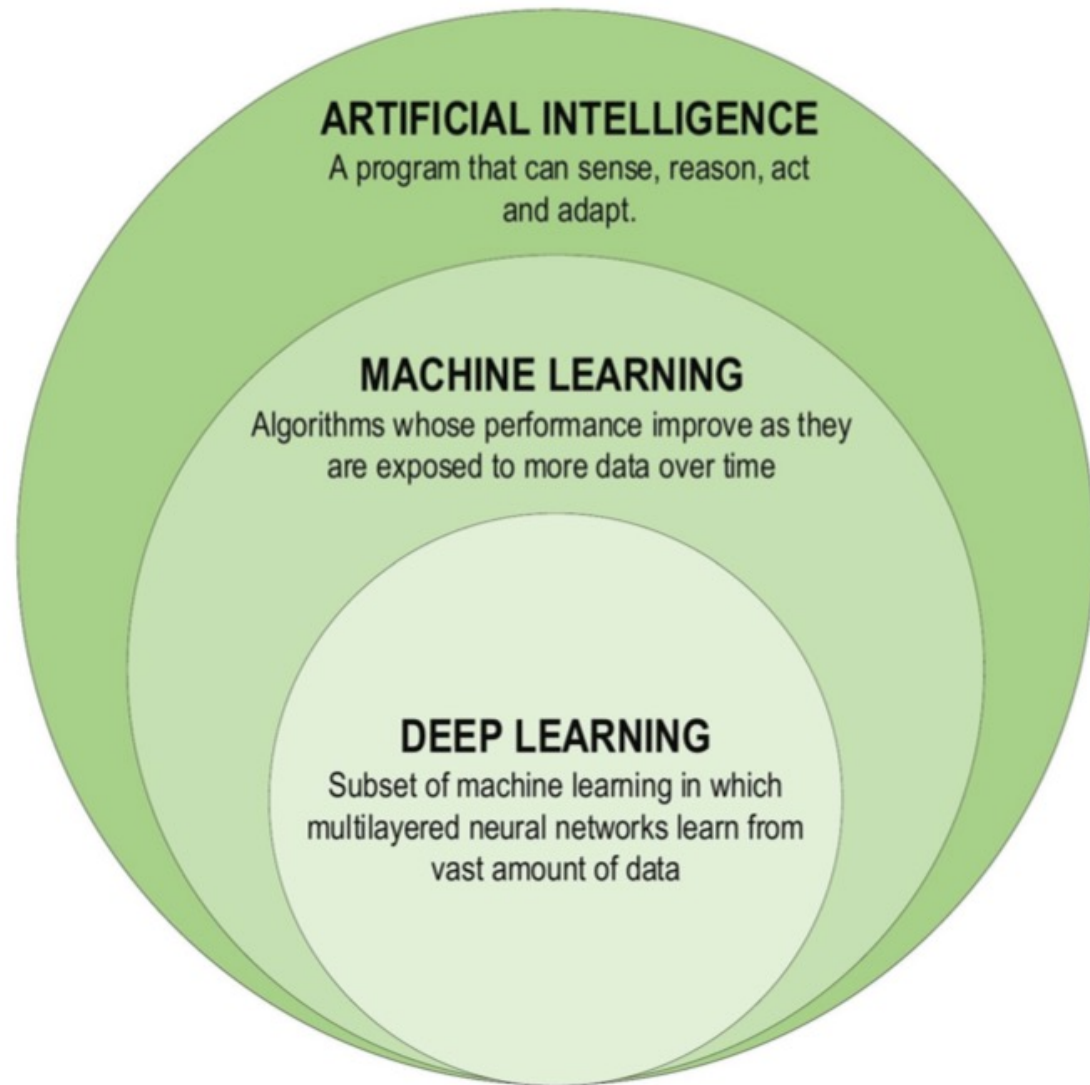




NEURAL NETWORKS

1.1 Introduction



NN Architectures

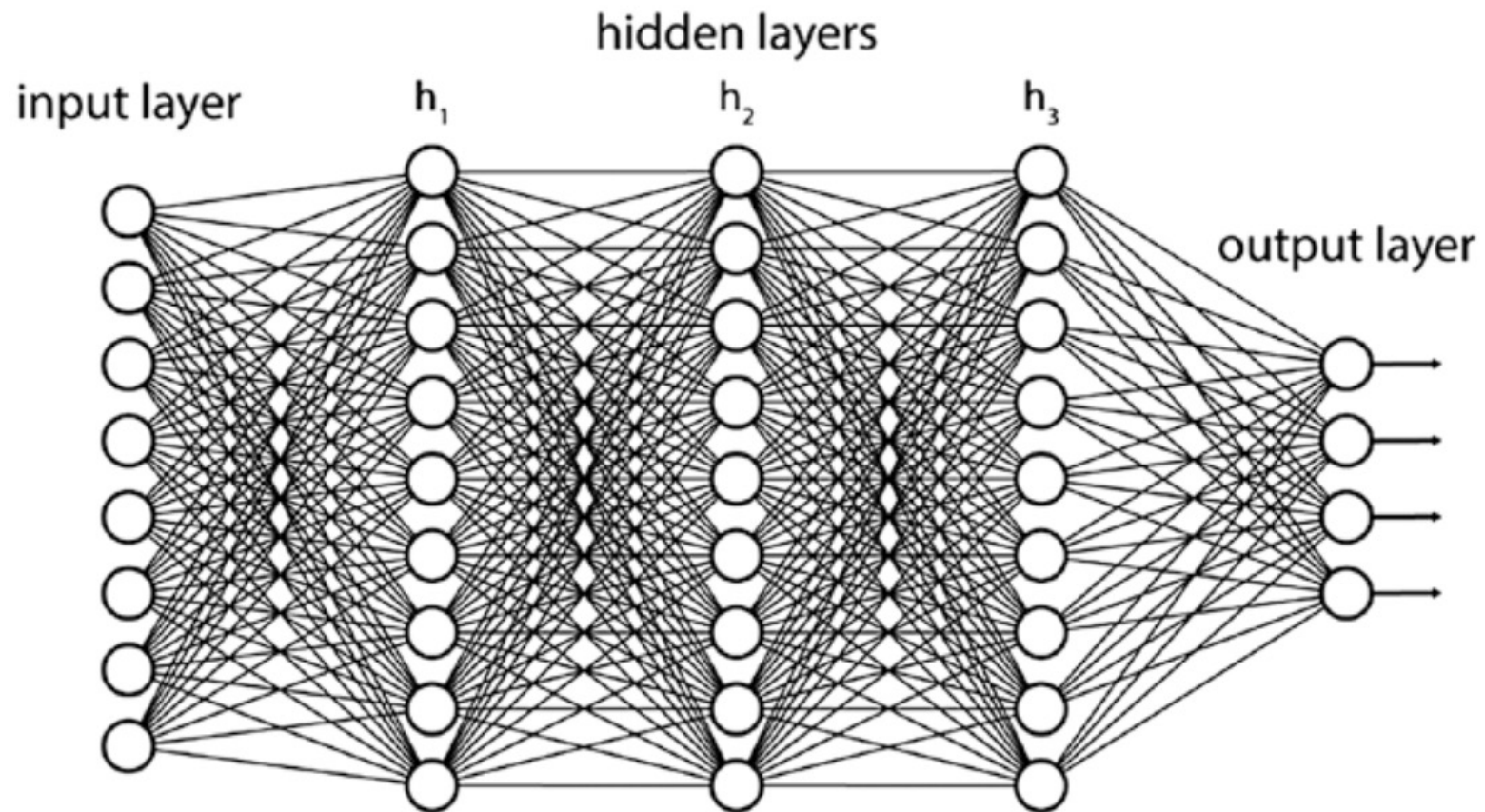
Neural Network Architectures

- The way the NN nodes connect allowing for the input data to be transformed into new meaningful representation of the data defines the NN architecture.
- The most simple NN architecture is the

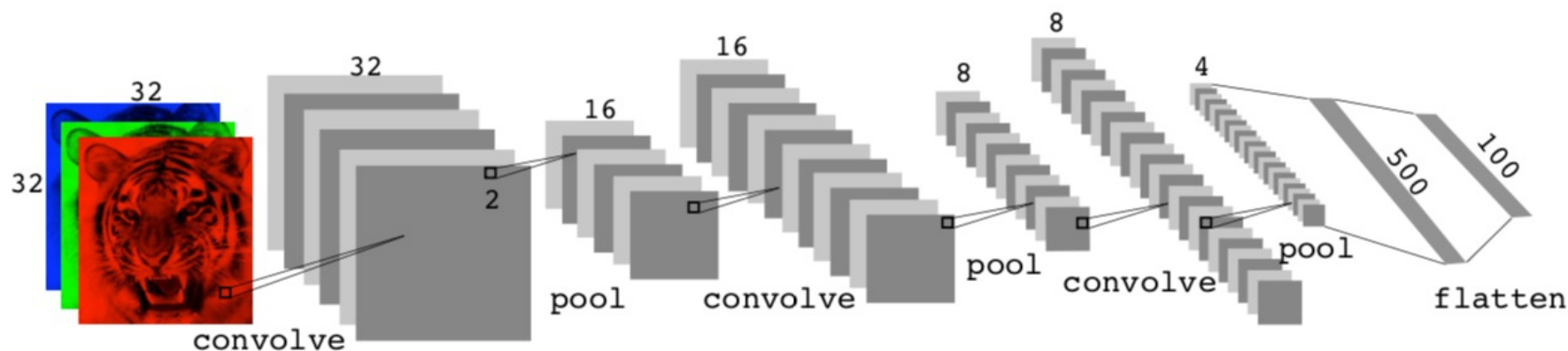
Neural Network Architectures

- Densely connected neural network (MLP)
- Convolutional Neural Networks (convnets, CNN)
- Recurrent Neural Networks (RNN)
- Long-Short Term Memory Networks (LSTM)
- Transformer Neural Networks
- Generative AI Networks

MLP (Sequence of connected layers)

