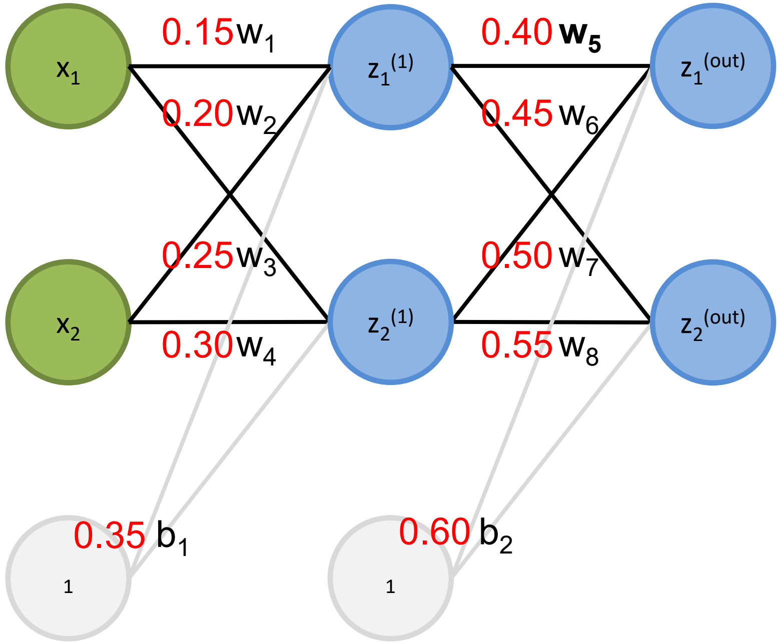
$$E_{z_2^{(out)}} = \frac{1}{2}(0.99 - 0.772928465)^2 = 0.023560026$$

$$E_{tot^{(out)}} = E_{z_1^{(out)}} + E_{z_2^{(out)}} = 0.298371109$$

https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Backpropagation example step by step

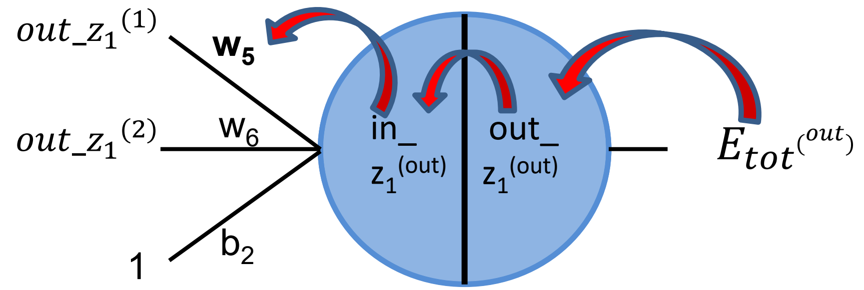
- Back propagation (output layer)



$\mathbf{w_5}$ influence on $E_{tot}{}^{(out)}$? $\frac{\partial E_{tot}{}^{(out)}}{\partial \mathrm{w}_5}$

Chain rule:

$$\frac{\partial E_{tot}{}^{(out)}}{\partial \mathrm{w}_5} = \frac{\partial E_{tot}{}^{(out)}}{\partial out\_z_1{}^{(out)}} * \frac{\partial out\_z_1{}^{(out)}}{\partial in\_z_1{}^{(out)}} * \frac{\partial in\_z_1{}^{(out)}}{\partial \mathrm{w}_5}$$



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Backpropagation example step by step

- Back propagation (output layer)

$$\frac{\partial E_{tot}{}^{(out)}}{\partial W_5} = \frac{\boldsymbol{\partial E_{tot}{}^{(out)}}}{\boldsymbol{\partial out\_z_1{}^{(out)}}} * \frac{\partial out\_z_1{}^{(out)}}{\partial in\_z_1{}^{(out)}} * \frac{\partial in\_z_1{}^{(out)}}{\partial W_5}$$

$$E_{tot}{}^{(out)} = E_{z_1}{}^{(out)} + E_{z_2}{}^{(out)}$$
$$= \frac{1}{2}\left(y_1 - out\_z_1{}^{(out)}\right)^2 + \frac{1}{2}\left(y_2 - out\_z_2{}^{(out)}\right)^2$$

$$\frac{\boldsymbol{\partial E_{tot}{}^{(out)}}}{\boldsymbol{\partial out\_z_1{}^{(out)}}} = 2 * \frac{1}{2}\left(y_1 - out_{z_1{}^{(out)}}\right)^{2-1} * -1 + 0$$
$$= out_{z_1{}^{(out)}} - target_{z_1{}^{(out)}}$$
$$= 0.75136507 - 0.01$$
$$= 0.74136507$$

