Neural Networks

Prof. Gheith Abandah

Reference: *Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow* by Aurélien Géron (O'Reilly). 2019, 978-1-492-03264-9.

Introduction

- YouTube Video: *But what *is* a Neural Network?* from 3Blue1Brown

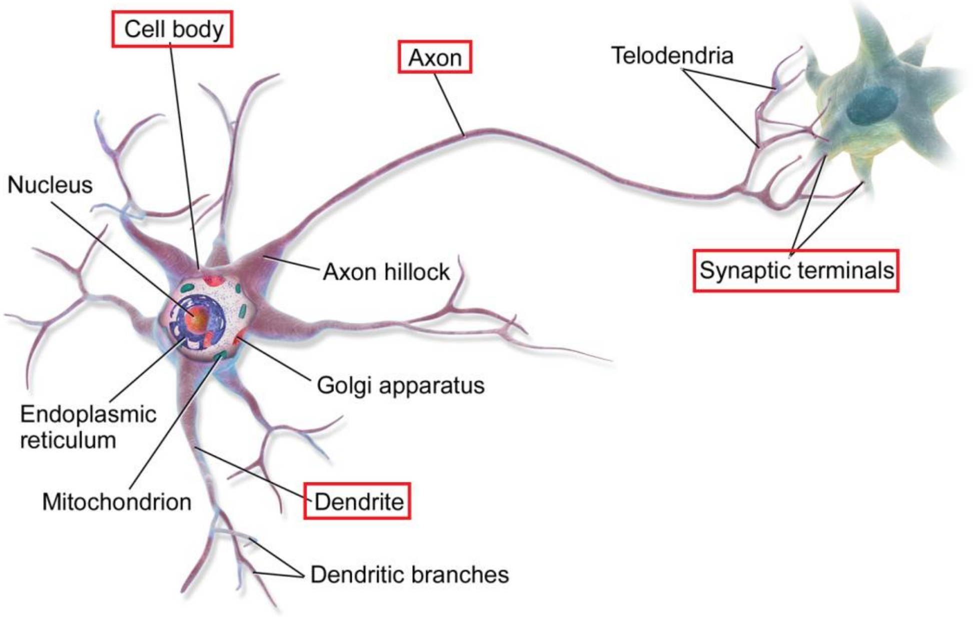
https://youtu.be/aircAruvnKk

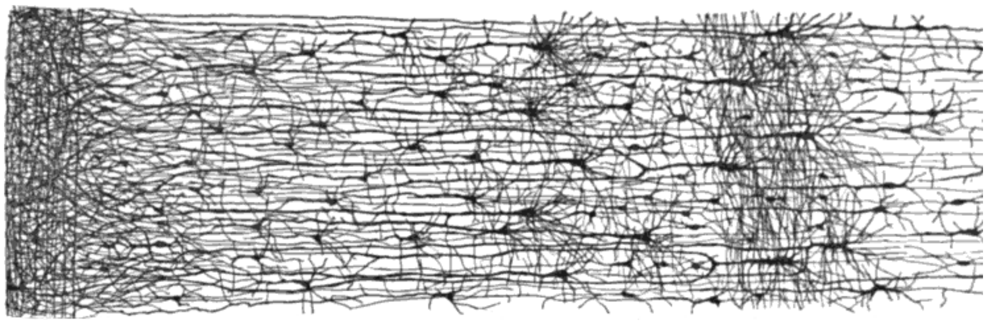
Outline

1. Introduction
2. The perceptron
3. Multi-layer perceptron (MLP)
4. Regression MLPs
5. Classification MLPs

1. Introduction

- *Artificial neural networks* (ANNs) are inspired by the brain's architecture.
- First suggested in 1943. Is now flourishing due to the availability of:
  - Data
  - Computing power
  - Better algorithms