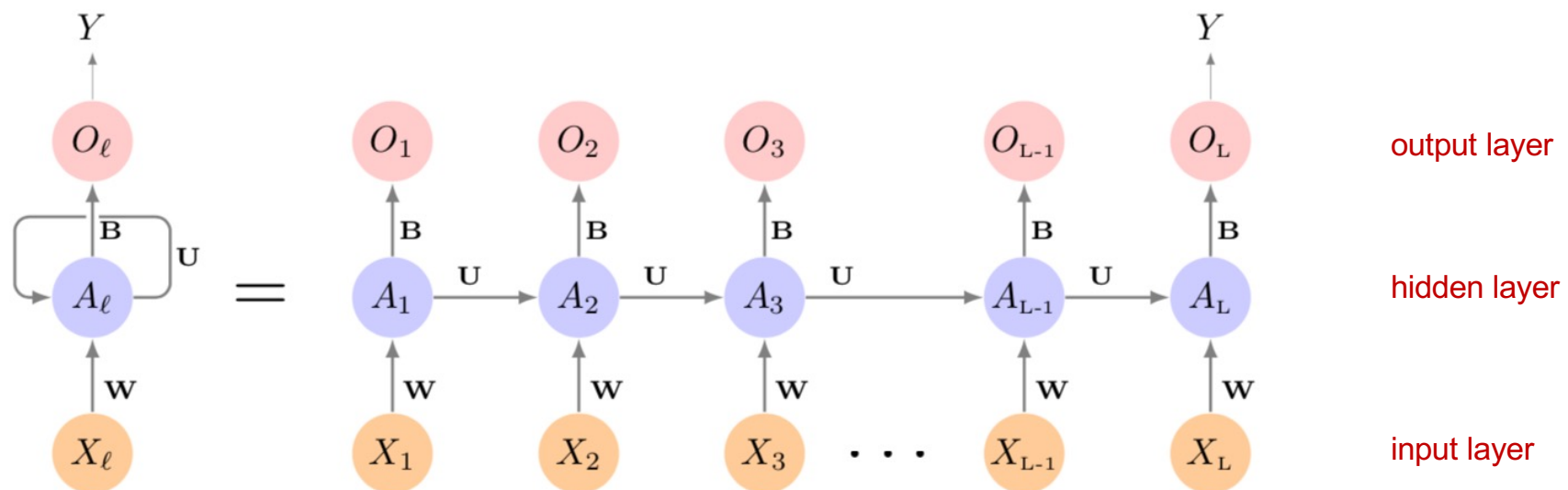


Deep CNN model for the CIFAR100 image classification



Convolution layers are interspersed with 2×2 max-pool layers, which reduce the size by a factor of 2 in both dimensions.

Simple Recurrent Neural Network (RNN)

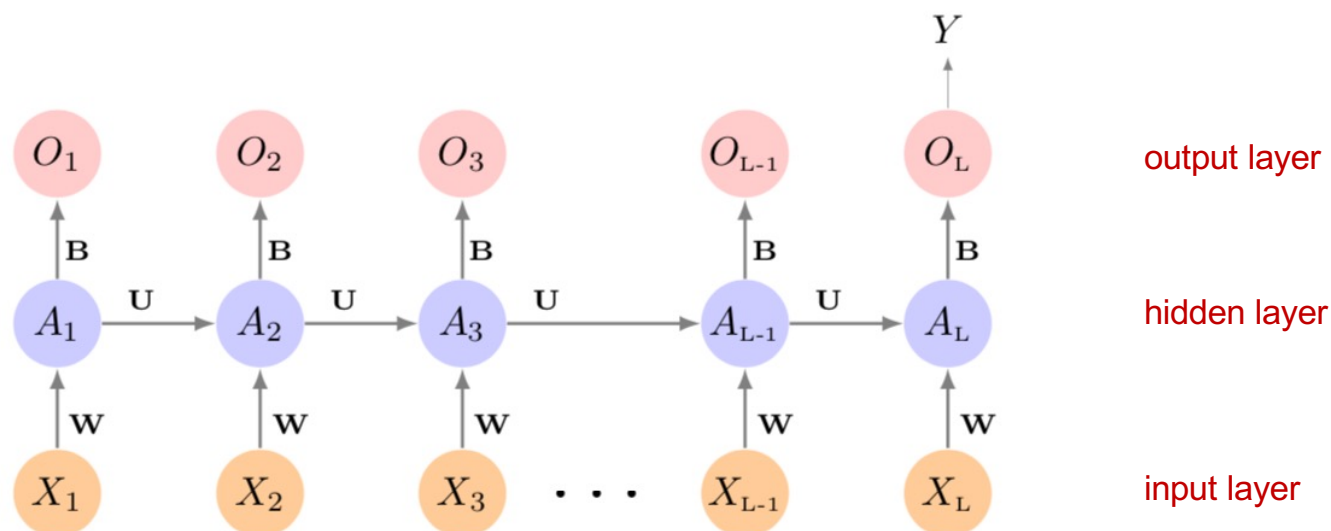


short representation
of the network

The network is unrolled
into a more explicit version

- The input is a sequence of vectors X_1, \dots, X_L the target is a single response Y
- The weights W , U and B are estimated as the sequence is processed

Simple Recurrent Neural Network (RNN)



- The NN processes the input sequence X sequentially
- Each X_i feeds into the hidden layer, which has as input the activation vector A_i from the previous element in the sequence producing the current activation vector A_i
- The output layer produces a sequence of predictions O_i from the current activation A_i , but typically only the last of these, O_L , is of relevance

Introduction

- sklearn is used for MLP (not for other DL architecture)
- Keras is the library for building most deep learning models
- Providing high-level operations for quick and easy implementation
- Tensor libraries are used for low-level operations (tensor manipulation and differentiation)
 - Tensorflow (by Google)
 - CNTK (by Microsoft)
 - Theano (by U. of Montreal)

Perceptron

Perceptron

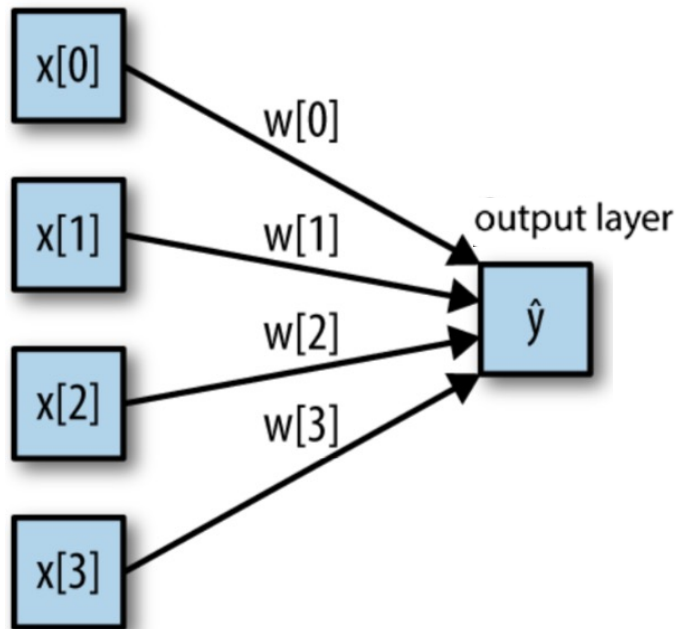
The Perceptron is the simplest NN model

It is used for **classification** when there are

- Two categories
- Linearly separable data

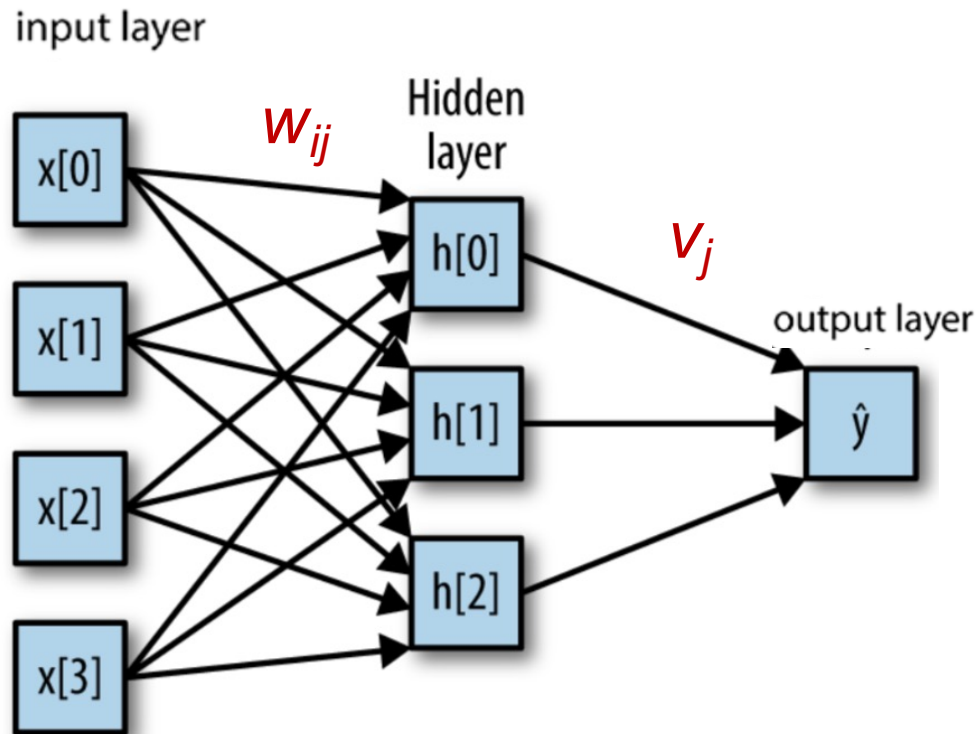
Perceptron (1 input and 1 output layer)

input layer



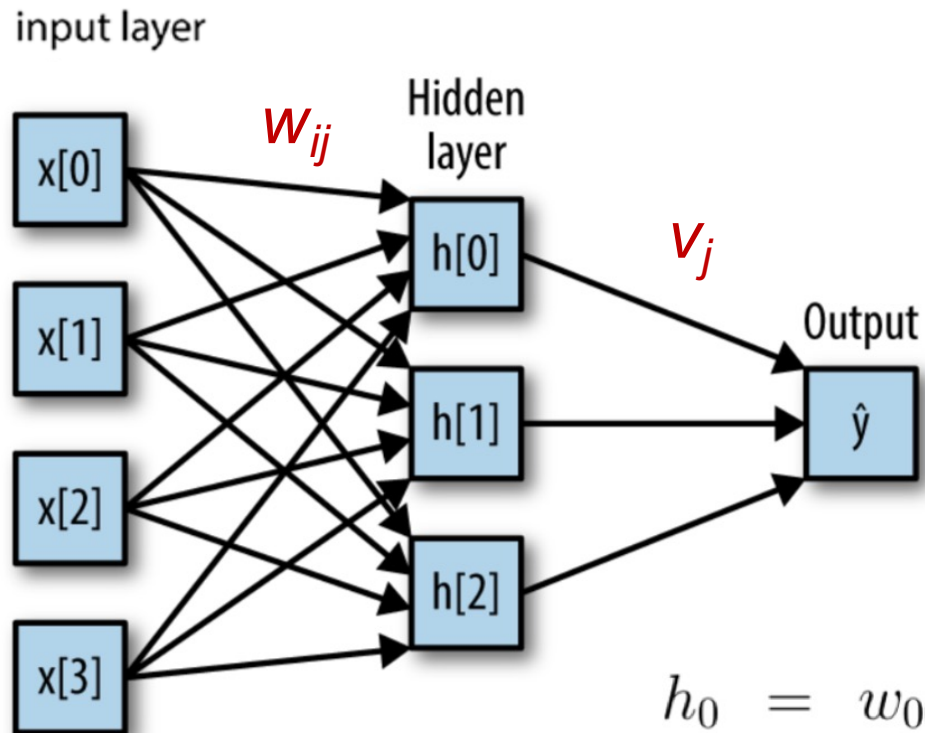
for each row $\hat{y} = w_0x_0 + w_1x_1 + w_2x_2 + w_3x_3$