Backpropagation example step by step

- Back propagation (output layer)

$$\frac{\partial E_{tot}{}^{(out)}}{\partial \mathrm{W}_5} = \frac{\partial E_{tot}{}^{(out)}}{\partial out\_z_1{}^{(out)}} * \frac{\partial \boldsymbol{out\_z_1}^{(out)}}{\partial \boldsymbol{in\_z_1}^{(out)}} * \frac{\partial in\_z_1{}^{(out)}}{\partial \mathrm{W}_5}$$

$$out_{z_1{}^{(out)}} = \frac{1}{1 + e^{-in\_z_1{}^{(out)}}}$$ (activation = sigmoid function)

Sigmoid → g'(x) = g(x)(1-g(x))

$$\frac{\partial \boldsymbol{out\_z_1}^{(out)}}{\partial \boldsymbol{in\_z_1}^{(out)}} = out_{z_1{}^{(out)}} * (1 - out\_z_1{}^{(out)})$$

$$= 0.75136507 * (1 - 0.75136507)$$

$$= 0.186815602$$

https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Backpropagation example step by step

- Back propagation (output layer)

$$\frac{\partial E_{tot}{}^{(out)}}{\partial \mathrm{w}_5} = \frac{\partial E_{tot}{}^{(out)}}{\partial out\_z_1{}^{(out)}} * \frac{\partial out\_z_1{}^{(out)}}{\partial in\_z_1{}^{(out)}} * \frac{\partial \boldsymbol{in\_z_1}{}^{(out)}}{\partial \mathbf{w}_5}$$

$$\mathrm{in\_z_1}^{(out)} = \mathrm{w}_5 * \mathrm{out\_z_1}^{(1)} + \mathrm{w}_6 * \mathrm{out\_z_2}^{(1)} + \mathrm{b}_2 * 1$$

$$\frac{\partial \boldsymbol{in\_z_1}{}^{(out)}}{\partial \mathbf{w}_5} = \mathrm{out\_z_1}^{(1)} + 0 + 0$$

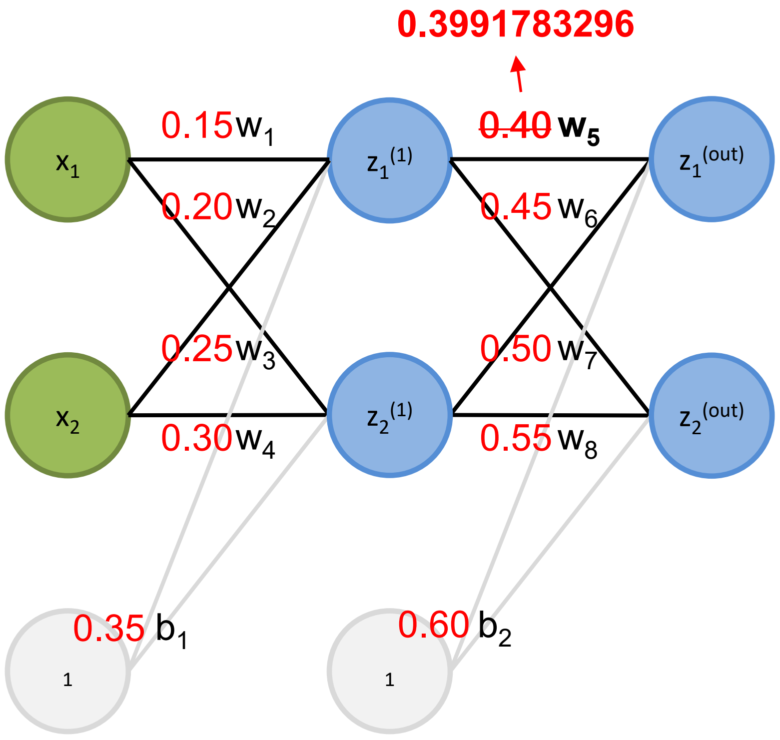
$$= \mathrm{out\_z_1}^{(1)}$$

$$= 0.593269992$$

https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Backpropagation example step by step