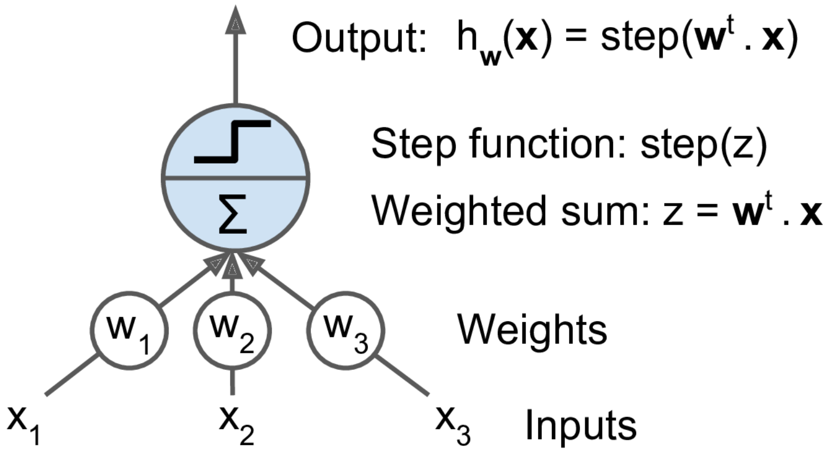




2. The Perceptron

- The *Perceptron* is a simple ANN, invented in 1957 and can perform linear binary classification or regression.

Linear threshold unit (LTU)



Output: $h_{\mathbf{w}}(\mathbf{x}) = \text{step}(\mathbf{w}^t \,.\, \mathbf{x})$

Step function: step(z)

Weighted sum: $z = \mathbf{w}^t \,.\, \mathbf{x}$

Weights

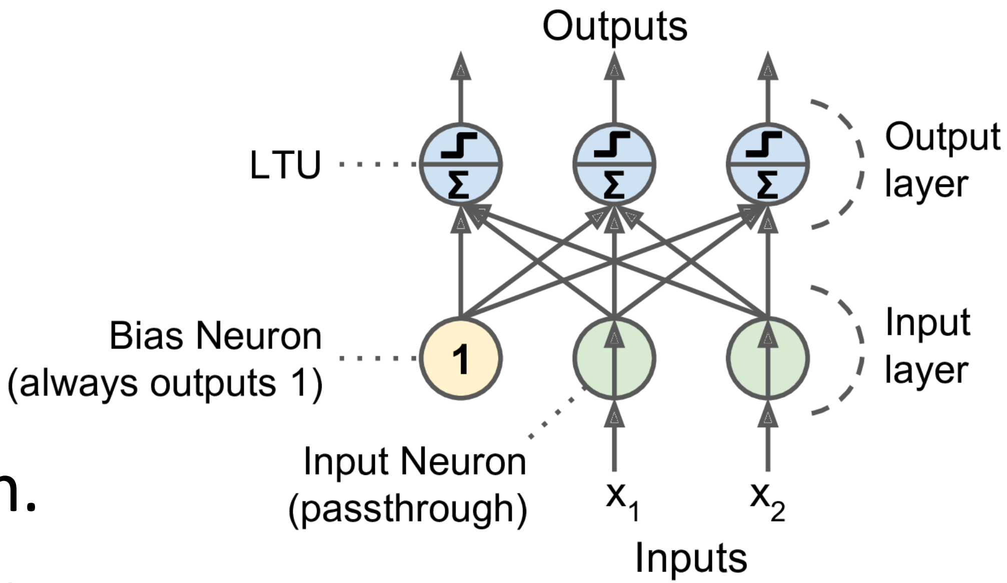
Inputs

- Common step functions:

$$\text{heaviside}\,(z) = \begin{cases} 0 & \text{if } z < 0 \\ 1 & \text{if } z \geq 0 \end{cases} \qquad \text{sgn}\,(z) = \begin{cases} -1 & \text{if } z < 0 \\ 0 & \text{if } z = 0 \\ +1 & \text{if } z > 0 \end{cases}$$