Multilayer Perceptron (MLP)



A perceptron supplemented with one or more hidden layers

Multilayer Perceptron (MLP)



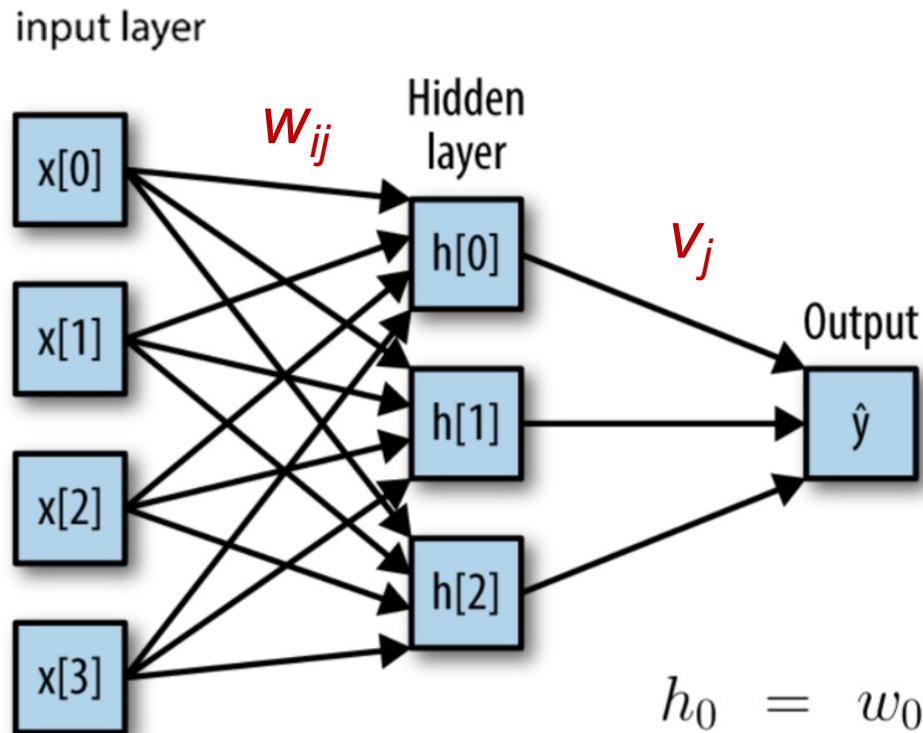
A perceptron
supplemented with
one or more hidden
layers

$$h_0 = w_{00}x_0 + w_{10}x_1 + w_{20}x_2 + w_{30}x_3 + b_0$$

$$h_1 = w_{01}x_0 + w_{11}x_1 + w_{21}x_2 + w_{31}x_3 + b_1$$

$$h_2 = w_{02}x_0 + w_{12}x_1 + w_{22}x_2 + w_{32}x_3 + b_2$$

Multilayer Perceptron



A generalization of linear model with multiple stages of processing to come to a decision (prediction or classification)

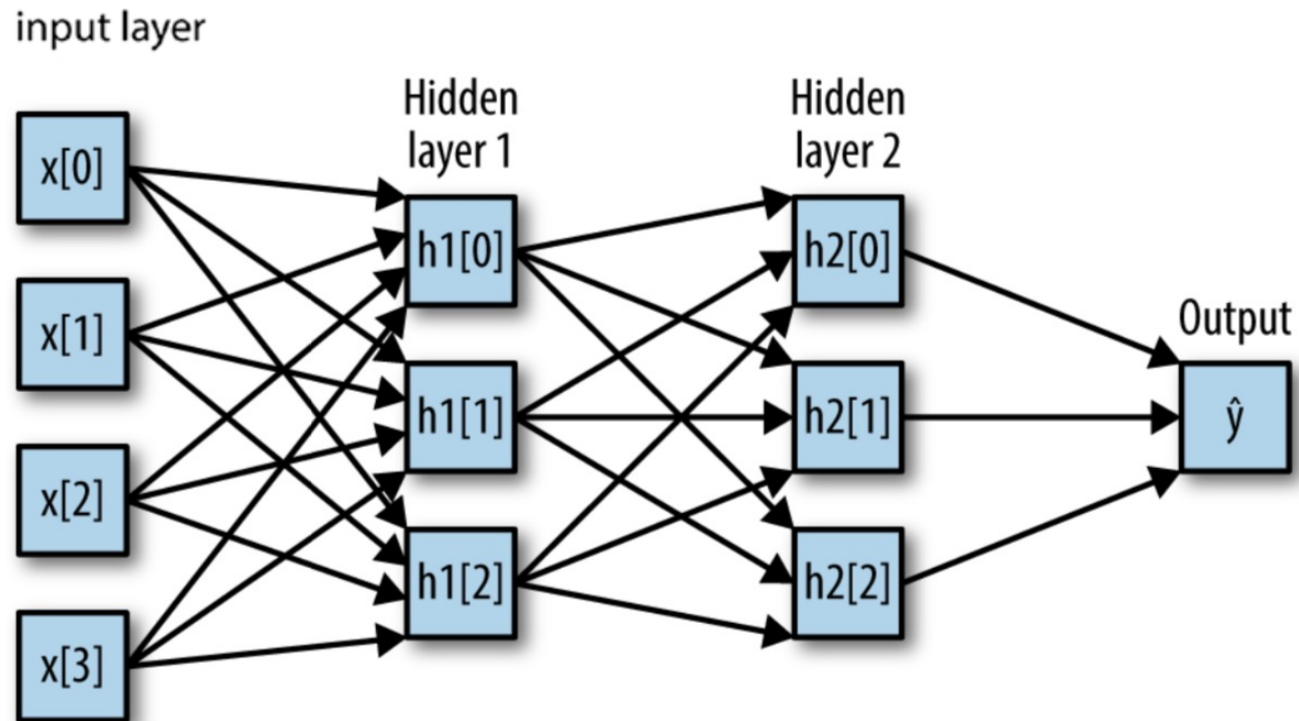
$$h_0 = w_{00}x_0 + w_{10}x_1 + w_{20}x_2 + w_{30}x_3 + b_0$$

$$h_1 = w_{01}x_0 + w_{11}x_1 + w_{21}x_2 + w_{31}x_3 + b_1$$

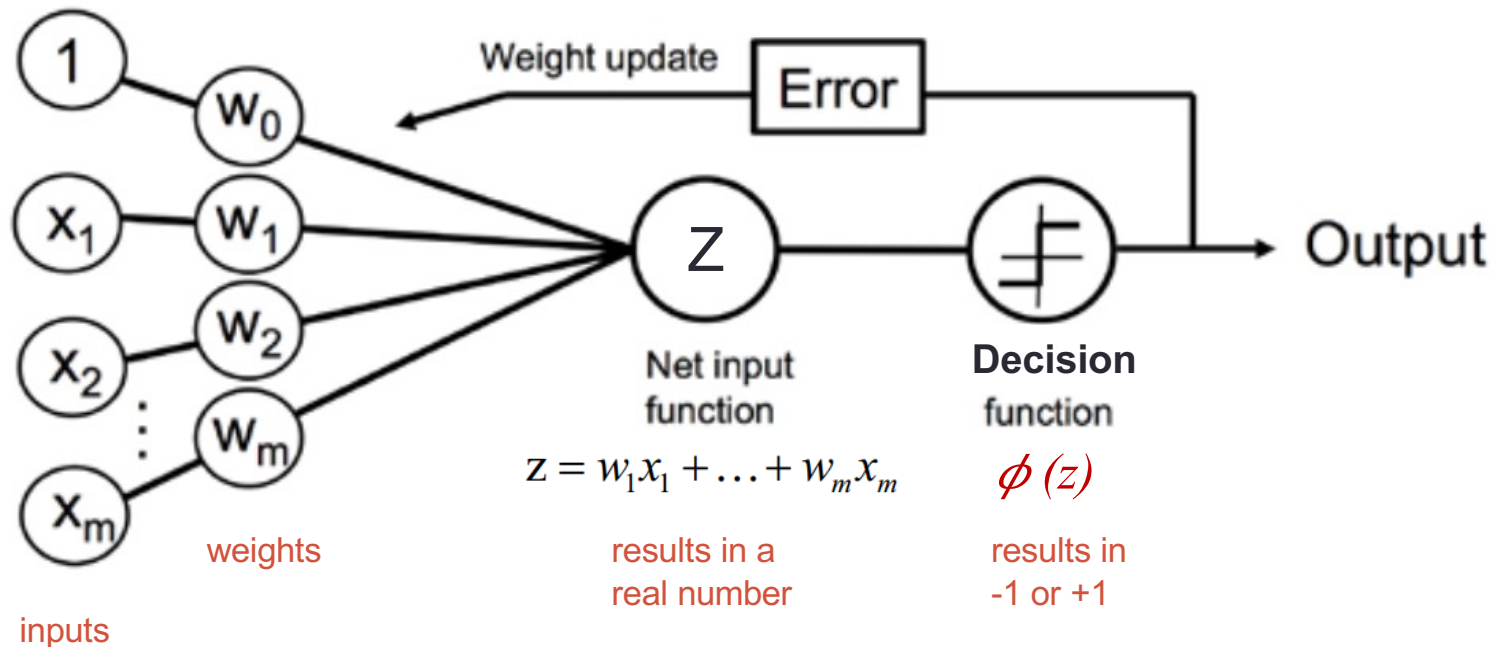
$$h_2 = w_{02}x_0 + w_{12}x_1 + w_{22}x_2 + w_{32}x_3 + b_2$$

$$\hat{y} = v_0h_0 + v_1h_1 + v_2h_2 + b$$

Multilayer Perceptron (two hidden layers)

