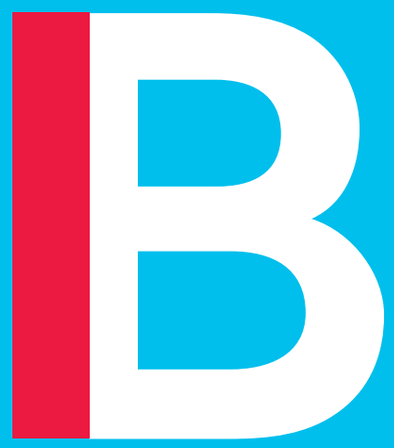
Imperial College
Business School

Imperial means
Intelligent Business

Machine Learning in Finance

Lecture 5
Introduction to Deep Learning



Arnaud de Servigny & Hachem Madmoun

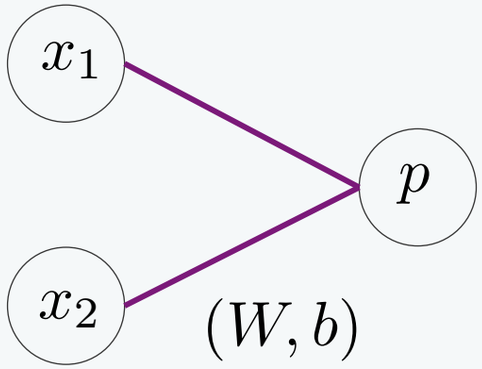
Outline:

- From Logistic Regression to Shallow Neural Networks
- Deep Neural Networks and Loss functions
- Deep Learning Techniques
- Programming Session

Part 1 : From Logistic Regression to Shallow Neural Networks

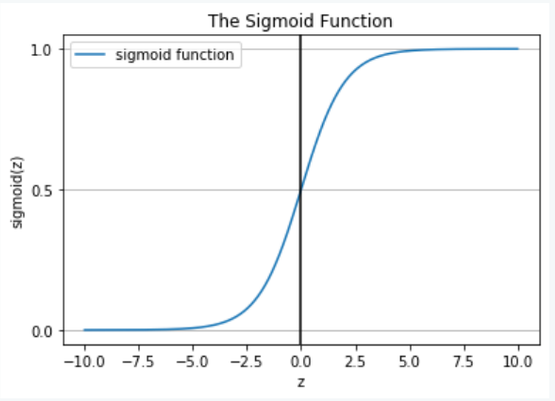
Logistic Regression

- The Logistic Regression Model predicts the probability of the positive class using the combination of linear decision function and a sigmoid function

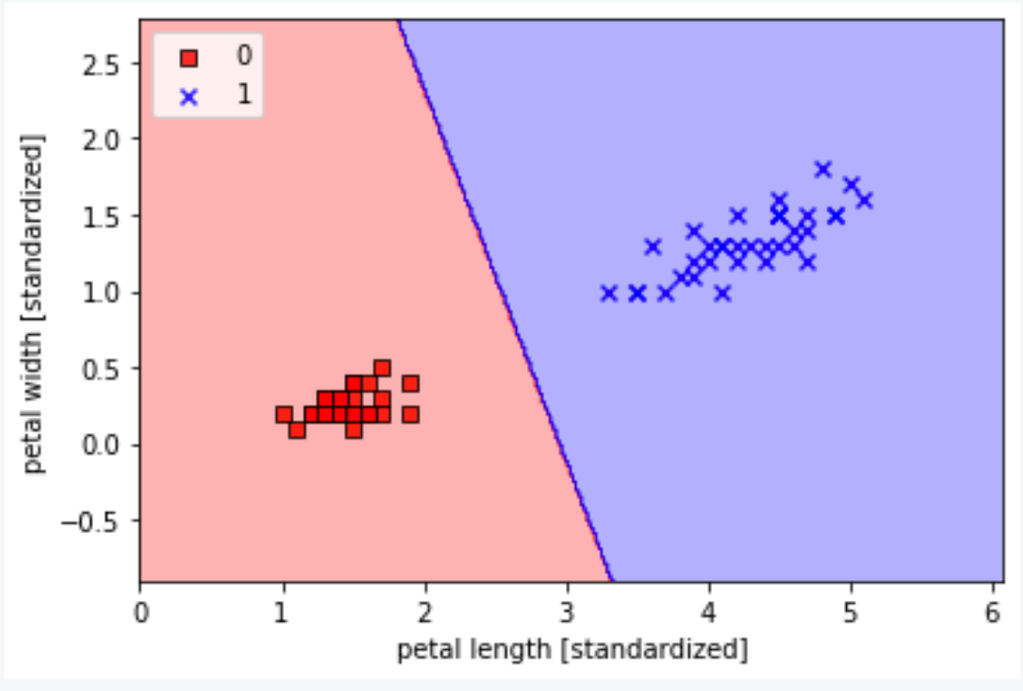


$$p = \mathbb{P}(Y = 1 | X_1 = x_1, X_2 = x_2)$$
$$= \sigma(W_1 x_1 + W_2 x_2 + b)$$

$$\sigma : z \mapsto \frac{1}{1 + e^{-z}}$$



- As the decision boundary is a **hyperplane,** the Logistic Regression model performs well on linearly separable classes.



Linearly inseparable data

- The basic idea to deal with linearly inseparable data is to create nonlinear combinations of the original features.

- We can then transform a two-dimensional dataset onto a three-dimensional feature space where the classes become linearly separable.

Original features:

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

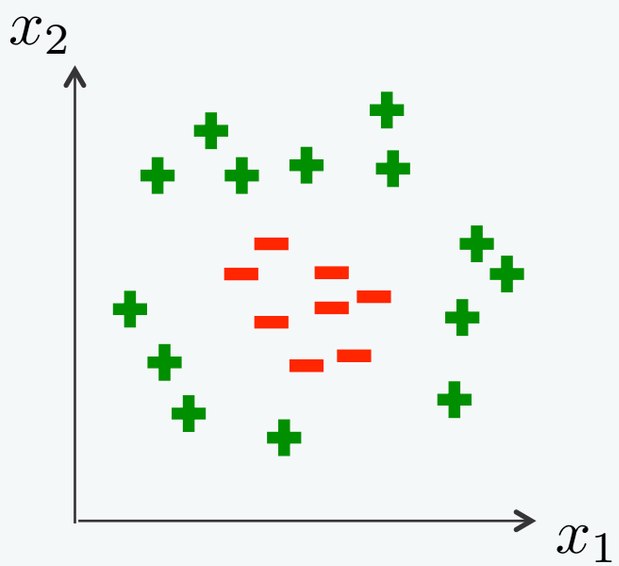
Transformation of the features:

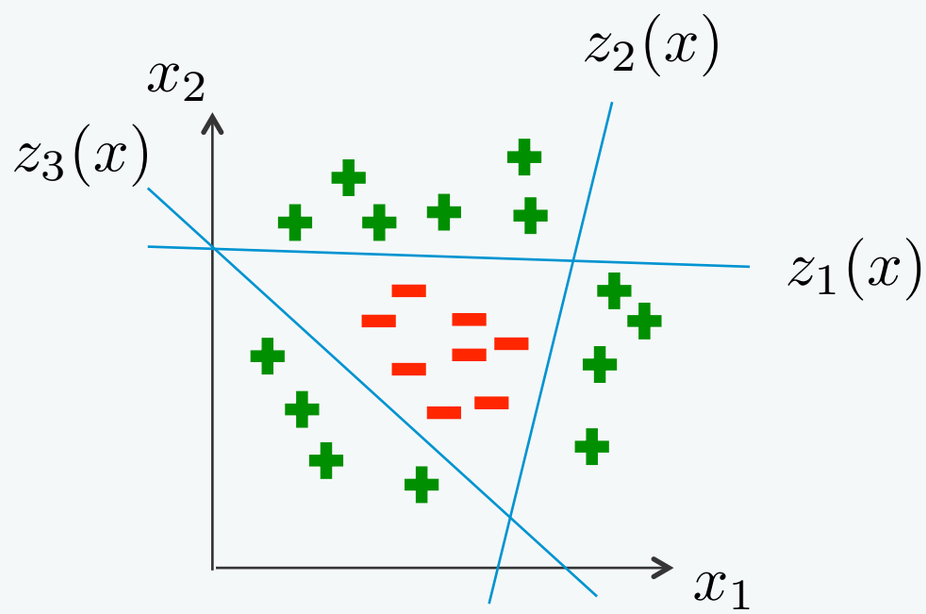
$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$$