2. The Perceptron

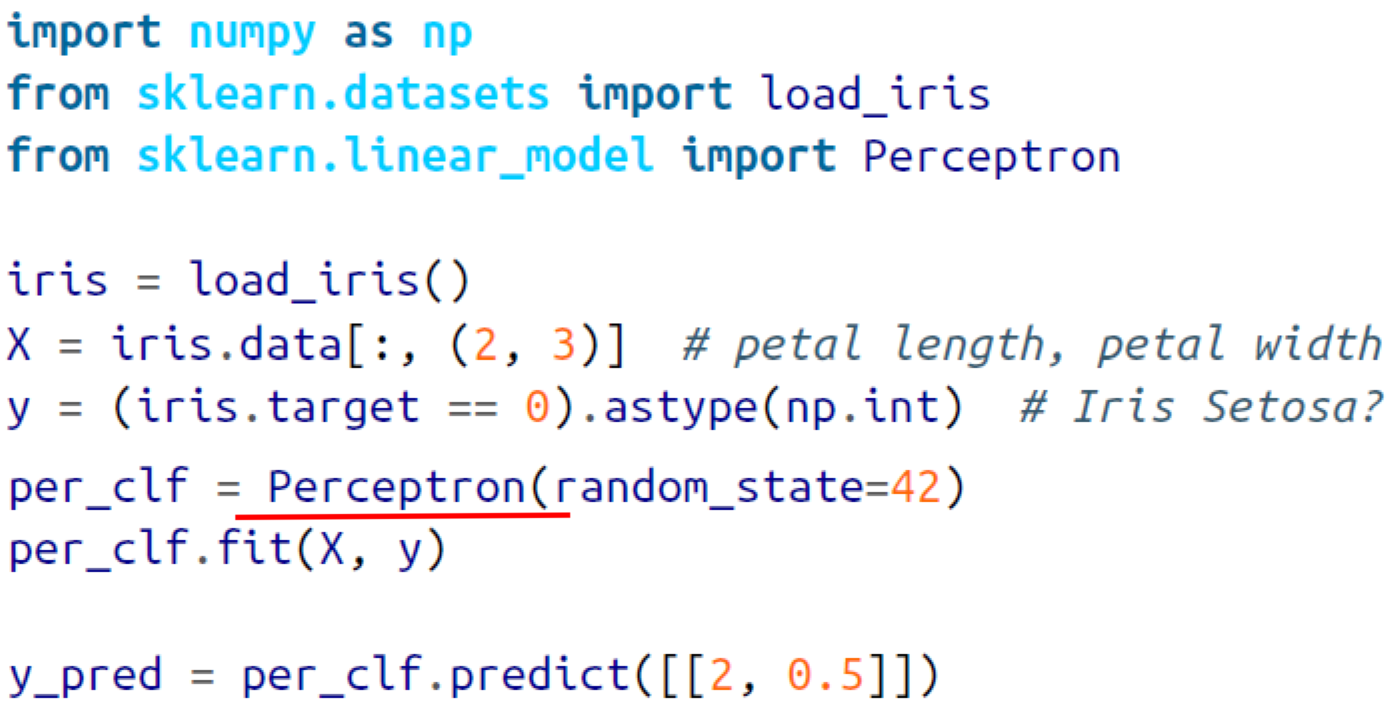
- The Perceptron has an *input layer* with *bias* and *output layer*.
- With multiple output nodes, it can perform multiclass classification.
- Hebbian learning "Cells that fire together, wire together."



$$\boxed{w_{i,j}^{(\text{next step})} = w_{i,j} + \eta\left(y_j - \hat{y}_j\right)x_i}$$