- Back propagation (output layer)



$$\frac{\partial E_{tot}{}^{(out)}}{\partial w_5} = \frac{\partial E_{tot}{}^{(out)}}{\partial out\_z_1{}^{(out)}} * \frac{\partial \text{out\_z}_1{}^{(\text{out})}}{\partial \text{in\_z}_1{}^{(\text{out})}} * \frac{\partial in\_z_1{}^{(out)}}{\partial w_5}$$

$$= 0.74136507 * 0.186815602 * 0.593269992$$

$$= 0.082167041$$

Gradient descent to decrease the error (with learning rate $\alpha = 0.01$) :

$$w_5 \leftarrow w_5 - \alpha * \frac{\partial E_{tot}{}^{(out)}}{\partial w_5}$$

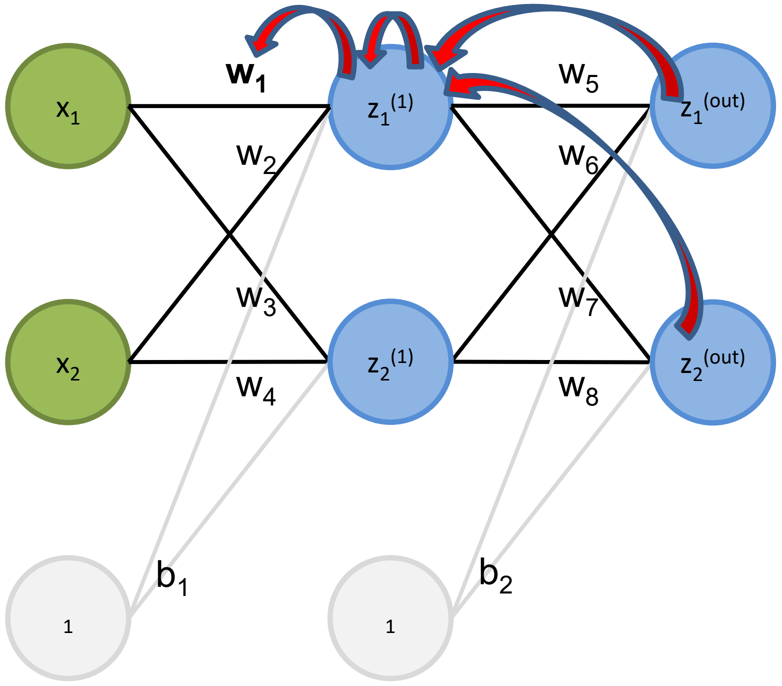
$$w_5 \leftarrow 0.40 - 0.01 * 0.082167041$$

$$w_5 \leftarrow 0.3991783296$$

https://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Backpropagation example step by step

- Backpropagation (hidden layer)



$$\frac{\partial E_{tot}{}^{(out)}}{\partial \mathbf{w_1}} = \underbrace{\frac{\partial E_{tot}{}^{(out)}}{\partial out\_z_1{}^{(1)}}} * \frac{\partial \mathrm{out\_z_1}{}^{(1)}}{\partial \mathrm{in\_z_1}{}^{(1)}} * \frac{\partial in\_z_1{}^{(1)}}{\partial \mathbf{w_1}}$$

$$\frac{\partial E_{tot}{}^{(out)}}{\partial out\_z_1{}^{(1)}} = \frac{\partial E_{z_1}{}^{(out)}}{\partial out\_z_1{}^{(1)}} + \frac{\partial E_{z_2}{}^{(out)}}{\partial out\_z_1{}^{(1)}}$$

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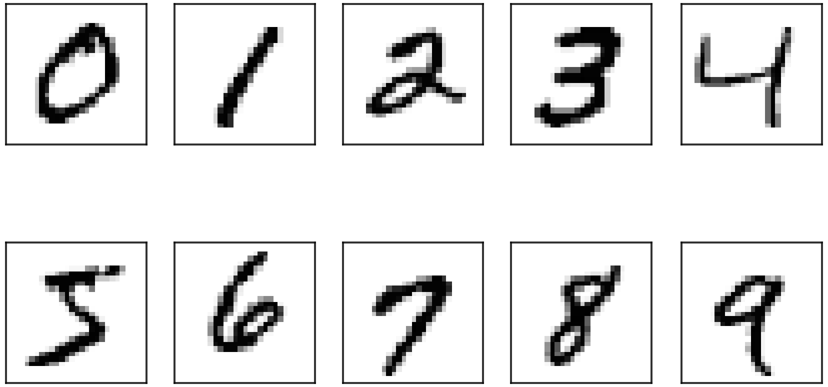