$$\forall i \in \{1, 2, 3\} :$$

$$z_i = \sigma(b_i^{(1)} + W_{1,i}^{(1)} x_1 + W_{2,i}^{(1)} x_2)$$

where $\sigma : z \mapsto \frac{1}{1 + e^{-z}}$

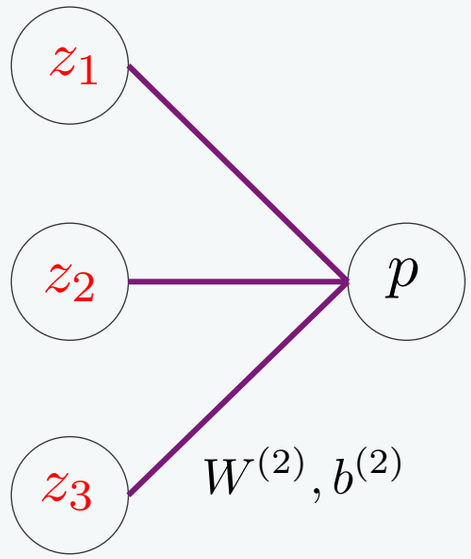




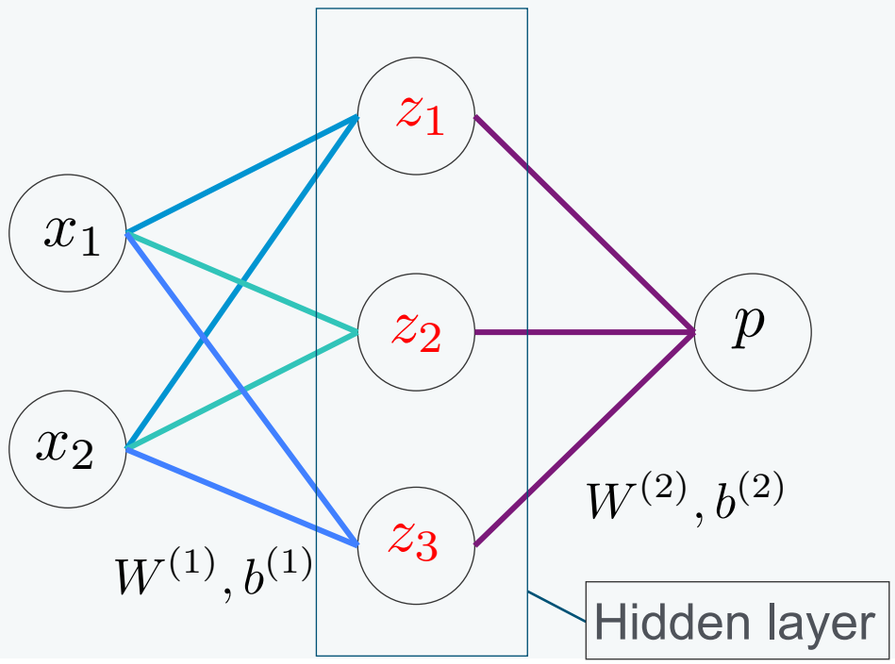
Shallow Neural Network

- After transforming the features, we can build a linear model on top of the new features:

$$p = \sigma(b^{(2)} + W_1^{(2)} z_1 + W_2^{(2)} z_2 + W_3^{(2)} z_3)$$



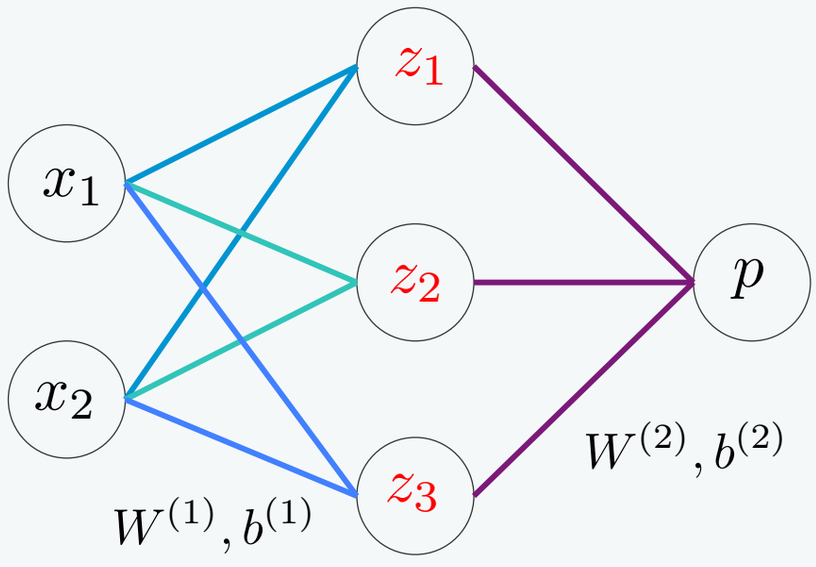
- This model is a basic example of an artificial neural network with **one hidden layer** containing **3 neurons**.



$$\forall i \in \{1, 2, 3\} \quad z_i = \sigma(b_i^{(1)} + W_{1,i}^{(1)} x_1 + W_{2,i}^{(1)} x_2)$$

$$p = \sigma(b^{(2)} + W_1^{(2)} z_1 + W_2^{(2)} z_2 + W_3^{(2)} z_3)$$

Interactive Session



- This is our model :

$$\forall i \in \{1,2,3\} \quad z_i = \sigma(b_i^{(1)} + W_{1,i}^{(1)} x_1 + W_{2,i}^{(1)} x_2)$$

$$p = \sigma(b^{(2)} + W_1^{(2)} z_1 + W_2^{(2)} z_2 + W_3^{(2)} z_3)$$

- Prove that without the activation function, the model becomes a simple **linear model**

$$p = \mathbf{U}x_1 + \mathbf{V}x_2 + \mathbf{b}$$

Training the Shallow Neural Network – Part 1 –

- We used Gradient Descent to learn the parameters of Logistic Regression, we can do the same for this shallow neural network model:

$$\forall i \in \{1,2,3\} \quad z_i = \sigma(b_i^{(1)} + W_{1,i}^{(1)} x_1 + W_{2,i}^{(1)} x_2)$$

$$p = \sigma(b^{(2)} + W_1^{(2)} z_1 + W_2^{(2)} z_2 + W_3^{(2)} z_3)$$

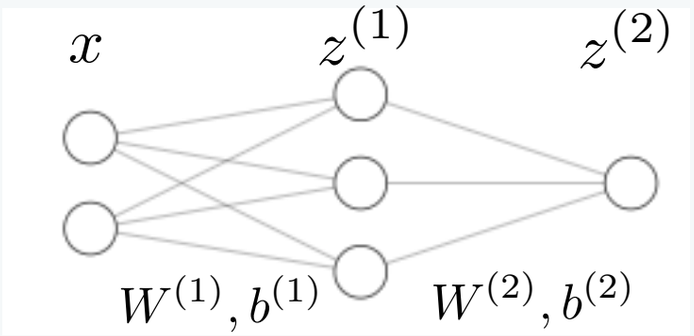
- The parameters θ of the model can be summerized as follows:

$$(W^{(1)} \in \mathbb{R}^{2\times 3}, b^{(1)} \in \mathbb{R}^3) \quad \text{and} \quad (W^{(2)} \in \mathbb{R}^{3\times 1}, b^{(2)} \in \mathbb{R})$$

- The Gradient Descent algorithm requires the use of **backpropagation.**

- **Backpropagation** consists in computing the gradient of the loss function J (that will be detailed later) with respect to each weight by the chain rule, iterating backward from the last layer.

Backpropagation



Chain rule

$$\frac{\partial J}{\partial W^{(1)}} = \frac{\partial J}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial W^{(1)}}$$

$$\frac{\partial J}{\partial W^{(2)}} = \frac{\partial J}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial W^{(2)}}$$

Training the Shallow Neural Network – Part 2 –

- The Gradient Descent algorithm consists in the following steps:
    - Initilize randomly θ_0
    - Fix a number of iterations K and a learning rate η and repeat K times:

$$\theta_{k+1} \leftarrow \theta_k - \eta \nabla_\theta J(\theta_k)$$

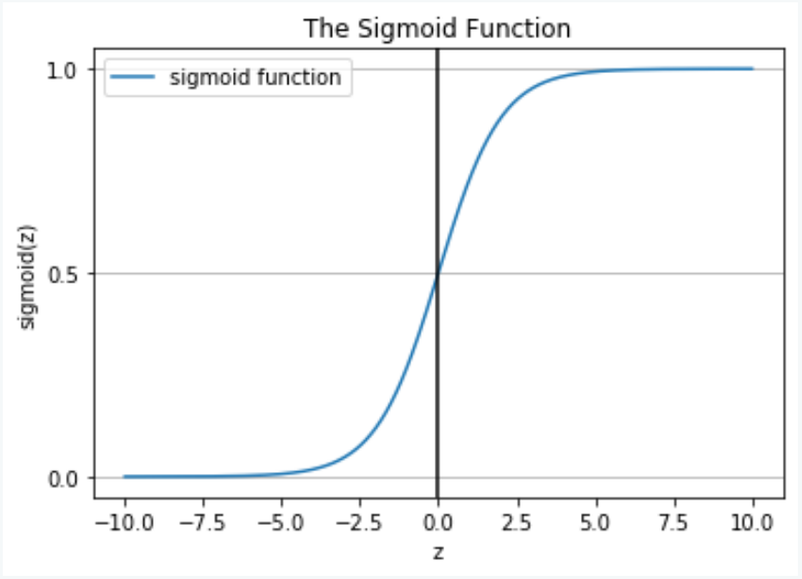
- J represents the loss function. We will detail later how to choose the appropriate one.

- We will also see in Lecture 7 several ways to improve the learning process:
    - By using Momentum.
    - By using adaptive learning rate.