2. The Perceptron

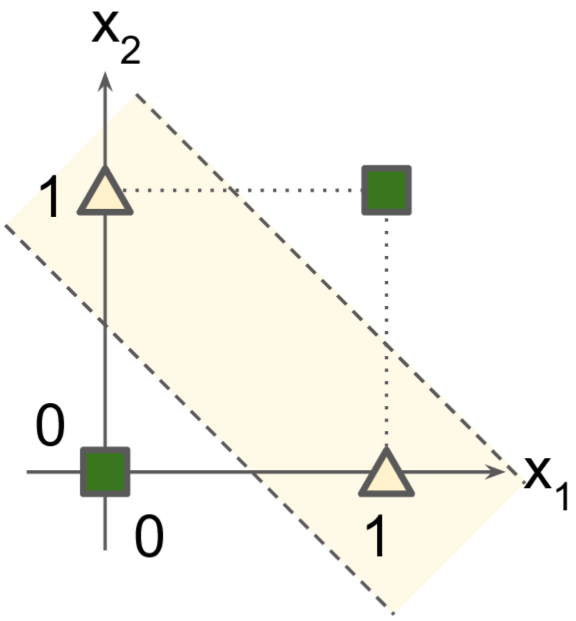
- Scikit-Learn provides a perceptron class.

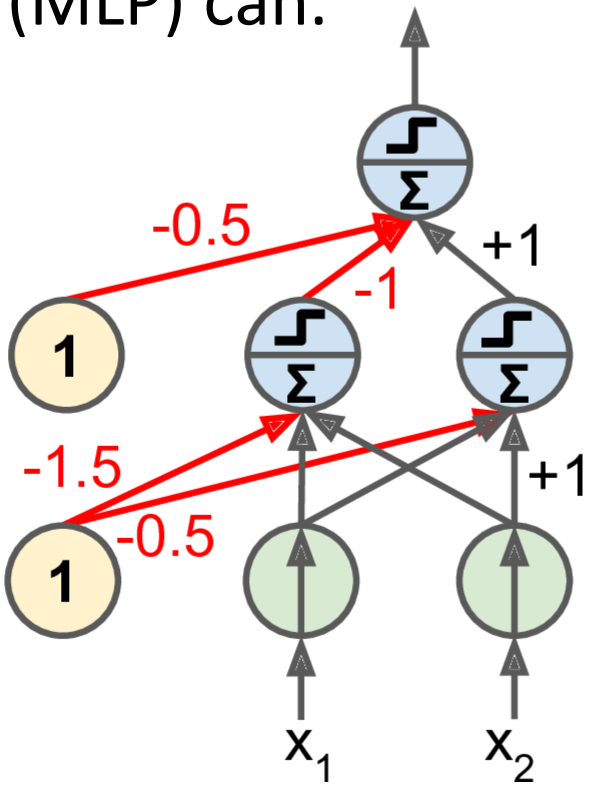


```python
import numpy as np
from sklearn.datasets import load_iris
from sklearn.linear_model import Perceptron

iris = load_iris()
X = iris.data[:, (2, 3)]  # petal length, petal width
y = (iris.target == 0).astype(np.int)  # Iris Setosa?
per_clf = Perceptron(random_state=42)
per_clf.fit(X, y)

y_pred = per_clf.predict([[2, 0.5]])
```

2. The Perceptron

- The perceptron cannot solve non-linear problems such as the XOR problem.
- The Multi-Layer Perceptron (MLP) can.