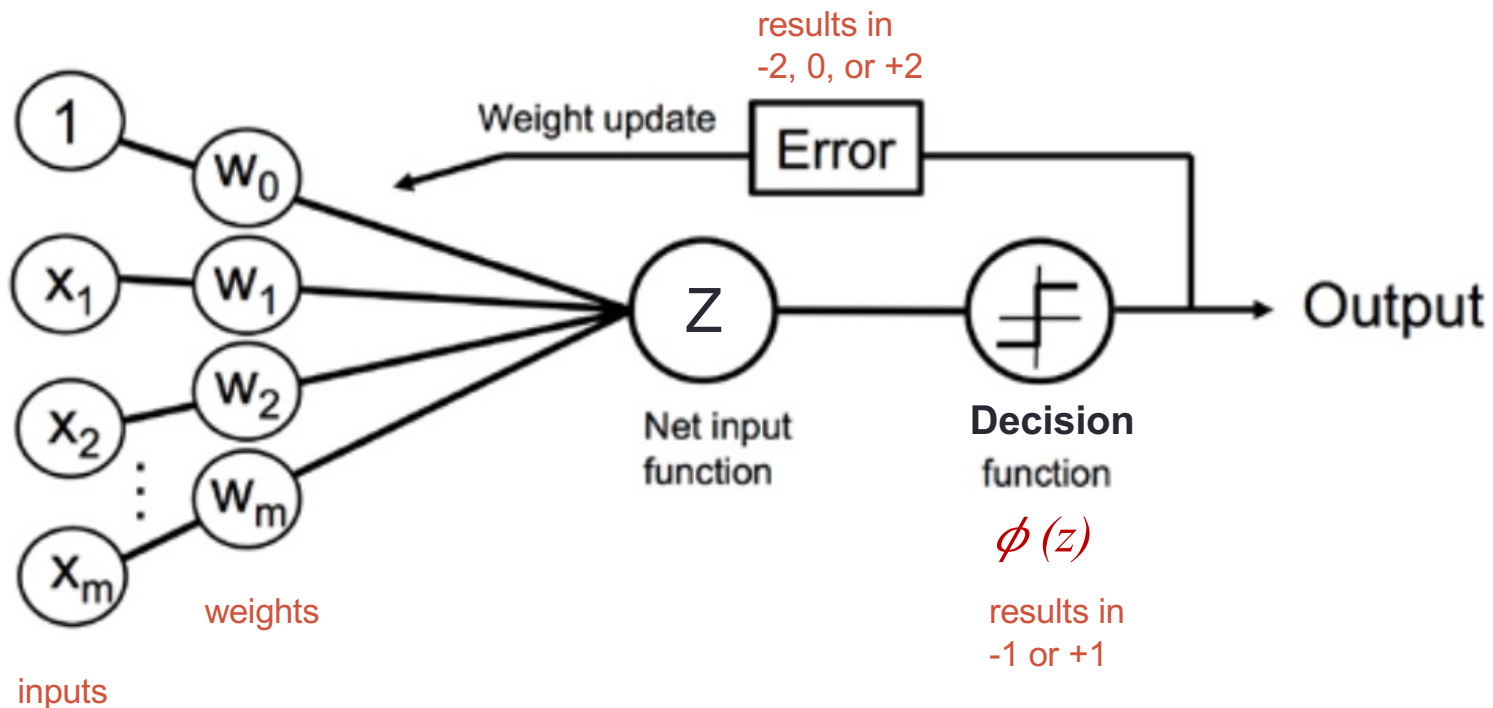


Perceptron



Combines **inputs** with **weights** to obtain the net input Z which is passed on to predict the category by means of a decision function $\phi(z)$ (also called threshold function)

Perceptron



- Predicted categories (**-1 or 1**) are compared to true categories to compute the error and update the weights.
- The process is repeated multiple times (epochs) until convergence (error is small enough).

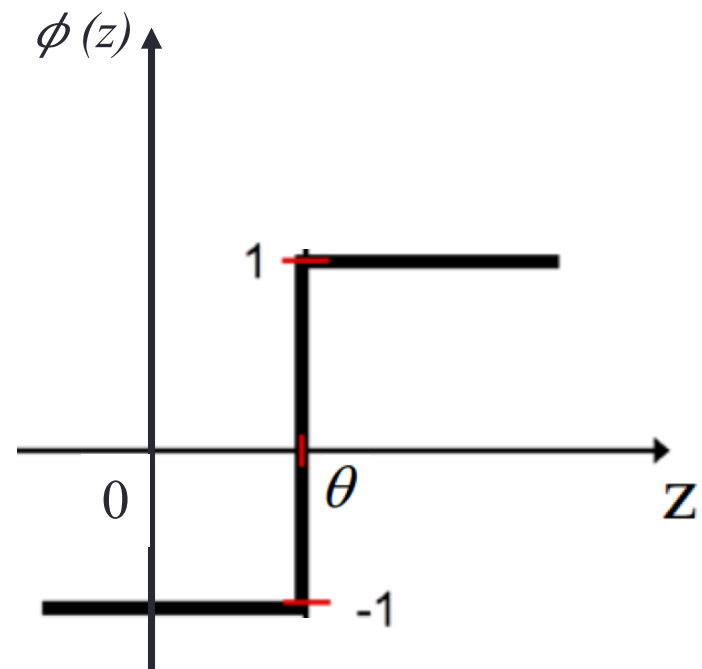
Perceptron

net input function $Z = w_1x_1 + \dots + w_mx_m$

decision function $\phi(z)$

$$\phi(z) = \begin{cases} 1 & \text{if } z \geq \theta \\ -1 & \text{otherwise} \end{cases}$$

θ is called the threshold



Perceptron

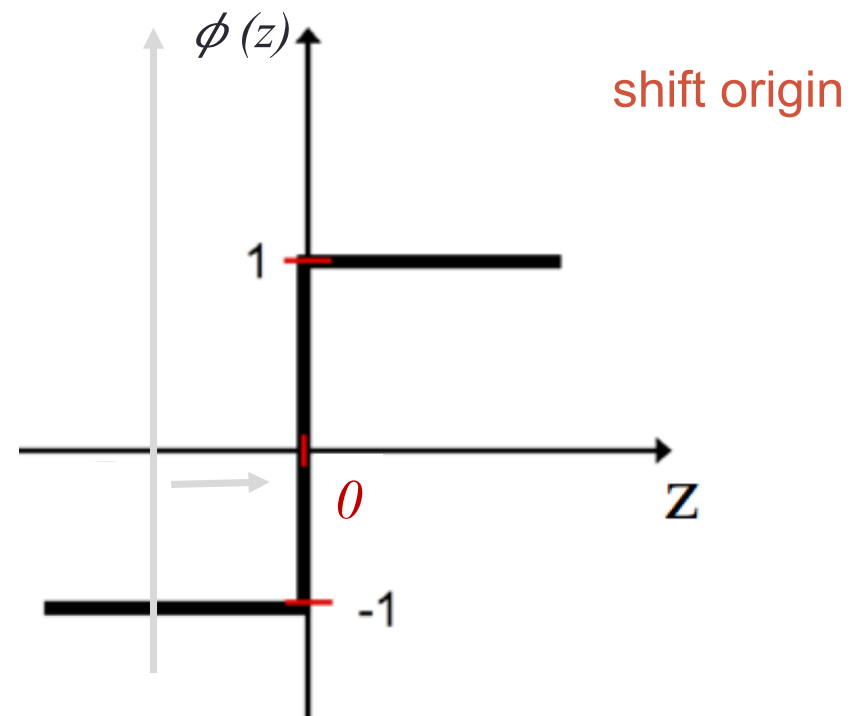
net input function

$$Z = w_0 x_0 + w_1 x_1 + \dots + w_m x_m$$

$$w_0 = -\theta \text{ and } x_0 = 1$$

decision function

$$\phi(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ -1 & \text{otherwise} \end{cases}$$



Perceptron

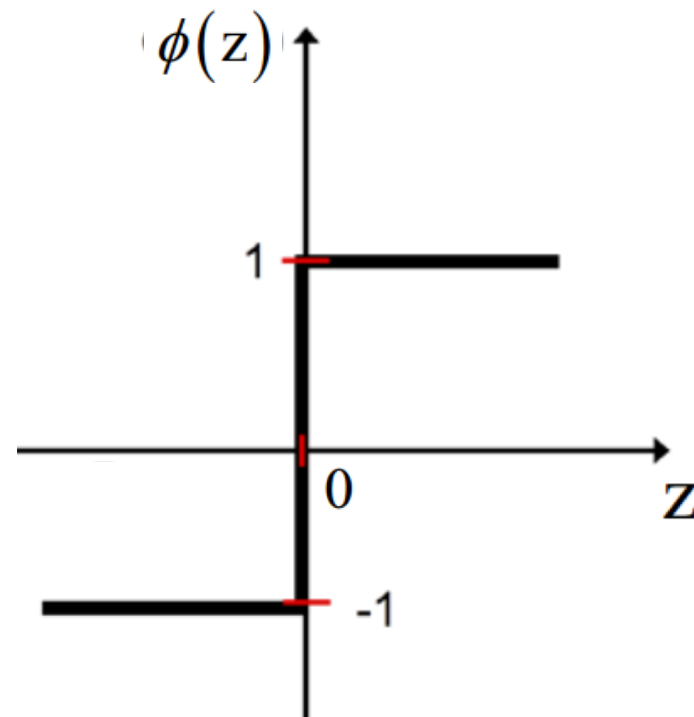
input function in
matrix notation

net input function $z = w_0x_0 + w_1x_1 + \dots + w_mx_m = \mathbf{w}^T \mathbf{x}$

$$w_0 = -\theta \text{ and } x_0 = 1$$

decision function

$$\phi(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ -1 & \text{otherwise} \end{cases}$$