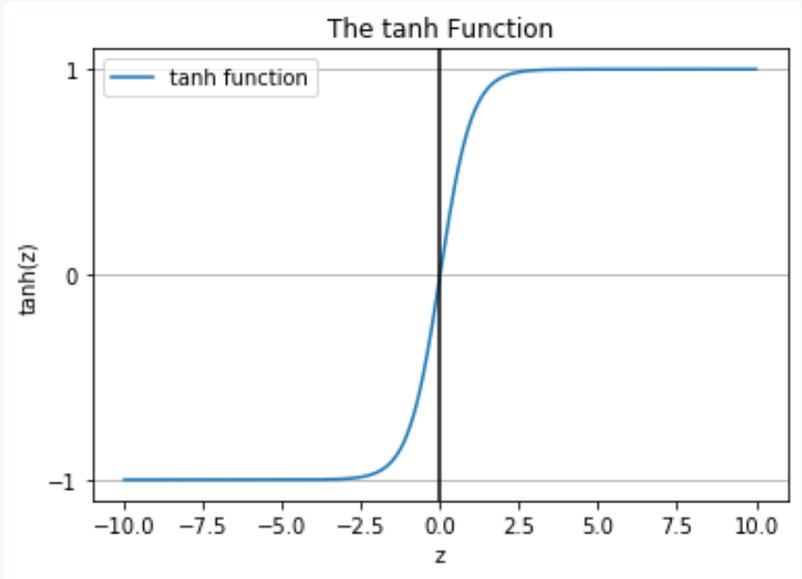
The activation functions – Part 1 –

- In the previous example, the non linearity results from the sigmoid function.
- The sigmoid function takes values in $[0, 1]$, which is convenient when we want to output a probability.
- However, we can still use other functions to introduce the non linearity in the intermediate layers.
- For instance, the hyperbolic tangent can also be used. It is just a scaled and shifted version of the sigmoid, so it has the same shape of the sigmoid with the advantage of taking values in $[-1, 1]$

$$\text{sigmoid}: \quad z \mapsto \frac{1}{1+\exp(-z)}$$



$$\tanh: \quad z \mapsto \frac{\exp(2z)-1}{\exp(2z)+1}$$



The activation functions – Part 2 –

- Although the sigmoid and tanh functions have good theoratical properties (both smooth, both diffentiable everywhere), they suffer from the **vanishig gradient problem**.

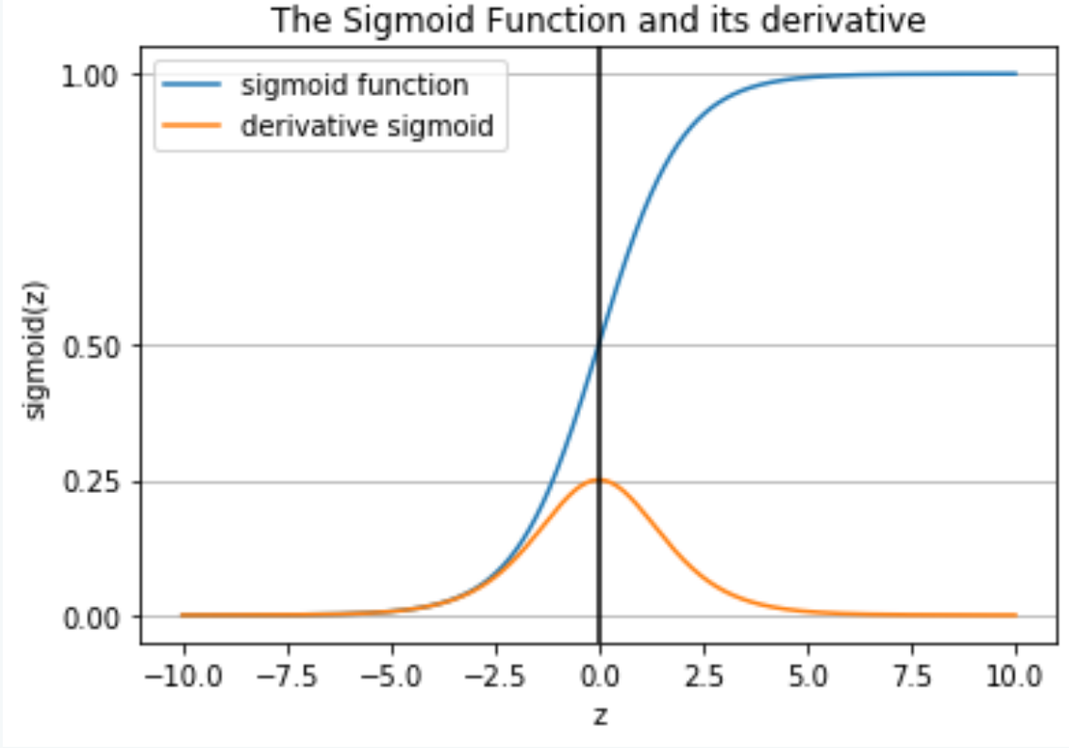
- To train the model we use **backpropagation.** However, the deeper the neural network is, the more terms have to be multipled due to the chain rule.

- For instance, with L layers:

$$\frac{\partial J}{\partial W^{(1)}} = \frac{\partial J}{\partial z^{(L)}} \frac{\partial z^{(L)}}{\partial z^{(L-1)}} \cdots \frac{\partial z^{(2)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial W^{(1)}}$$

- The problem with the sigmoid function is that its derivative has a maximum value of 0.25.

- So if we use a deep neural networks with sigmoid activation functions, we will end up multiplying several small numbers, which leads to the vanishing gradient problem.



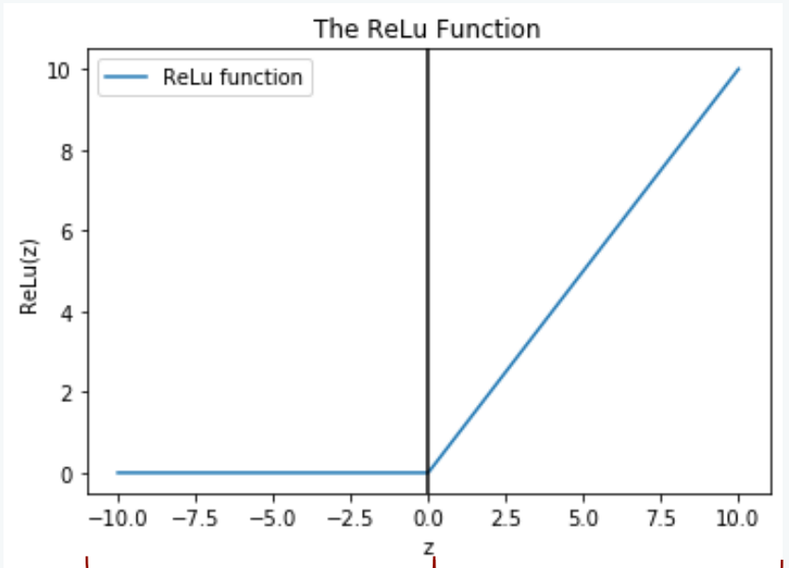
The activation functions – Part 3 –

- A simple solution to the previous vanishing gradient problem is to use the following activations functions:

$$\text{ReLu} : z \mapsto \max(0, z)$$

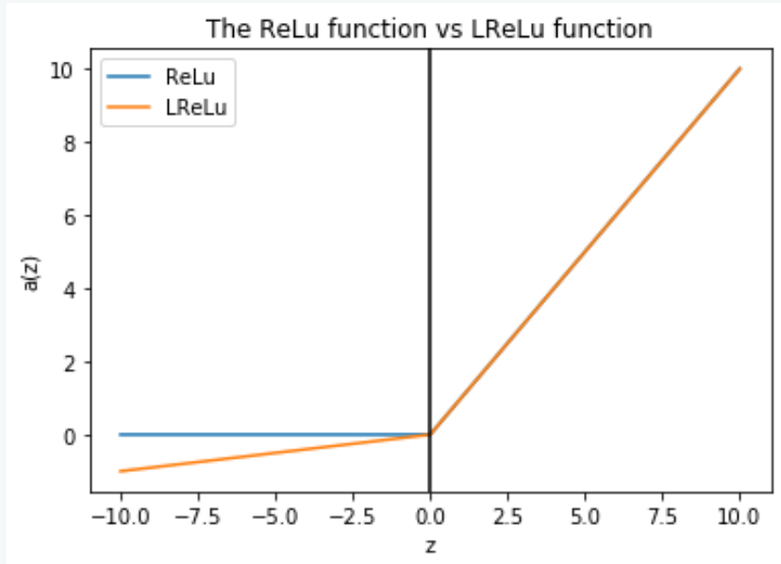
$$\text{Leaky Relu} : z \mapsto \begin{cases} z & \text{if} \quad z \neq 0 \\ \alpha z & \text{if} \quad z < 0 \end{cases}$$