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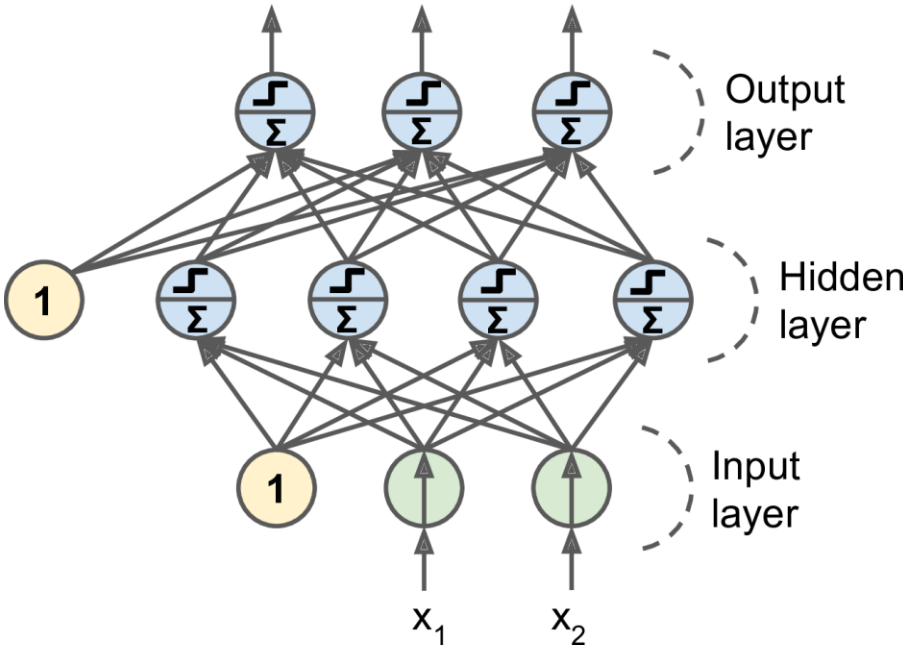
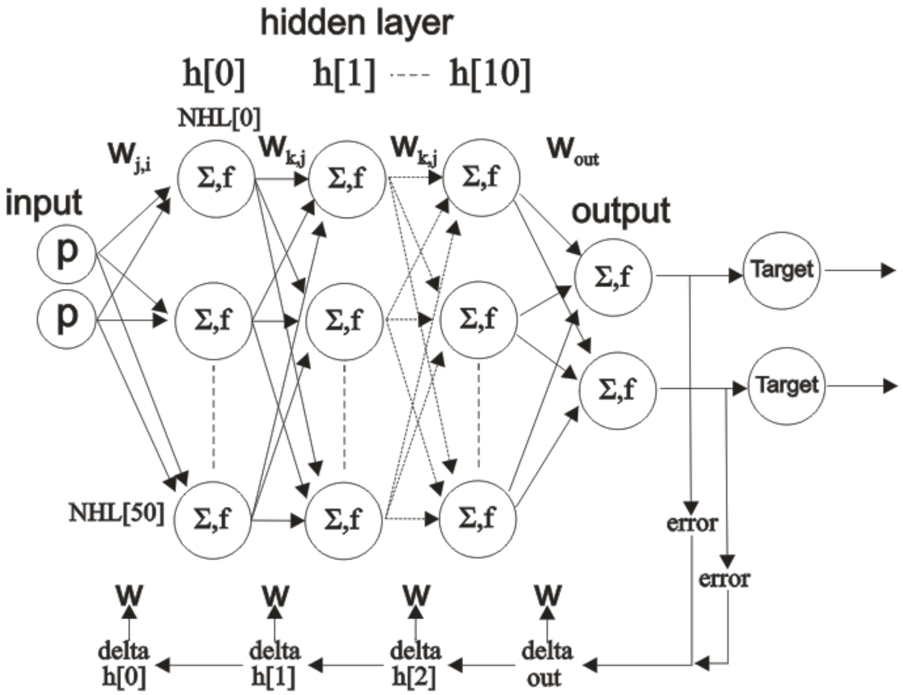
3. Multi-Layer Perceptron (MLP)

- An MLP is composed of a (pass-through) input layer, one or more layers of LTUs, called *hidden layers*, and a final layer of LTUs called the output layer.
- When an ANN has two or more hidden layers, it is called a *deep neural network* (DNN).



3. Multi-Layer Perceptron (MLP)

- Trained using the *backpropagation training algorithm*.
  - For each training instance the algorithm first makes a prediction (*forward pass*), measures the error,
  - then goes through each layer in reverse to measure the error contribution from each connection (*reverse pass*),
  - and finally slightly tweaks the connection weights to reduce the error (*Gradient Descent step*).