Jupyter Notebook

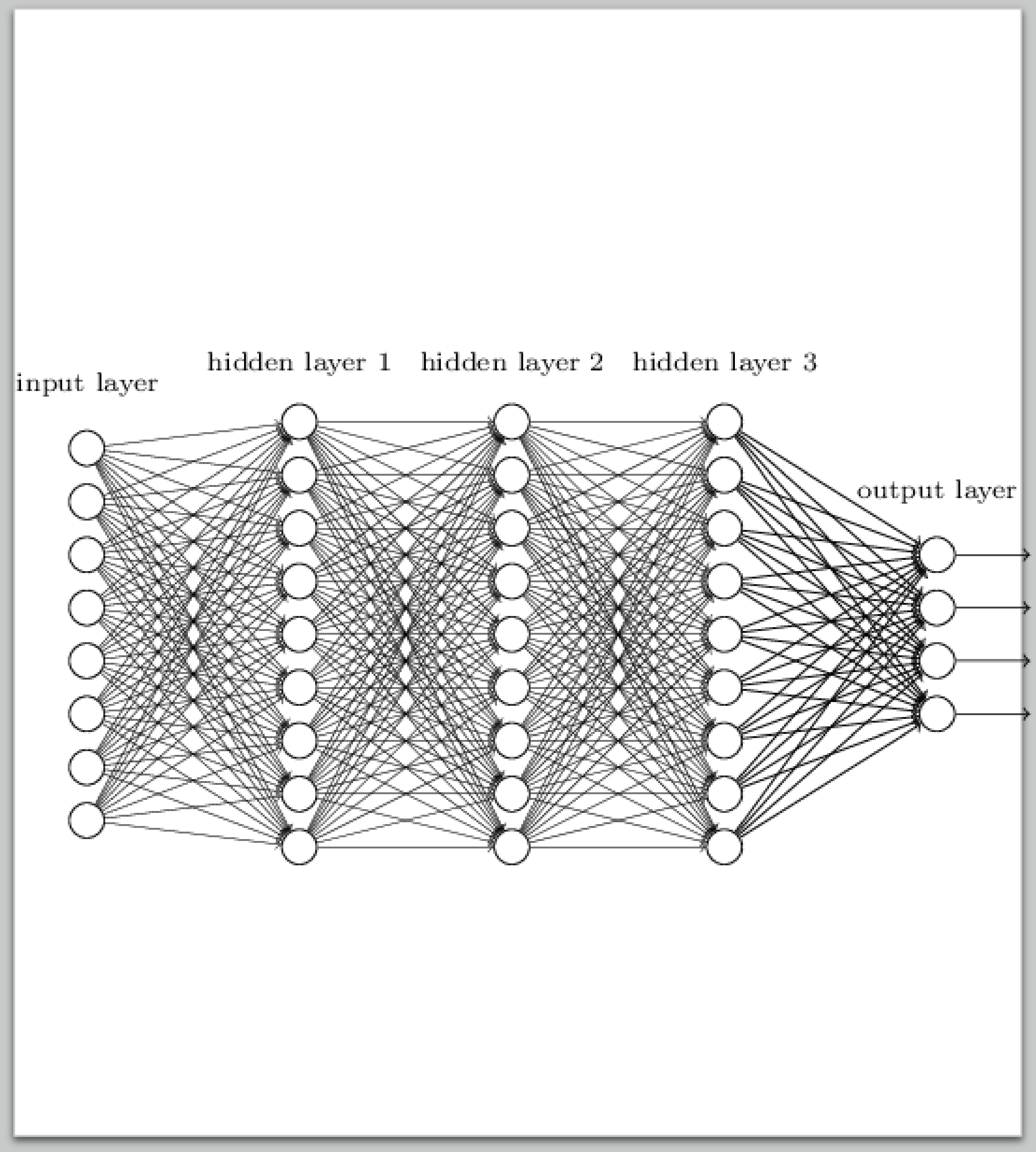
Multi-Layer Perceptron Coding Example

(Classifying Handwritten Digits)

SUMMARY

- Multi-Layer Perceptron Architecture
  - Multiple Hidden Layers
  - Nonlinear Activation Functions

- Training: Backpropagation algorithm
  - Example step by step



Resources

- Coding Libraries
  - ConvnetJS: a toy 2D classification with 2-layer neural network. [link]
  - Python Machine Learning (3rd Edition) by Sebastian Raschka at https://github.com/rasbt/python-machine-learning-book-3rd-edition

- Book Chapters
  - Chapter 6.7, 6.8 Introduction to Data Mining by Kumar et al.