$$\text{Softplus} : z \mapsto \log(1 + \exp(z))$$

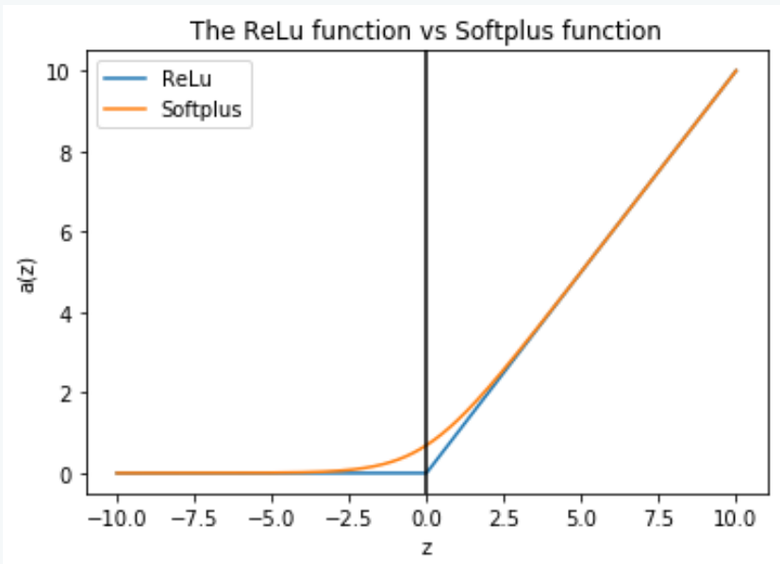


the gradient in the left side is vanished

The right side is not vanishing



Fixing the left side of the ReLu



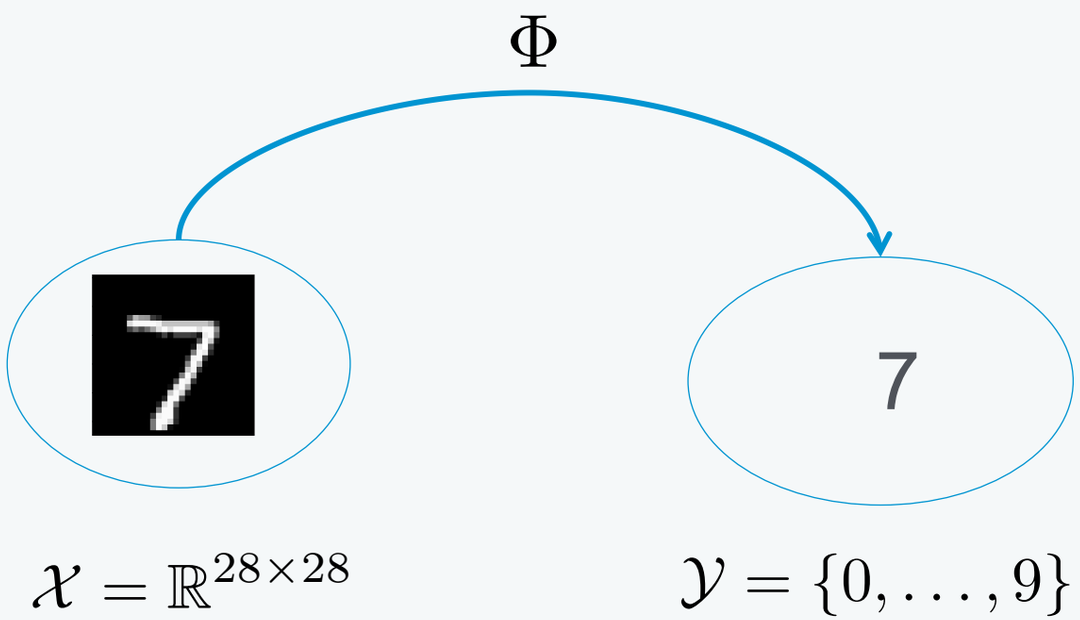
Looks linear on the right side

- Apart from the last activation function that should be chosen according to the problem (we will see later why we should use sigmoid for binary classification, softmax for multiclass classification and no activation function for regression), it is essential to compare a handful of different activation functions for the other layers, as we do for any other hyperparameter.

Universal Approximation Theory

- Universal Approximation Theory proves that any continuous function Φ can be approximated under some regularity conditions as closely as wanted by a shallow neural network. But it will require exponentially many neurons in terms of the dimension of the problem.

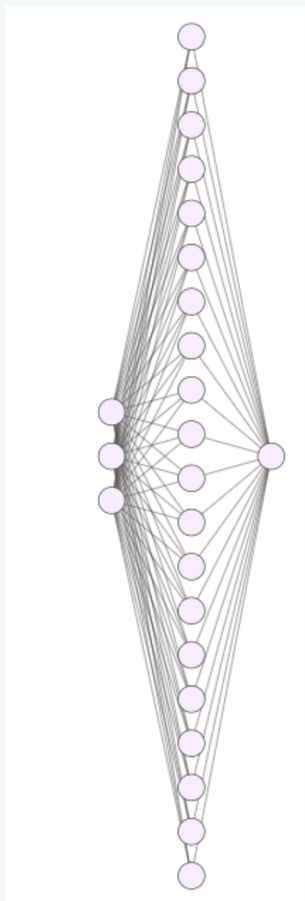
- Reference : [Pinkus 1999 : Approximation theory of the MLP model in neural networks]



The classification problem is of dimension:

d = 784

Theoratically, it should require exp(d) neurons in the hidden layer



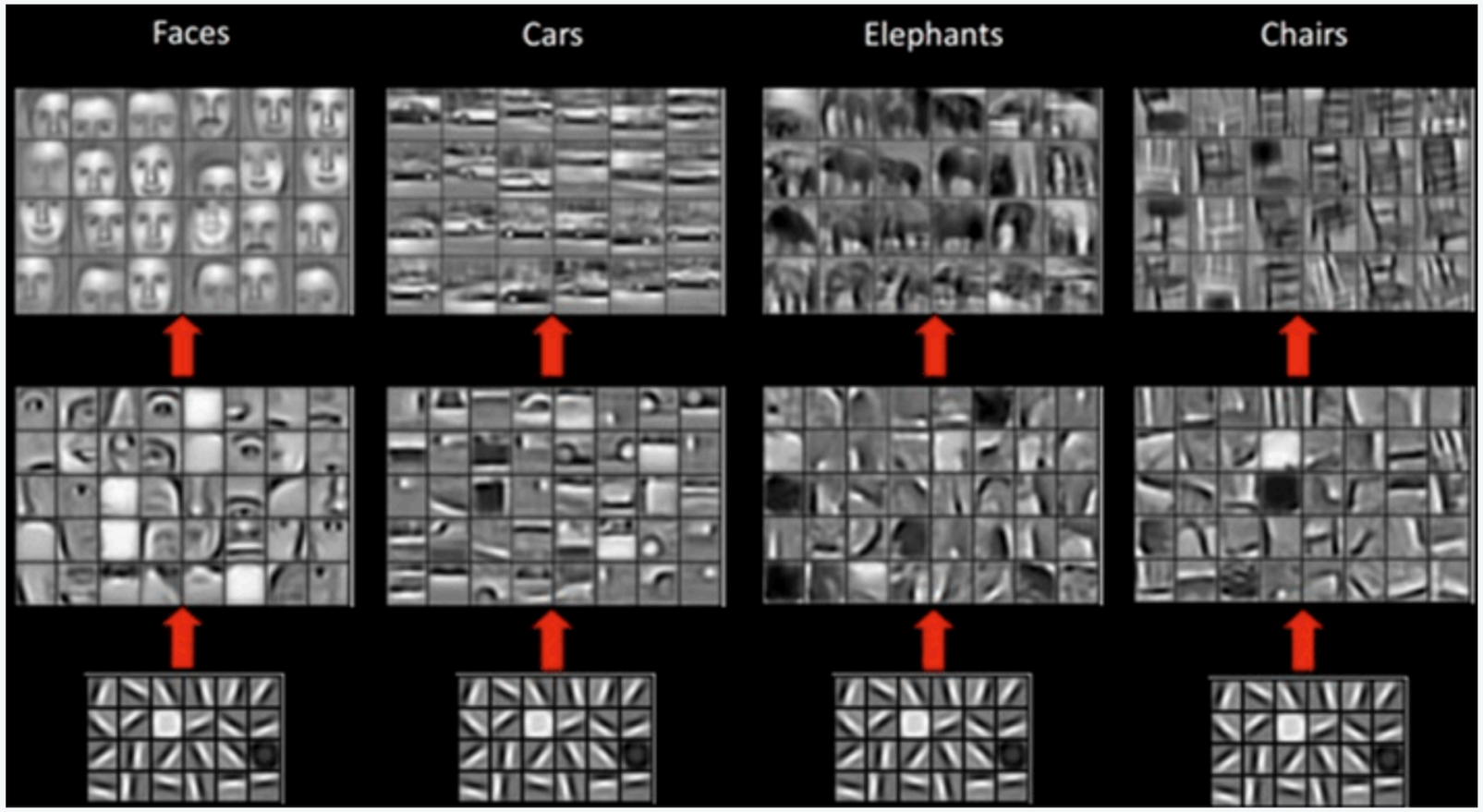
- Although Multilayer Networks are less understood theoratically compared with Shallow Networks, it turns out deeper networks perform better for a given number of parameters in practice.

Part 2 : Deep Neural Networks and Loss functions

Why deeper Networks ?