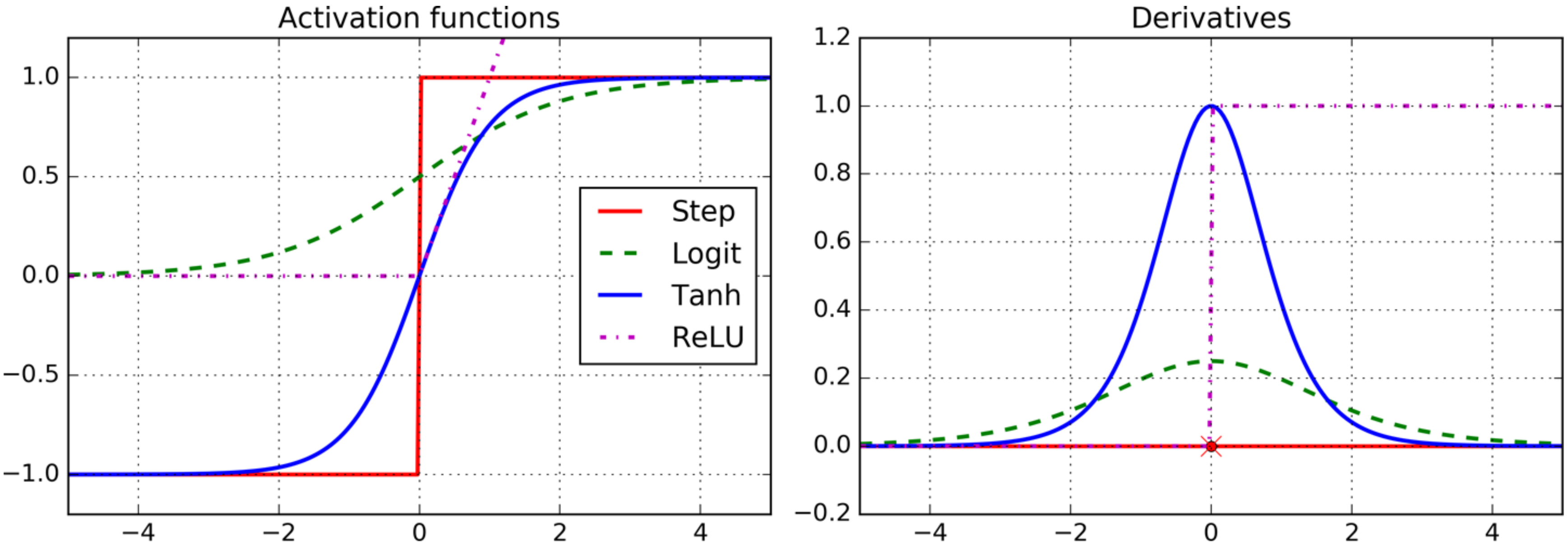
3. Multi-Layer Perceptron (MLP)

- **Common activation functions**: logistic, hyperbolic tangent, and rectified linear unit.