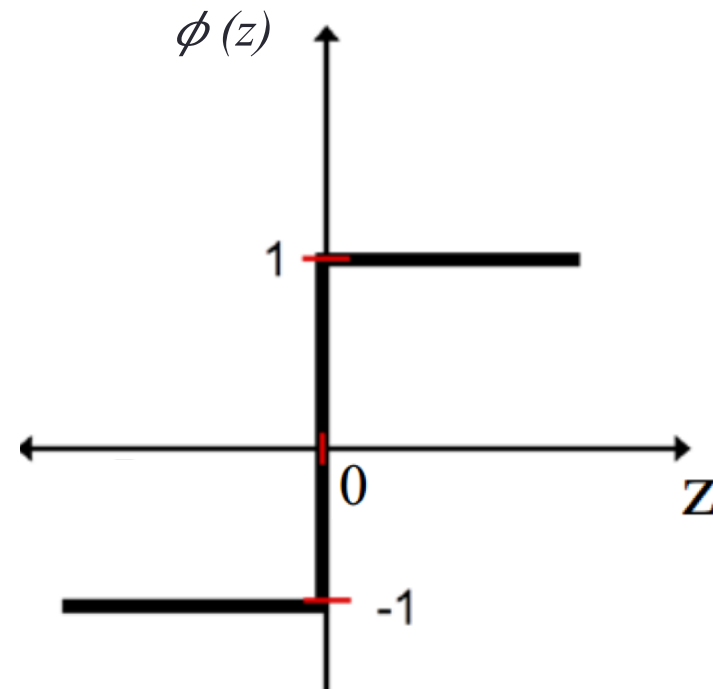
Perceptron

threshold function $\phi(z)$

$$\phi(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

input function

$$z = \mathbf{w}^T \mathbf{x}$$



Perceptron learning rule

- For each column, randomly initialize the weights w_1, \dots, w_p

- For each row $i = 1, \dots, n$

find $\hat{y}_i = \phi(z_i)$

find the error $(y_i - \hat{y}_i)$

update the weights $w_j = w_j + \Delta w_j$

using $\Delta w_j = \lambda(y_i - \hat{y}_i) x_{ij}$

for each column $j = 1, \dots, p$

- Repeat N times

Perceptron learning rule

- For each column, randomly initialize the weights w_1, \dots, w_p
- For each row $i = 1, \dots, n$

find $\hat{y}_i = \phi(z_i)$

prediction is +1 or -1

find the error $(y_i - \hat{y}_i)$

update the weights $w_j = w_j + \Delta w_j$

using $\Delta w_j = \lambda(y_i - \hat{y}_i) x_{ij}$

for each column $j = 1, \dots, p$

- Repeat N times

Perceptron learning rule

- For each column, randomly initialize the weights w_1, \dots, w_p
- For each row $i = 1, \dots, n$

find $\hat{y}_i = \phi(z_i)$

find the error $(y_i - \hat{y}_i)$

error is -2, 0, or +2

update the weights $w_j = w_j + \Delta w_j$

using $\Delta w_j = \lambda(y_i - \hat{y}_i) x_{ij}$

for each column $j = 1, \dots, p$

- Repeat N times

Perceptron learning rule

- For each column, randomly initialize the weights w_1, \dots, w_p

- For each row $i = 1, \dots, n$

find $\hat{y}_i = \phi(z_i)$

find the error $(y_i - \hat{y}_i)$

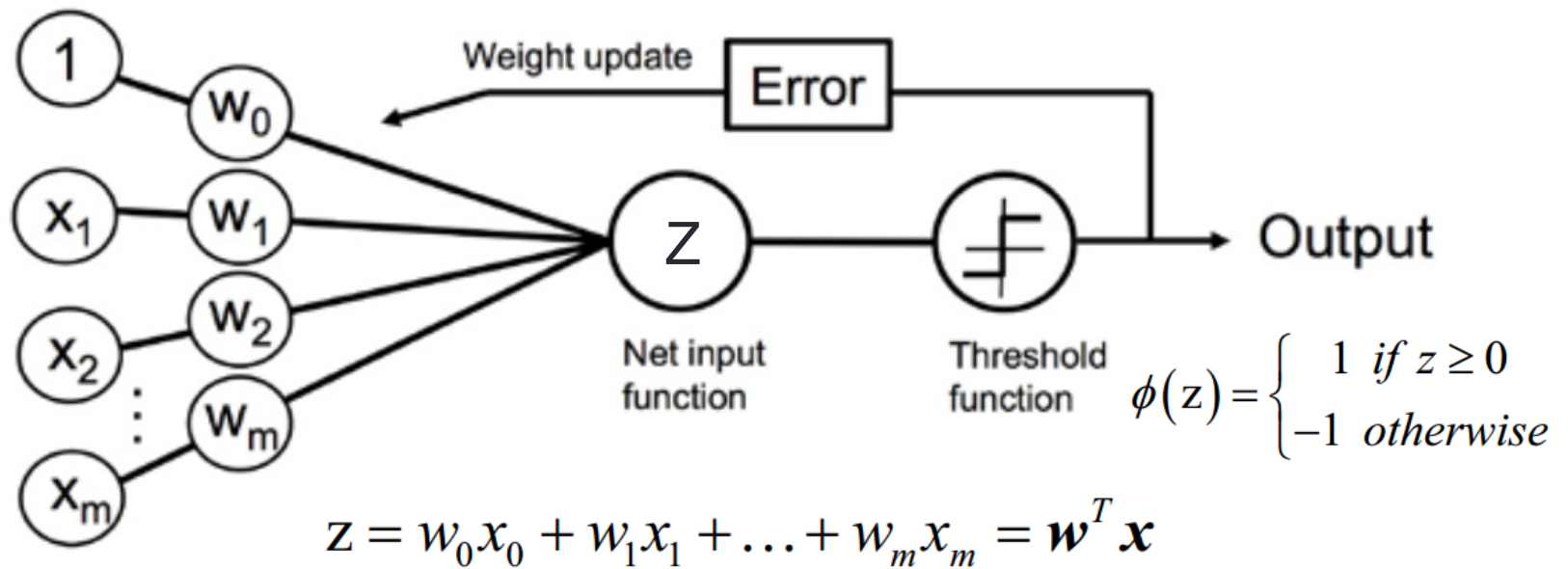
update the weights $w_j = w_j + \Delta w_j$

using $\Delta w_j = \lambda(y_i - \hat{y}_i) x_{ij}$

for each column $j = 1, \dots, p$

- Repeat N times

Perceptron learning rule



Adaline

ADaptive Linear NEuron (Adaline)

- Similar to the Perceptron
- The Perceptron compares the true categories with predicted categories (+1 or -1)
- Adaline compares the true categories with the result of the adaline activation function (a real number)
- Activation function is denoted by $\phi(z)$

ADaptive Linear NEuron (Adaline)

- Find $Z = w_1x_1 + \dots + w_mx_m$
- net input z is transformed using **Activation function**

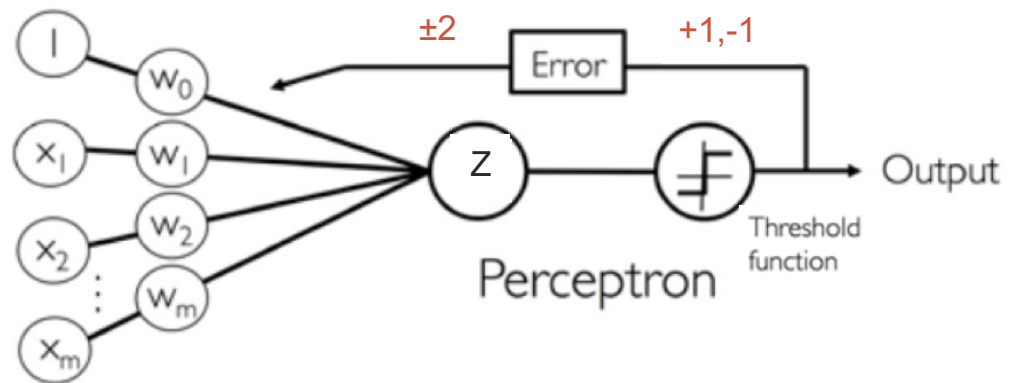
$$\phi(z) = z$$

- Update weights N times
- Prediction is given by **decision function**

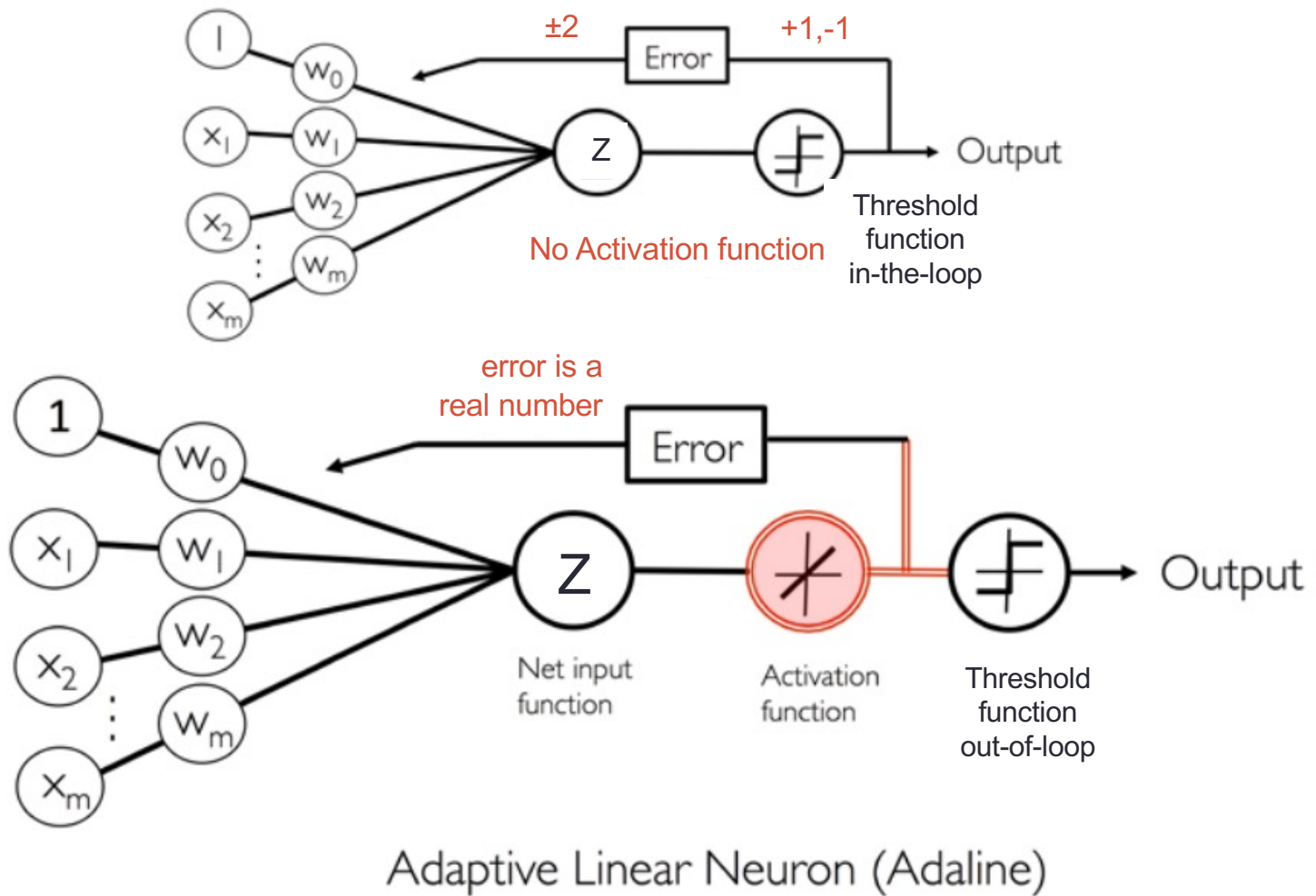
using the updated weights

$$\hat{y} = \begin{cases} 1 & \text{if } z > 0 \\ -1 & \text{if } z \leq 0 \end{cases}$$