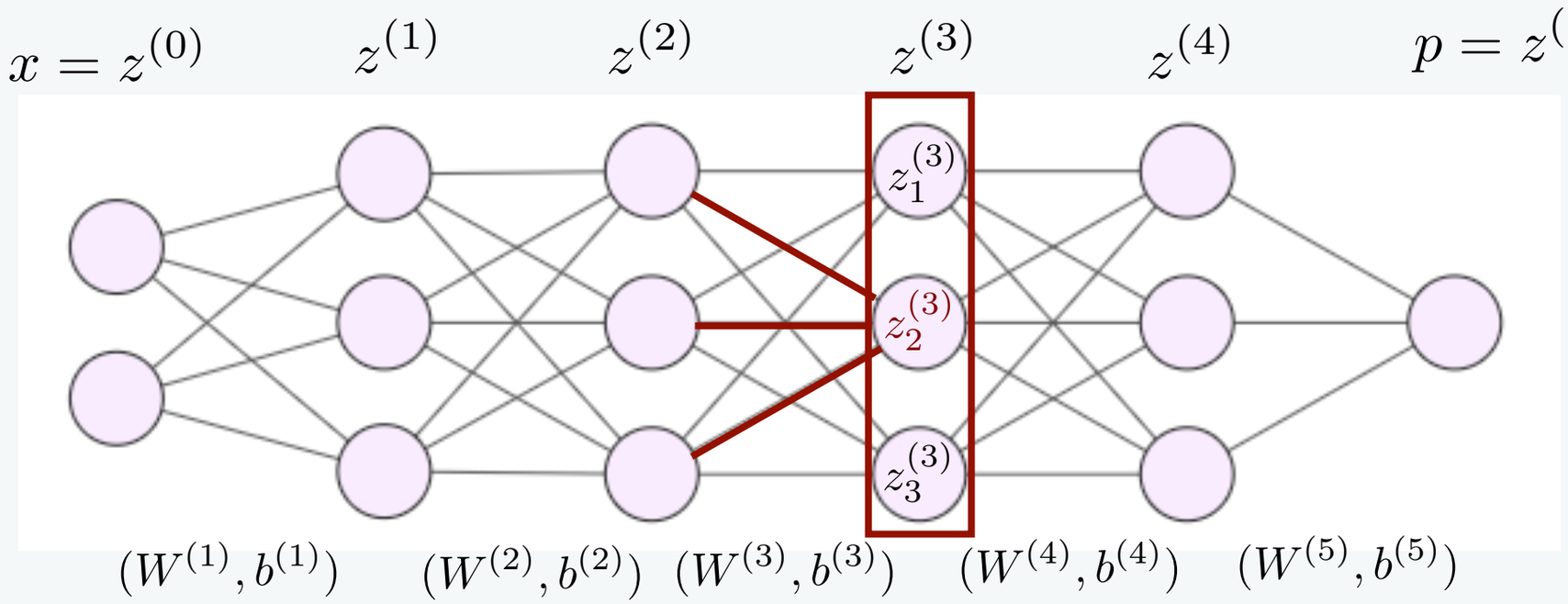
- Each neural network layer is a feature transformation.
- Deeper layers learn increasingly complex features.
- We have introduced a specific type of layers called the **Dense Layers**. We will introduce other types of transformations in future lectures. For instance, the Convolutional layer is typically used for images.

- The first convolution layer will learn small local patterns such as edges.
- Deeper layers will learn larger patterns made of the features of the previous layers, and so on.



Forward Propagation for Binary Classification – Part 1 –

- Let's keep the example of binary classification, but with a deeper model (i.e, with multiple layers and multiple neurons per layer)



- On a neuron level : $$z_2^{(3)} = \sigma(W_{12}^{(3)} z_1^{(2)} + W_{22}^{(3)} z_2^{(2)} + W_{32}^{(3)} z_3^{(2)} + b^{(3)})$$

- On a layer level:

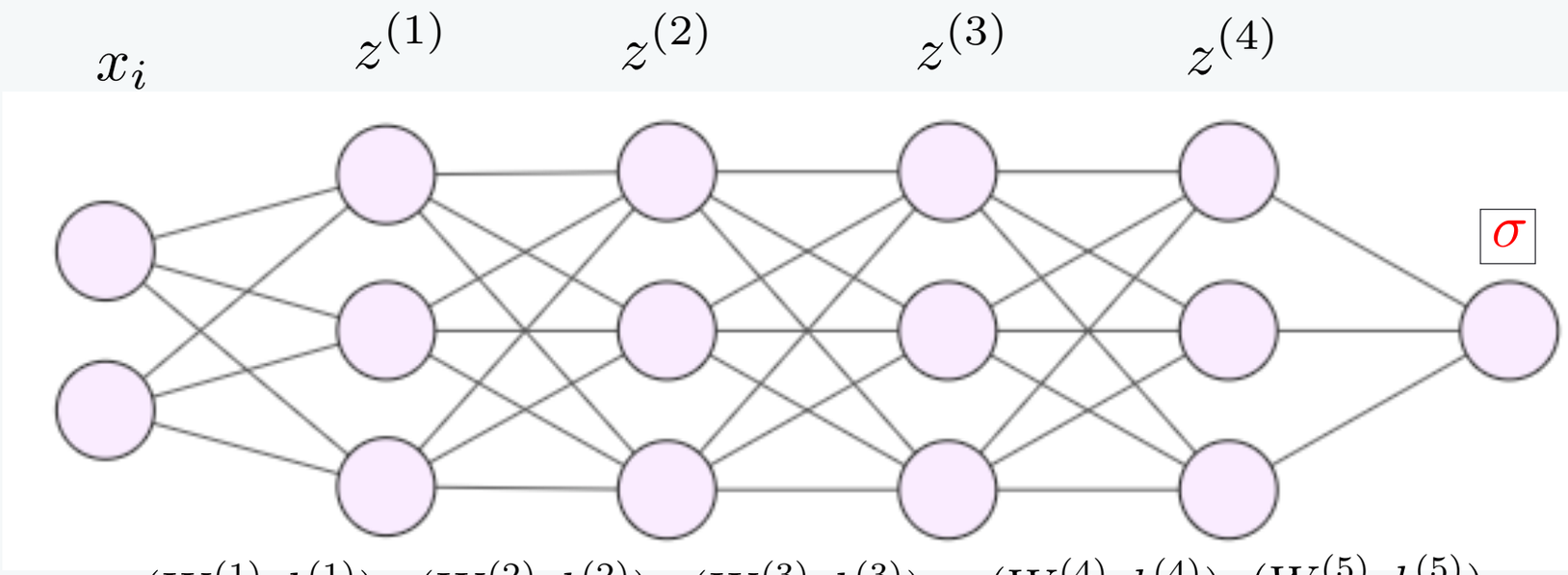
$$W^{(3)^T} = \begin{pmatrix} W_{11}^{(3)} & W_{21}^{(3)} & W_{31}^{(3)} \\ W_{12}^{(3)} & W_{22}^{(3)} & W_{32}^{(3)} \\ W_{13}^{(3)} & W_{23}^{(3)} & W_{33}^{(3)} \end{pmatrix} \qquad z^{(2)} = \begin{pmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{pmatrix} \Bigg\} \rightarrow$$

$$\forall l \in \{1, \ldots, 5\}$$

$$z^{(l)} = \sigma(W^{(l)^T} z^{(l-1)} + b^{(l)})$$

Forward Propagation for Binary Classification – Part 2 –

$$x_i = \begin{pmatrix} \text{length} \\ \text{width} \end{pmatrix}$$



- In the previous example, the forward propagation can be summerized as follows:

$$\forall i \in \{1, \dots, N\} \quad p_i = f_\theta(x_i) \qquad \text{where} \qquad \theta = \left\{ (W^{(i)}, b^{(i)}); i \in \{1, \dots, 5\} \right\}$$

- The forward propagation outputs the probability of the positive class: $p_i = \mathbb{P}(Y = 1 | X = x_i)$

- As the forward propagation outputs a probability in the range $[0, 1]$, the last activation function should be a **sigmoid function**.