$$\sigma(z) = 1 \,/\, (1 + \exp(-z))$$

$$tanh\ (z) = 2\sigma(2z) - 1$$

$$\mathrm{ReLU}\ (z) = \max\ (0, z)$$



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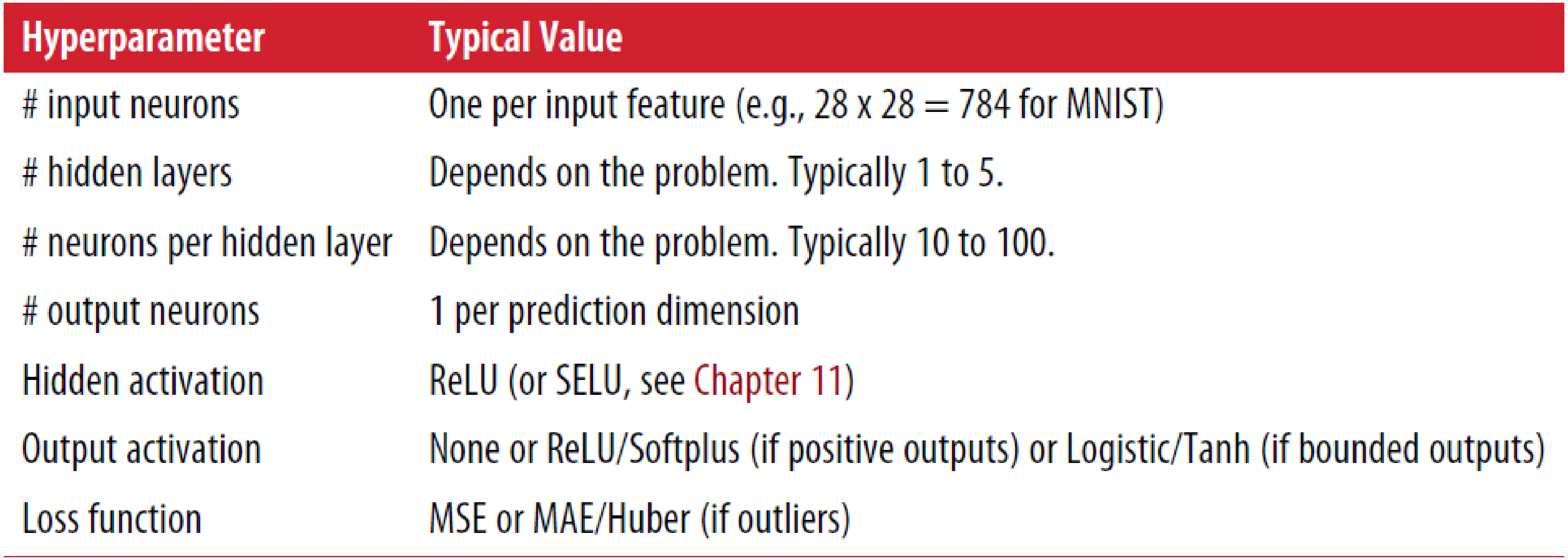
4. Regression MLPs

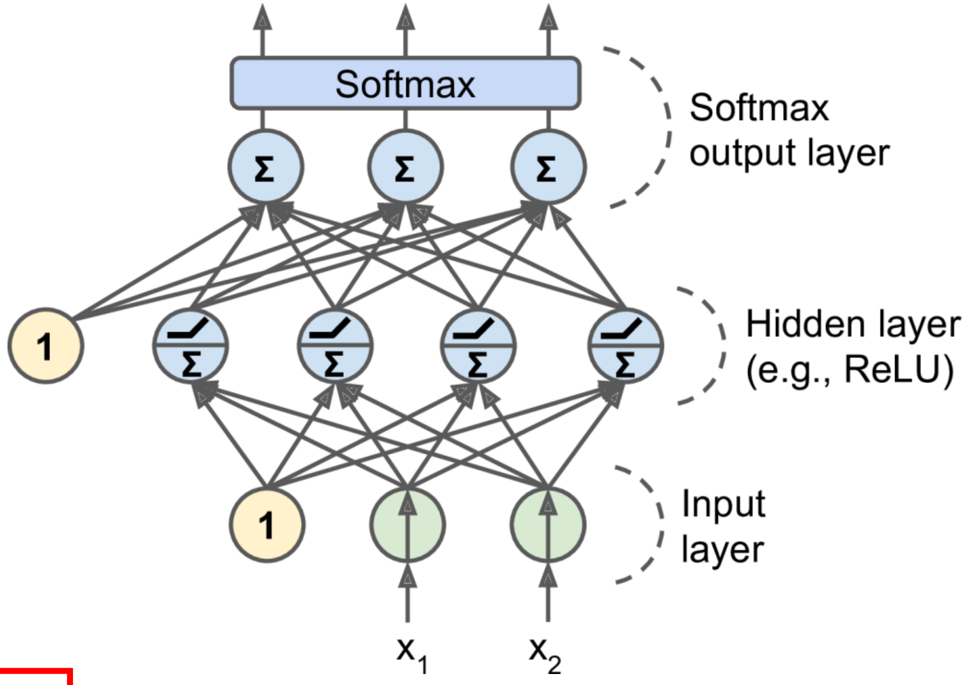
- Typical MLP architecture for **regression**:



Hyperparameter	Typical Value
# input neurons	One per input feature (e.g., 28 x 28 = 784 for MNIST)
# hidden layers	Depends on the problem. Typically 1 to 5.
# neurons per hidden layer	Depends on the problem. Typically 10 to 100.
# output neurons	1 per prediction dimension
Hidden activation	ReLU (or SELU, see Chapter 11)
Output activation	None or ReLU/Softplus (if positive outputs) or Logistic/Tanh (if bounded outputs)
Loss function	MSE or MAE/Huber (if outliers)

5. Classification MLPs

- For **classification**, the output layer uses the *softmax function*.
- The output of each neuron corresponds to the estimated probability of the corresponding class.

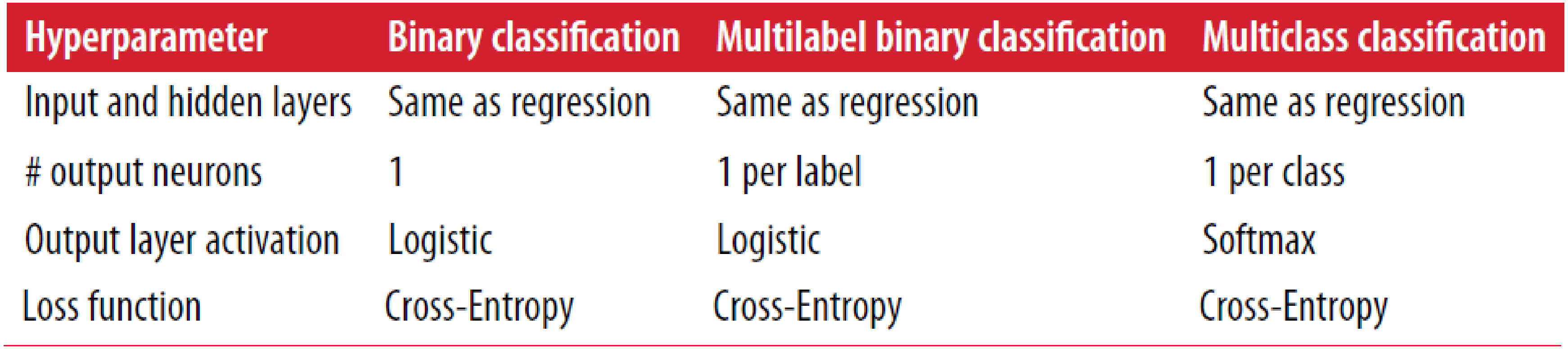


$$\hat{p}_k = \sigma(\mathbf{s}(\mathbf{x}))_k = \frac{\exp\left(s_k(\mathbf{x})\right)}{\sum_{j=1}^{K} \exp\left(s_j(\mathbf{x})\right)}$$

$$\hat{y} = \underset{k}{\operatorname{argmax}}\ \sigma(\mathbf{s}(\mathbf{x}))_k$$

5. Classification MLPs

- Typical MLP architecture for **classification**:



Hyperparameter	Binary classification	Multilabel binary classification	Multiclass classification
Input and hidden layers	Same as regression	Same as regression	Same as regression
# output neurons	1	1 per label	1 per class
Output layer activation	Logistic	Logistic	Softmax
Loss function	Cross-Entropy	Cross-Entropy	Cross-Entropy

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