Perceptron



Adaline vs Perceptron



Adaline learning rule

- Randomly initialize the weights w_1, \dots, w_p
- For each row $i = 1, \dots, n$

$$\text{find } z_i = w_1 x_{1i} + \dots + w_p x_{pi}$$

find the error $(y_i - z_i)$

error is a real number

$$\text{update the weights } w_j = w_j + \Delta w_j$$

$$\text{using } \Delta w_j = \lambda \sum_{i=1}^n (y_i - \phi(z_i)) x_{ij}$$

for each column $j = 1, \dots, p$

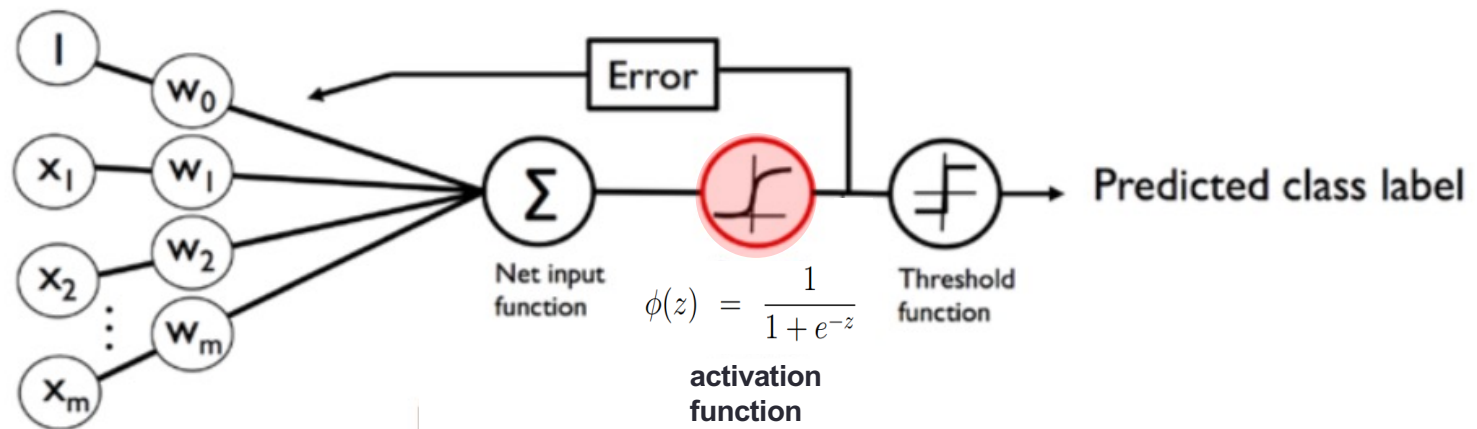
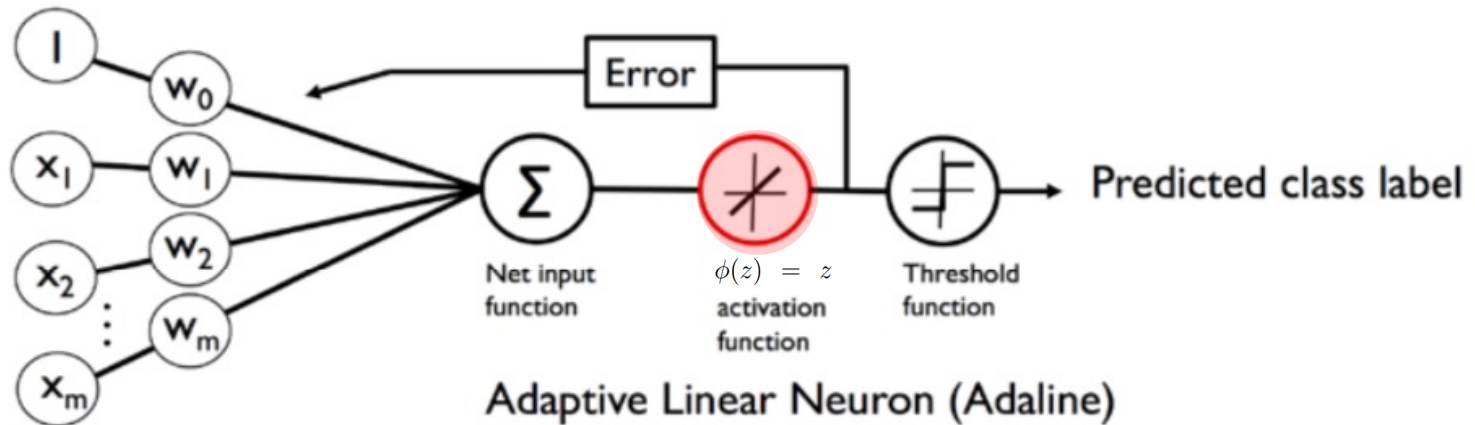
- Repeat N times, then predict with decision function

Logistic Regression

Logistic Regression

- A special case of Adaline with different activation function and loss function

Adaline vs Logistic Regression



Adaline

- activation function

$$\phi(z) = z \quad \text{where} \quad z = w_1 x_1 + \cdots + w_p x_p$$

- loss function

$$\begin{aligned} J(w) &= \sum_{i=1}^n (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^n (y_i - \phi(z_i))^2 = \sum_{i=1}^n (y_i - z_i)^2 \end{aligned}$$

Logistic Regression

- activation function

$$\phi(z) = \frac{1}{1 + e^{-z}} \quad \text{where} \quad z = w_1 x_1 + \cdots + w_p x_p$$

- loss function

$$J(w) = - \sum_{i=1}^n [y_i \log \phi(z_i) + (1 - y_i) \log(1 - \phi(z_i))]$$

Logistic Regression

- Categories labeled as 0 and +1
- Activation function

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

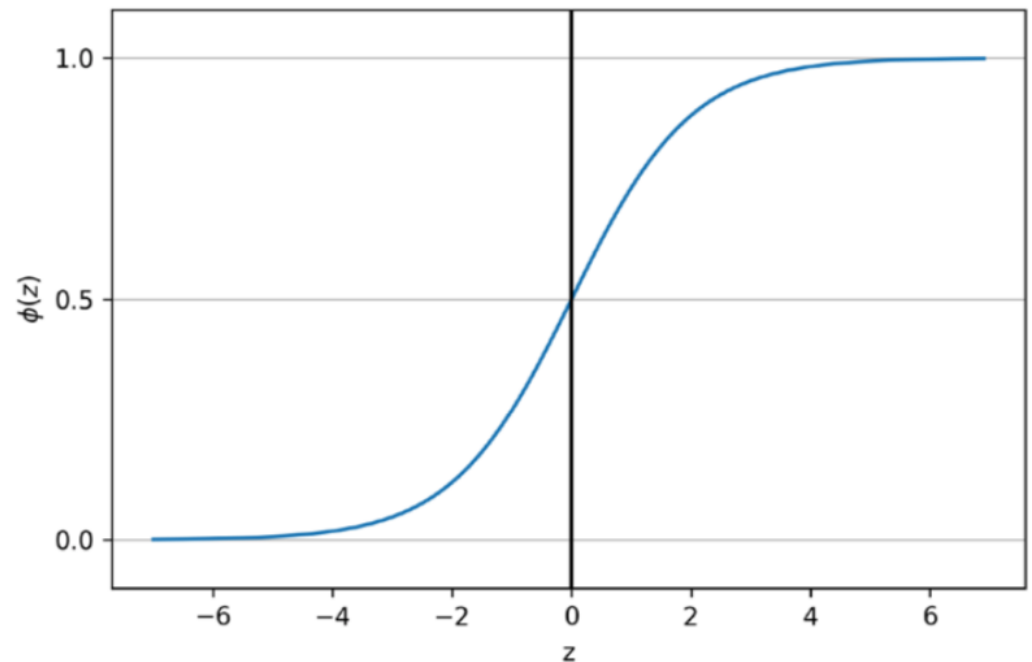
- Decision function (Threshold function)

$$\hat{y} = \begin{cases} 1 & \text{if } \phi(z) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

Logistic Regression

- Activation function

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



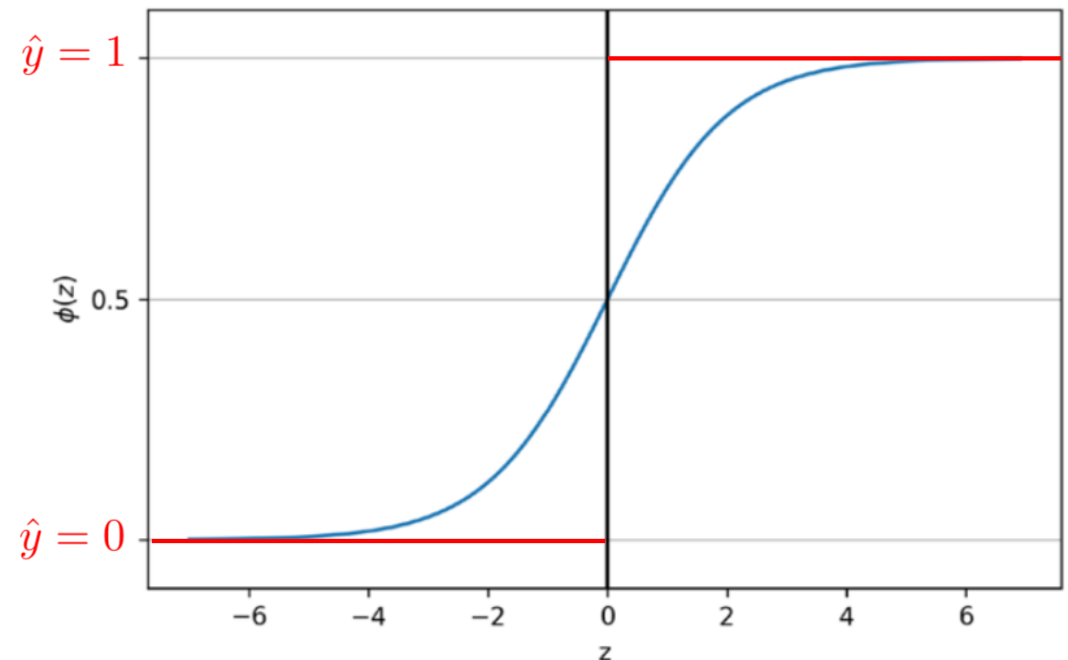
- Decision function

$$\hat{y} = \begin{cases} 1 & \text{if } \phi(z) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