Loss function for Binary Classification – Part 1 –

$$\Rightarrow x_1 = \begin{pmatrix} \text{length} \\ \text{width} \end{pmatrix} \Rightarrow \boxed{f_\theta} \Rightarrow p_1 = f_\theta(x_1) = \mathbb{P}(Y = 1 | X = x_1)$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$\Rightarrow x_i = \begin{pmatrix} \text{length} \\ \text{width} \end{pmatrix} \Rightarrow \boxed{f_\theta} \Rightarrow p_i = f_\theta(x_i) = \mathbb{P}(Y = 1 | X = x_i)$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$\Rightarrow x_N = \begin{pmatrix} \text{length} \\ \text{width} \end{pmatrix} \Rightarrow \boxed{f_\theta} \Rightarrow p_N = f_\theta(x_N) = \mathbb{P}(Y = 1 | X = x_N)$$

- From the dataset $(x_i, y_i)_{1 \leq i \leq N}$ and the model: $Y|X = x_i \sim \mathcal{B}(p_i)$ where $\mathcal{B}$ stands for the Bernoulli distribution, our objective is to maximize the following likelihood :

$$\mathcal{L}(\theta) = \prod_{i=1}^{N} \mathbb{P}(Y = y_i | X = x_i) = \prod_{i=1}^{N} f_\theta(x_i)^{y_i} (1 - f_\theta(x_i))^{1 - y_i}$$

Loss function for Binary Classification – Part 2 –

- As usual, instead of maximizing the likelihood, we prefer to minimize the normalized negative log-likelihood (called the loss function J)

$$
\begin{aligned}
J(\theta) &= -\frac{1}{N}\log(\mathcal{L}(\theta)) \\
&= -\frac{1}{N}\log\left(\prod_{i=1}^{N} f_\theta(x_i)^{y_i}(1-f_\theta(x_i))^{1-y_i}\right) \\
&= -\frac{1}{N}\sum_{i=1}^{N}\log\left(f_\theta(x_i)^{y_i}(1-f_\theta(x_i))^{1-y_i}\right) \\
&= -\frac{1}{N}\sum_{i=1}^{N}\{y_i\log(f_\theta(x_i)) + (1-y_i)\log(1-f_\theta(x_i))\}
\end{aligned}
$$

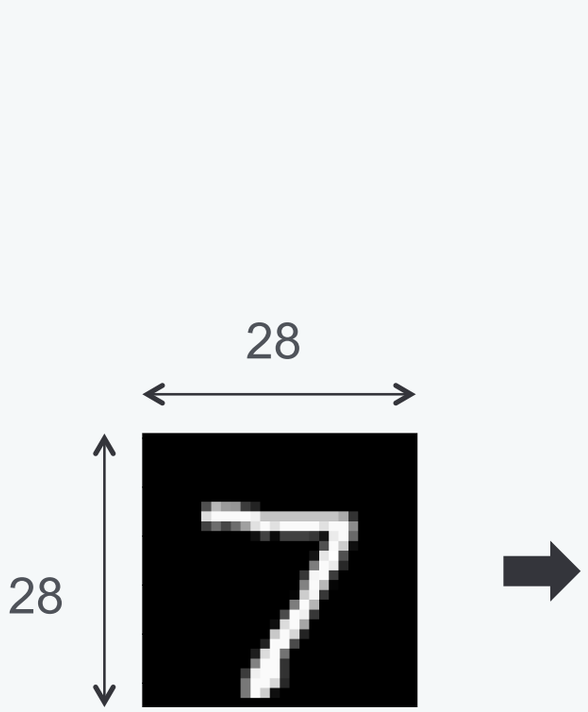
- Thus, the loss function for binary classification is the following **binary cross-entropy**:

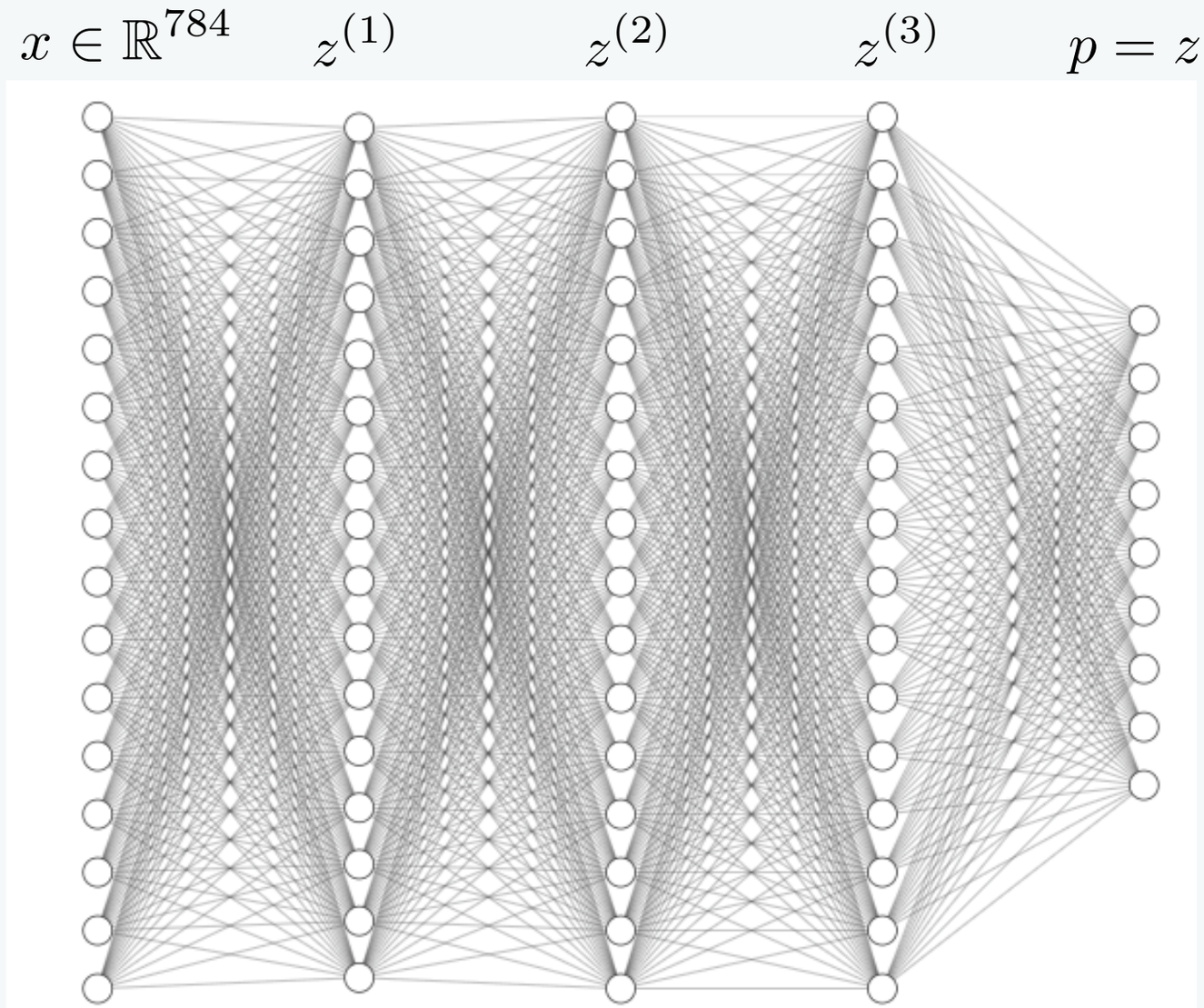
$$
\boxed{J(\theta) = -\frac{1}{N}\sum_{i=1}^{N}\{y_i\log(f_\theta(x_i)) + (1-y_i)\log(1-f_\theta(x_i))\}}
$$

Forward Propagation for Multiclass Classification – Part 1 –

- The multiclass classification consists in predicting one of K categories.

- Let's take the example of the MNIST dataset. The objective is to predict a category among the set of numbers $\{0, 1, \ldots, 9\}$ based on an image of shape (28, 28) that we can flatten into a 784 dimensional input vector.





Forward Propagation for Multiclass Classification – Part 2 –

- If we want the output to be discrete distribution over all the possible categories (10 in our example), the last layer must have 10 neurons and the activation function must be the **softmax activation function**.

- The softmax activation function transforms a vector of size K into a probability distribution. It first uses the exponential function to turn the real numbers into positive ones, then a classic normalization is performed.

$$\begin{pmatrix} w_1 \\ \vdots \\ w_i \\ \vdots \\ w_K \end{pmatrix}$$

Output of the last layer before applying the activation function

Applying the Softmax activation function

$$\forall i \in \{1, \ldots, K\} \quad p_i = \frac{e^{w_i}}{\sum_{j=1} e^{w_j}}$$

$$\forall i \in \{1, \ldots, K\} \quad p_i \geq 0$$

$$\sum_{i=1}^{K} p_i = 1$$

$$\begin{pmatrix} p_1 \\ \vdots \\ p_i \\ \vdots \\ p_K \end{pmatrix}$$

Output of the last layer after applying the activation function

Categorical Distribution – One hot encoding –

- As we have seen before, , the categorical distribution (also called multinomial distribution) models the outcome of a random variable that can take K possible categories.