Logistic Regression

- Activation function

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



- Decision function

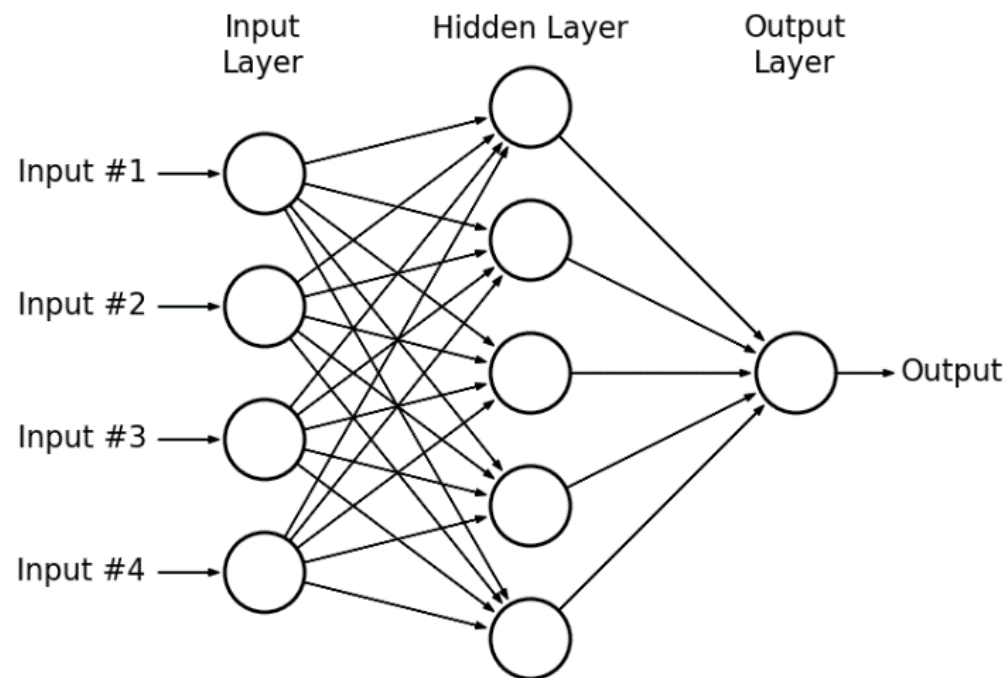
$$\hat{y} = \begin{cases} 1 & \text{if } \phi(z) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

$$\hat{y} = \begin{cases} 1 & \text{if } z \geq 0.0 \\ 0 & \text{otherwise} \end{cases}$$

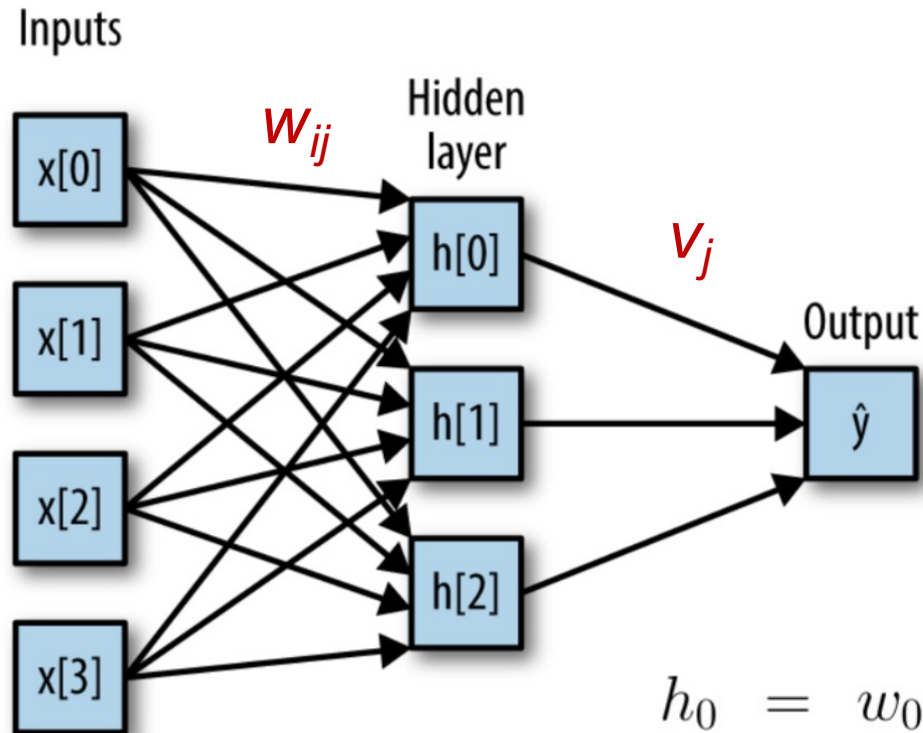
Multilayer Perceptron

Multilayer Perceptron

A Perceptron with at least one intermediate layer



Multilayer Perceptron (MLP)



A generalization of linear model with multiple stages of processing to come to a decision (prediction or classification)

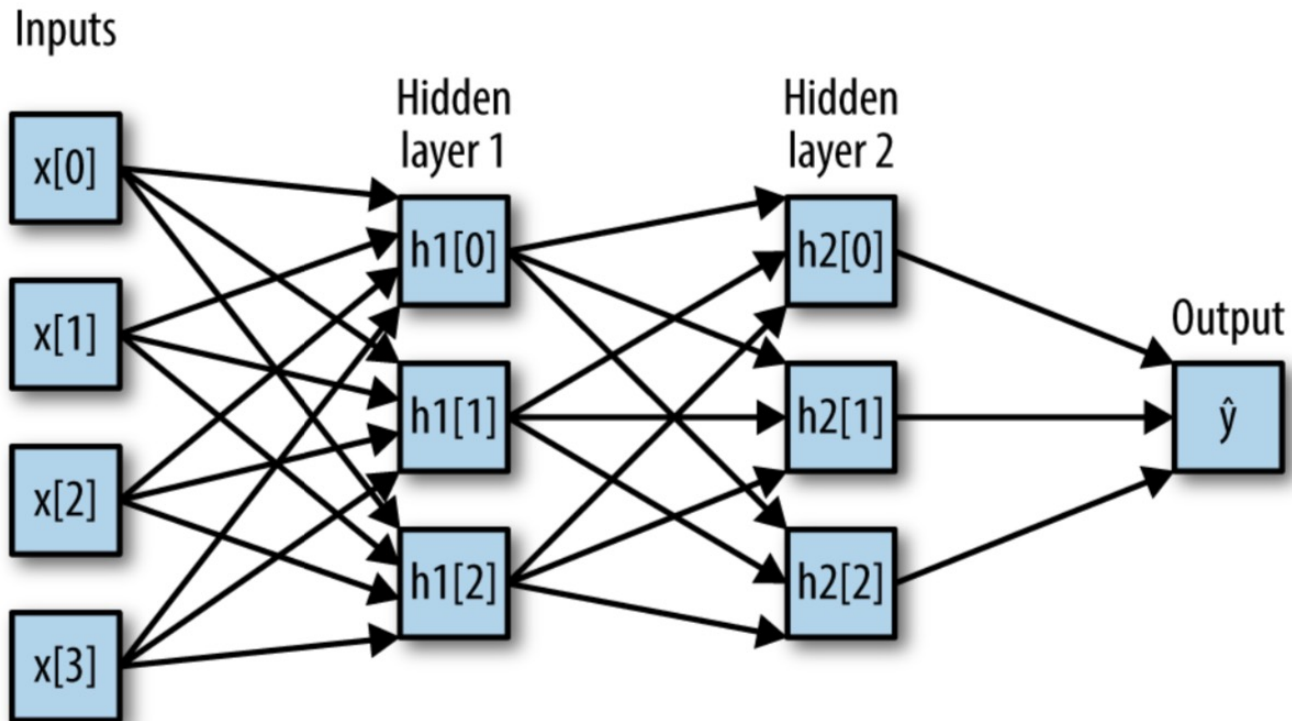
$$h_0 = w_{00}x_0 + w_{10}x_1 + w_{20}x_2 + w_{30}x_3 + b_0$$

$$h_1 = w_{01}x_0 + w_{11}x_1 + w_{21}x_2 + w_{31}x_3 + b_1$$

$$h_2 = w_{02}x_0 + w_{12}x_1 + w_{22}x_2 + w_{32}x_3 + b_2$$

$$\hat{y} = v_0h_0 + v_1h_1 + v_2h_2 + b$$

Multilayer Perceptron (MLP)

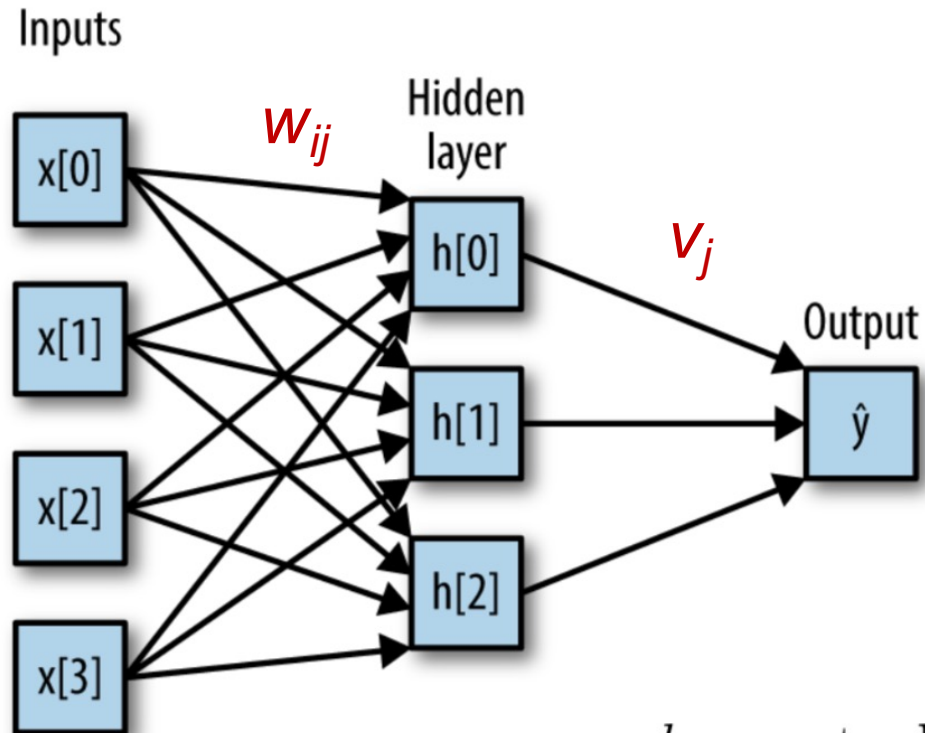


May have multiple hidden layers

Activation Functions

- Activation functions are used to let the NN become a nonlinear model (for classification or regression)
- They help in the convergence of the learning algorithm
- Common Activation functions
 - **tanh** MLP, RNN
 - **ReLU** MLP, CNN
 - **softmax** (multi-class classification)