- Let X be a random variable than can take K possible values, each value k with probability π_k

$$\forall k \in \{1, \dots, K\} \quad \mathbb{P}(X = k) = \pi_k$$

- We say that X follows a Multinomial distribution:

$$X \sim \mathcal{M}(1, \pi_1, \dots, \pi_K) \quad \text{where} \quad \forall k \in \{1, \dots K\} \quad \pi_k \geq 0 \quad \text{and} \quad \sum_{k=1}^{K} \pi_k$$

- We usually use **one hot encoding** to represent the discrete random variable X, which consists in encoding X with a random variable $Y = (Y_1, \dots, Y_K)^T$ such that

$$\forall k \in \{1, \dots, K\} \quad Y_k = 1_{\{X=k\}}$$

- Which means:

$$\{X = k\} \iff Y = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow \text{k-th position}$$

- Thus:

$$\forall k \in \{1, \dots, K\} \quad \mathbb{P}(X = k) = \mathbb{P}(Y_k = 1)$$

Loss function for Multiclass Classification – Part 1 –

$$\Rightarrow \quad x_1 \in \mathbb{R}^{784} \quad \Rightarrow \quad \boxed{f_\theta} \quad \Rightarrow \quad p_1 = f_\theta(x_1) = \begin{pmatrix} p_1^1 \\ \vdots \\ p_1^k \\ \vdots \\ p_1^K \end{pmatrix} = \begin{pmatrix} \mathbb{P}(Y_1 = 1 | X = x_1) \\ \vdots \\ \mathbb{P}(Y_k = 1 | X = x_1) \\ \vdots \\ \mathbb{P}(Y_K = 1 | X = x_1) \end{pmatrix}$$

$\vdots$ $\qquad$ $\vdots$ $\qquad$ $\vdots$

$$\Rightarrow \quad x_i \in \mathbb{R}^{784} \quad \Rightarrow \quad \boxed{f_\theta} \quad \Rightarrow \quad p_i = f_\theta(x_i) = \begin{pmatrix} p_i^1 \\ \vdots \\ p_i^k \\ \vdots \\ p_i^K \end{pmatrix} = \begin{pmatrix} \mathbb{P}(Y_1 = 1 | X = x_i) \\ \vdots \\ \mathbb{P}(Y_k = 1 | X = x_i) \\ \vdots \\ \mathbb{P}(Y_K = 1 | X = x_i) \end{pmatrix}$$

$\vdots$ $\qquad$ $\vdots$ $\qquad$ $\vdots$

$$\Rightarrow \quad x_N \in \mathbb{R}^{784} \quad \Rightarrow \quad \boxed{f_\theta} \quad \Rightarrow \quad p_N = f_\theta(x_N) = \begin{pmatrix} p_N^1 \\ \vdots \\ p_N^k \\ \vdots \\ p_N^K \end{pmatrix} = \begin{pmatrix} \mathbb{P}(Y_1 = 1 | X = x_N) \\ \vdots \\ \mathbb{P}(Y_k = 1 | X = x_N) \\ \vdots \\ \mathbb{P}(Y_K = 1 | X = x_N) \end{pmatrix}$$

Loss function for Multiclass Classification – Part 2 –

- The targets should be one hot encoded too.

$$[y_i]_{1\leq i\leq N} = \begin{pmatrix} 4 \\ 3 \\ 2 \\ 6 \\ 9 \\ 0 \end{pmatrix} \quad \Rightarrow \quad [\hat{y}_i^k]_{\substack{1\leq i\leq N \\ 1\leq k\leq K}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

- Which means: $\forall i \in \{1,\dots,N\}\ \forall k \in \{1,\dots,K\} \quad y_i = k \quad \Longleftrightarrow \quad \hat{y}_i^k = 1$

- From the dataset $(x_i, y_i)_{1\leq i\leq N}$ and the model: $Y|X = x_i \sim \mathcal{M}(1, p_i^1, \dots, p_i^K)$ where $\mathcal{M}$ stands for the Multinomial distribution, our objective is to maximize the following likelihood :

$$\mathcal{L}(\theta) = \prod_{i=1}^{N} \mathbb{P}(Y = y_i|X = x_i) = \prod_{i=1}^{N} \boxed{\prod_{k=1}^{K} {p_i^k}^{\hat{y}_i^k}}$$

$$\prod_{k=1}^{K} {p_i^k}^{\hat{y}_i^k} = p_i^l \quad \Longleftrightarrow \quad \hat{y}_i^l = 1$$

Loss function for Multiclass Classification – Part 3 –

- As before, instead of maximizing the likelihood, we prefer to minimize the normalized negative log-likelihood (called the loss function J)

$$J(\theta) = -\frac{1}{N}\log(\mathcal{L}(\theta))$$

$$= -\frac{1}{N}\log\left(\prod_{i=1}^{N}\prod_{k=1}^{K} {p_i^k}^{\hat{y}_i^k}\right)$$

$$= -\frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{K}\hat{y}_i^k\log(p_i^k)$$

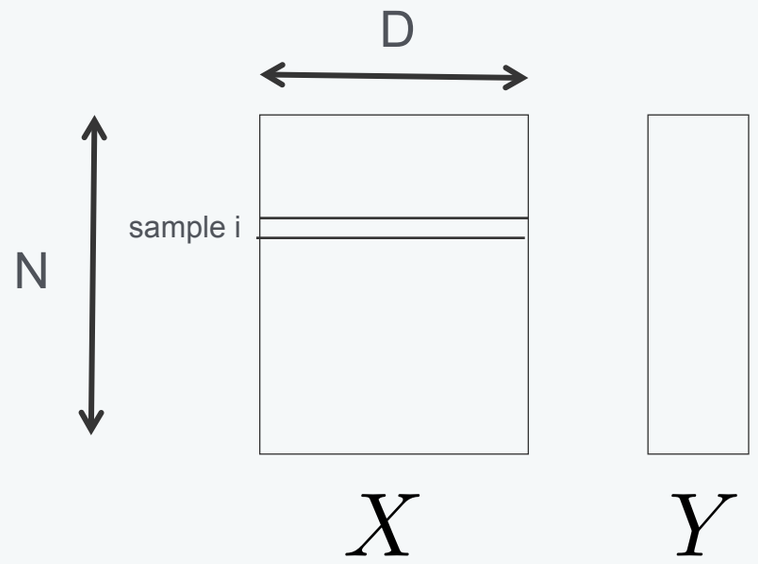
- Thus, the loss function for multiclass classification is the following **categorical cross-entropy**:

$$\boxed{J(\theta) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{K}\hat{y}_i^k\log(p_i^k)}$$

Part 3 : Deep Learning Techniques

Optimization Techniques: - Gradient Descent -

- Data:



- Parameters:

$$\theta = \left\{ (W^{(k)}, b^{(k)}); k \in \{1, \ldots, K\} \right\}$$

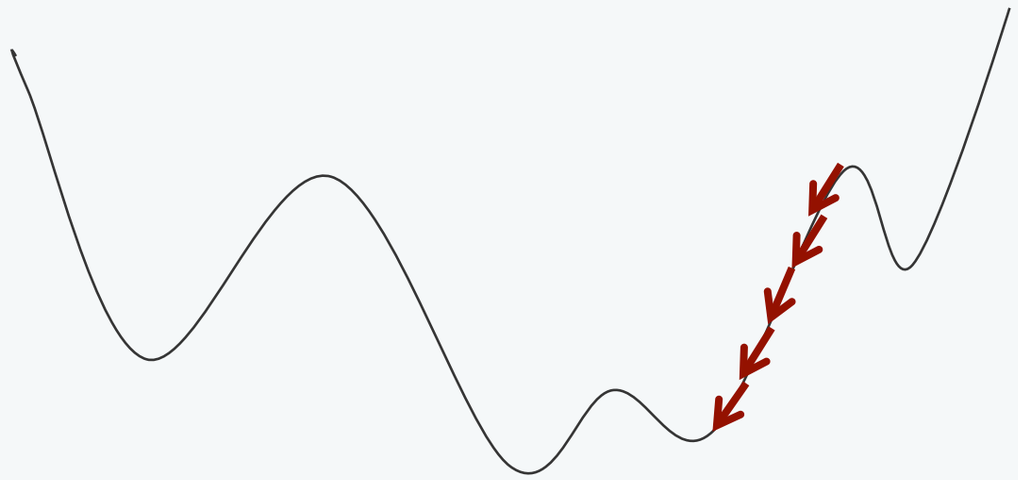
- Loss function for the dataset:

$$\underbrace{J_{\text{dataset}}(\theta)}_{\text{loss of the dataset}} = \frac{1}{N} \sum_{i=1}^{N} \underbrace{J(\theta, i)}_{\text{loss for sample i}}$$

- Algorithm:

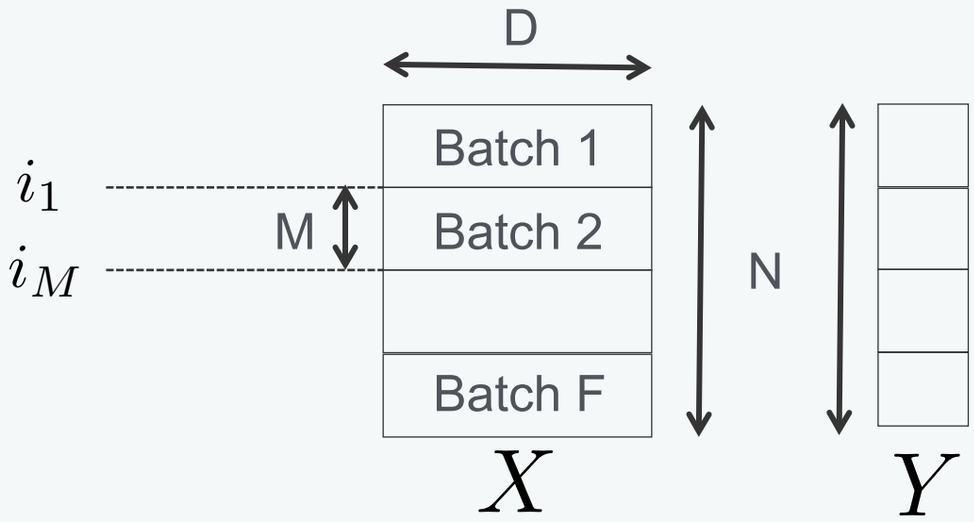
  - Initilize randomly θ_0
  - Fix a number of iterations N_{iter} and a learning rate η and repeat:

$$\theta_{k+1} \leftarrow \theta_k - \eta \nabla_\theta J_{\text{dataset}}(\theta_k)$$



Optimization Techniques: - Stochastic Gradient Descent -

- Data:



Number of batches

$$F = \text{int}(N/M)$$

- Parameters:

$$\theta = \left\{ (W^{(k)}, b^{(k)}); k \in \{1, \ldots, K\} \right\}$$

- Loss function for a batch:

$$\underbrace{J_{\text{batch}}(\theta)}_{\text{loss of the batch}} = \frac{1}{M} \sum_{i=i_1}^{i_M} \underbrace{J(\theta, i)}_{\text{loss for sample i}}$$

- Algorithm:

- Initilize randomly θ_0
- Repeat N_{epochs} times:
  - Shuffle the data and split it into batches of size M.
  - Update the weights for each batch in $\{1, \ldots, F\}$

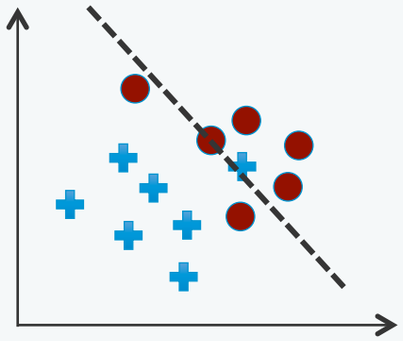
$$\theta_{k+1} \leftarrow \theta_k - \eta \nabla_\theta J_{\text{batch}}(\theta_k)$$

Fighting the Overfitting problem – 1 –

- There are a lot of hyperparameters to tune when using Neural Networks:
  - The number of hidden layers, the number of neuros per hidden layer.
  - The activations functions
  - The number of epochs, the batch size and the learning rate (and other hyperparameters for more sophisticated optimization algorithms), etc.

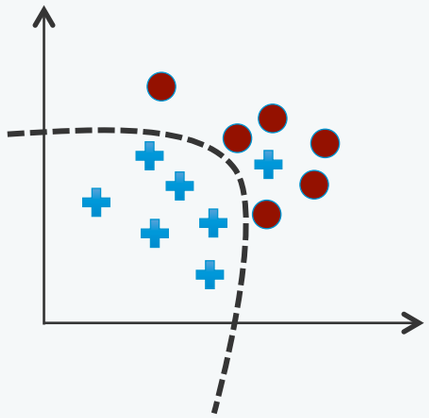
- The main issue when designing the architecture of a neural network (i.e, choosing the hyperparameters) is to make sure we keep the balance between the **optimization** task and the **generalization** purpose.

Underfitting



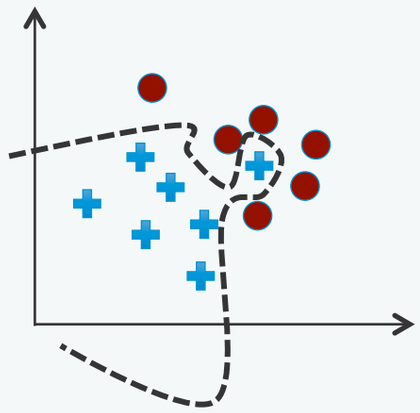
Complexity of $\mathcal{G}$ too small (high bias)

Good Compromise



Complexity of $\mathcal{G}$: neither too big, nor too small.

Overfitting

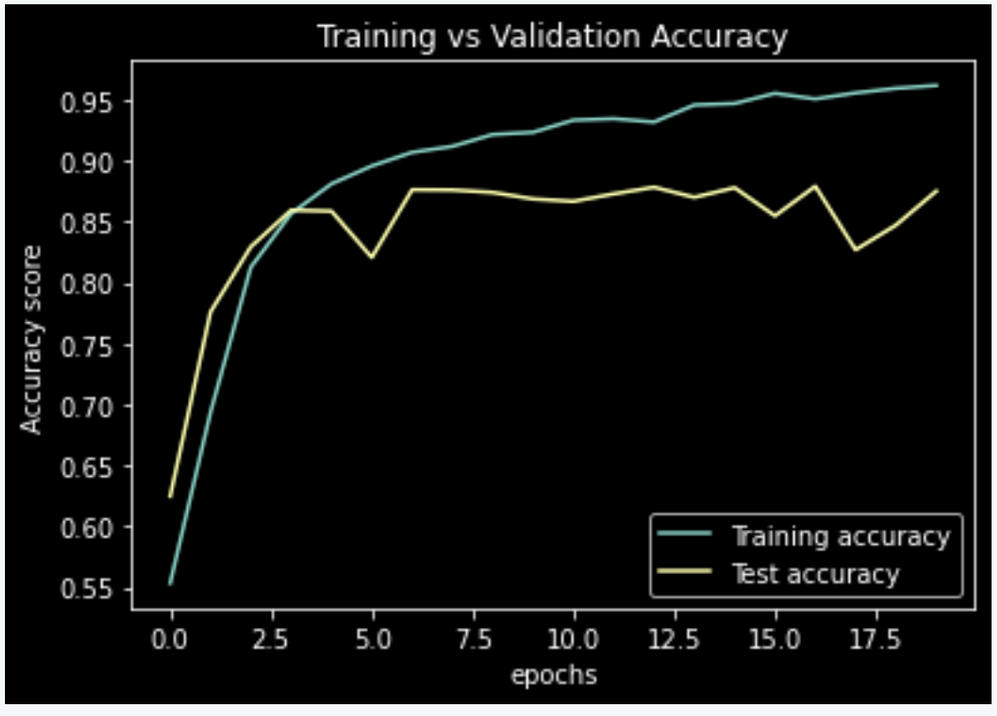


Complexity of $\mathcal{G}$ too big (high variance)

Fighting the Overfitting problem – 2 –

- At the beginning of the training process, **optimization** and **generalization** are correlated. Both the training and the validation metrics are improving.

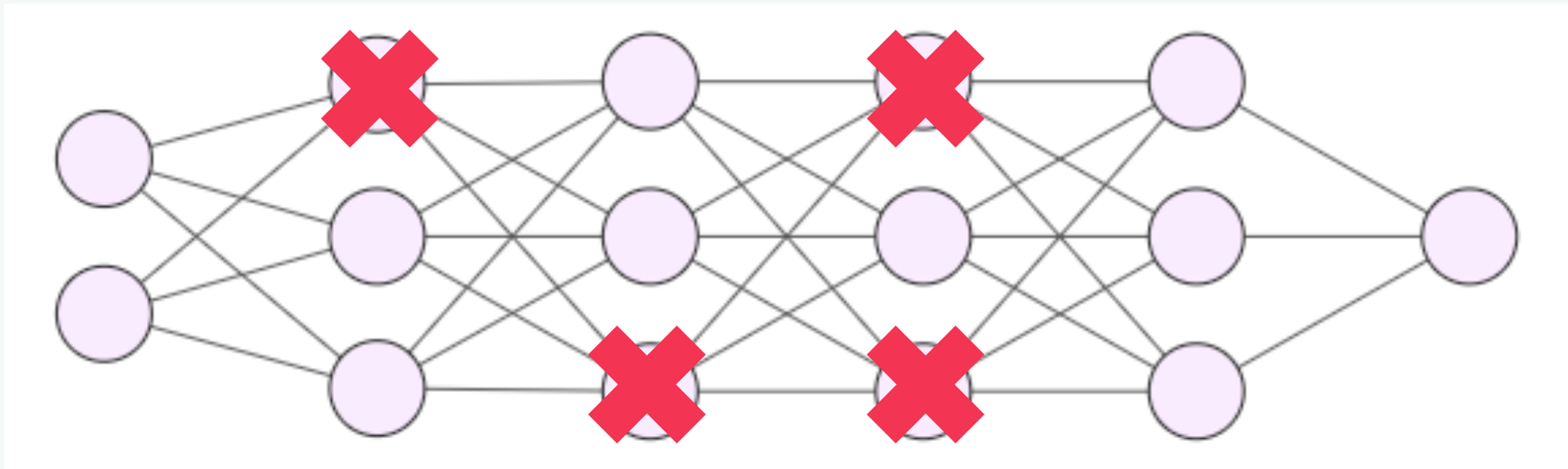
- After some iterations, generalization stops improving, validation metrics start degrading because the model is then learning some patterns that are specific to the training data and irrelevant to new data. The model is simply **overfitting**.



Fighting the Overfitting problem – 3 –

- To overcome the overfitting problem, we can add more samples or reduce the compexity of the network. We can also test several regularization techniques:

    - **Dropout** applied to a layer, consists of randomly "dropping out" (i.e. setting to zero) a number of output features of the layer during training. The "dropout rate" is the fraction of the features that are being zeroed-out; it is usually set between 0.2 and 0.5.



- **Weight regularization**: it consists in adding to the loss function of the network a cost associated with having large weights. For the cost, we can use the $\mathcal{L}^1$ norm of the weights or the $\mathcal{L}^2$ norm.

Programming Session

Go to the following link and take Quiz 5 :

https://mlfbg.github.io/MachineLearningInFinance/