MLP – tanh activation function



Activation functions are used to let the NN become a nonlinear model

$$h_0 = \tanh(w_{00}x_0 + w_{10}x_1 + w_{20}x_2 + w_{30}x_3 + b_0)$$

$$h_1 = \tanh(w_{01}x_0 + w_{11}x_1 + w_{21}x_2 + w_{31}x_3 + b_1)$$

$$h_2 = \tanh(w_{02}x_0 + w_{12}x_1 + w_{22}x_2 + w_{32}x_3 + b_2)$$

$$\hat{y} = v_0h_0 + v_1h_1 + v_2h_2 + b$$

Common Activation Functions

Logistic
(sigmoid)

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



Hyperbolic
Tangent
(tanh)

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



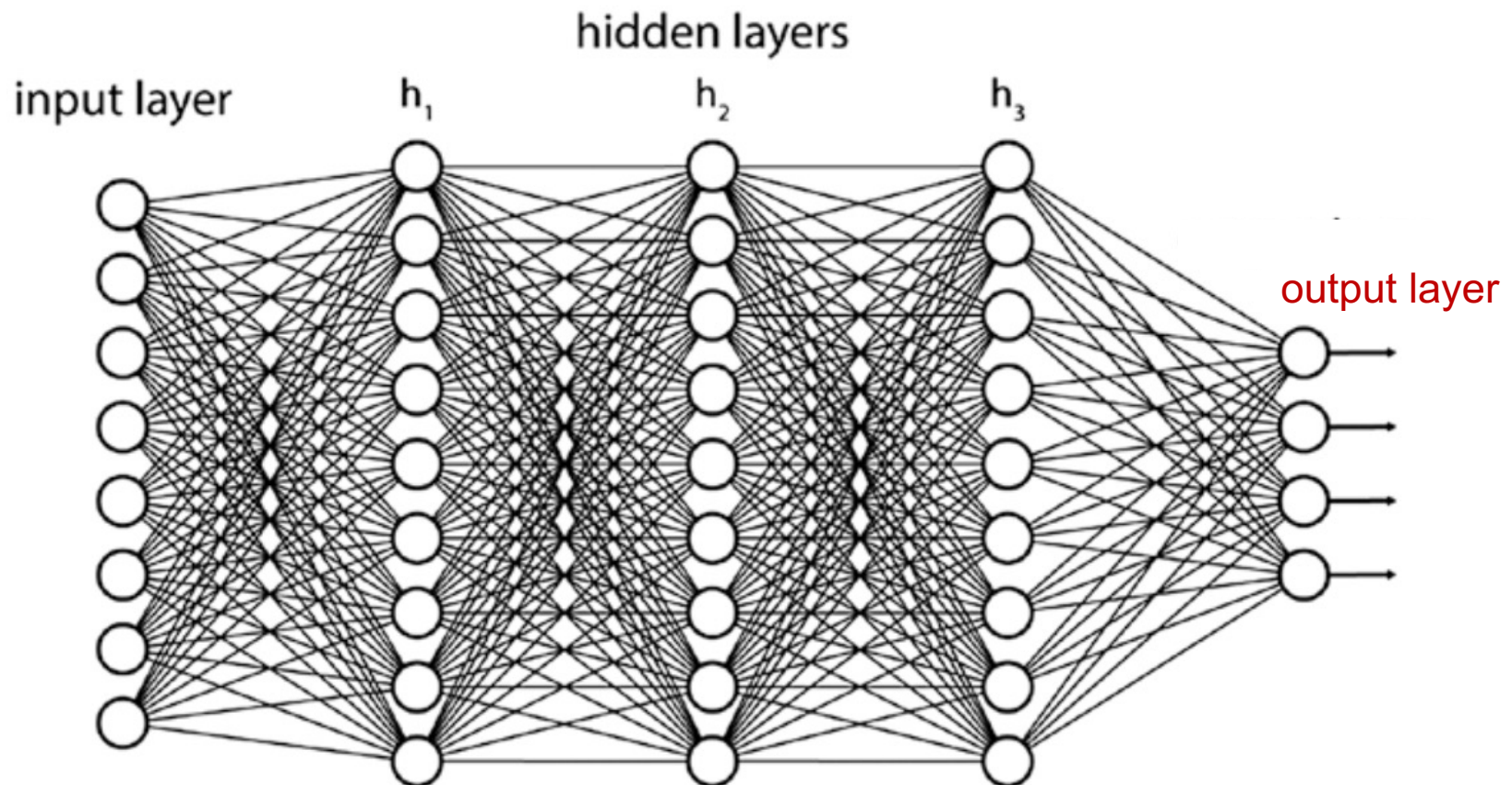
ReLU
(Rectified
Linear Unit)

$$\phi(z) = \begin{cases} 0 & z < 0 \\ z & z > 0 \end{cases}$$



Deep Neural Network

Model may have thousands of parameters (regression coefficients)



Notes

- Scale the data before building NN models
- NN layer is called **Dense** if *all* nodes are connected with nodes from neighbor layers
- NN is called Multilayer Perceptron (MLP) if all layers are dense

Notes

- For small datasets use a small number of hidden layers otherwise risk of overfitting
- Consider increasing the number of hidden layers with larger datasets
- NN **hyperparameters**:
 - number of hidden layers
 - number of nodes per layer
 - learning rate λ

Example 1 – Multilayer Perceptron

Example 1 – Multilayer Perceptron

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

```
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score
from sklearn.metrics import confusion_matrix
from sklearn.neural_network import MLPClassifier
```

```
df = pd.read_csv('moons.csv')
df
```

	feature1	feature2	label
0	0.161278	1.040189	0
1	-0.198249	0.650045	0
2	0.718082	-0.387594	1

```
y = df.label
X = df.drop(['label'],axis=1)
```

```
y.value_counts()
```

```
1    100
0    100
```

```
X_train, X_test, y_train, y_test = train_test_split(X,y, stratify=y,
                                                    random_state=42)
```

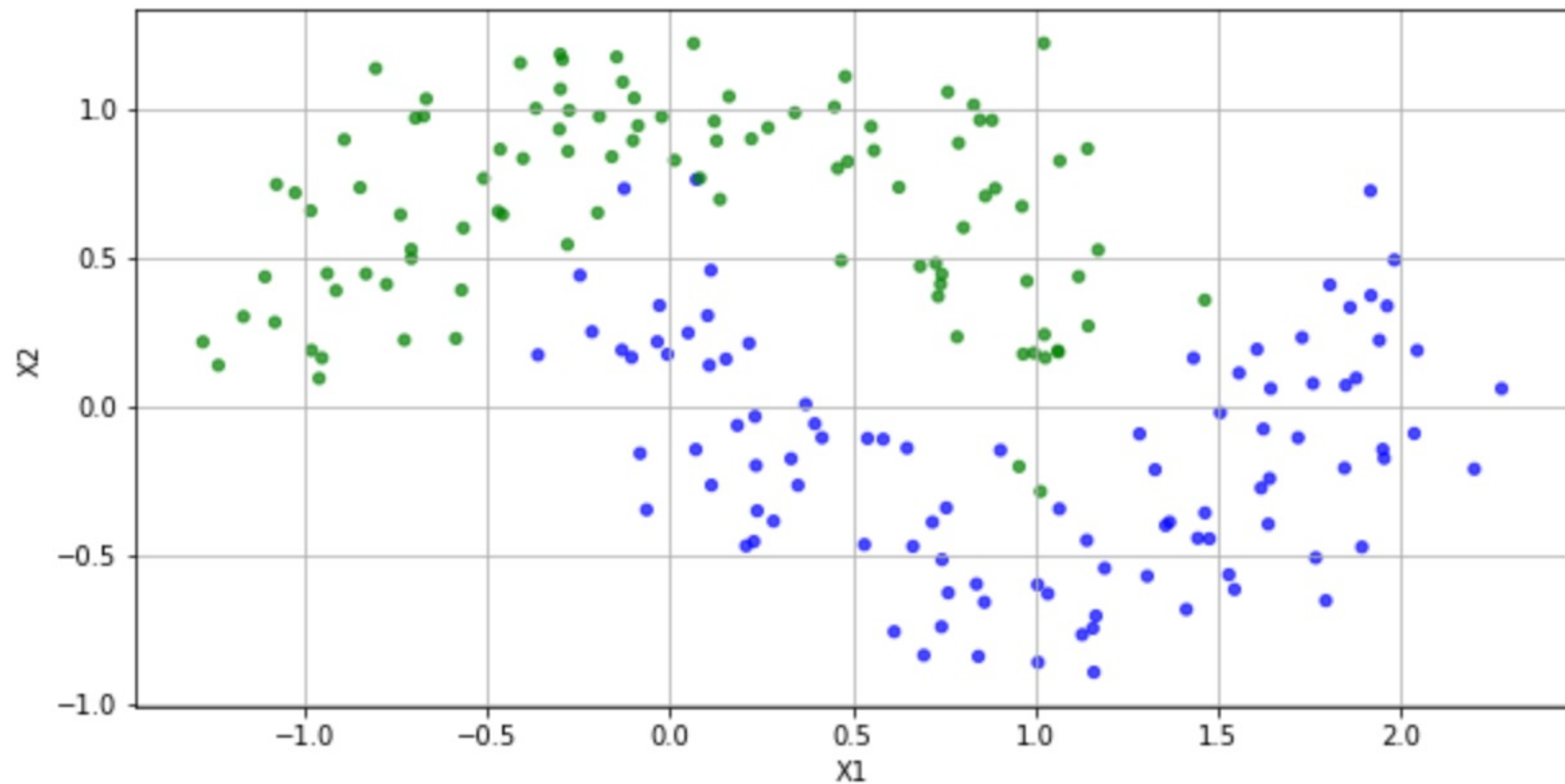
```
X_train = X_train.values
```

```
X_test = X_test.values
```

train set 75%

Example 1 – Nonlinearly separable data

```
plt.figure(figsize=(10,5))  
plt.scatter(X.feature1, X.feature2, s=18, c=colors, alpha=0.7)  
plt.xlabel('X1')  
plt.ylabel('X2')  
plt.grid()
```



Example 1 – Function to display boundary

```
def plot1(model, X, y, h=0.01, pad=0.25):
    x_min, x_max = X[:, 0].min()-pad, X[:, 0].max()+pad
    y_min, y_max = X[:, 1].min()-pad, X[:, 1].max()+pad
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))

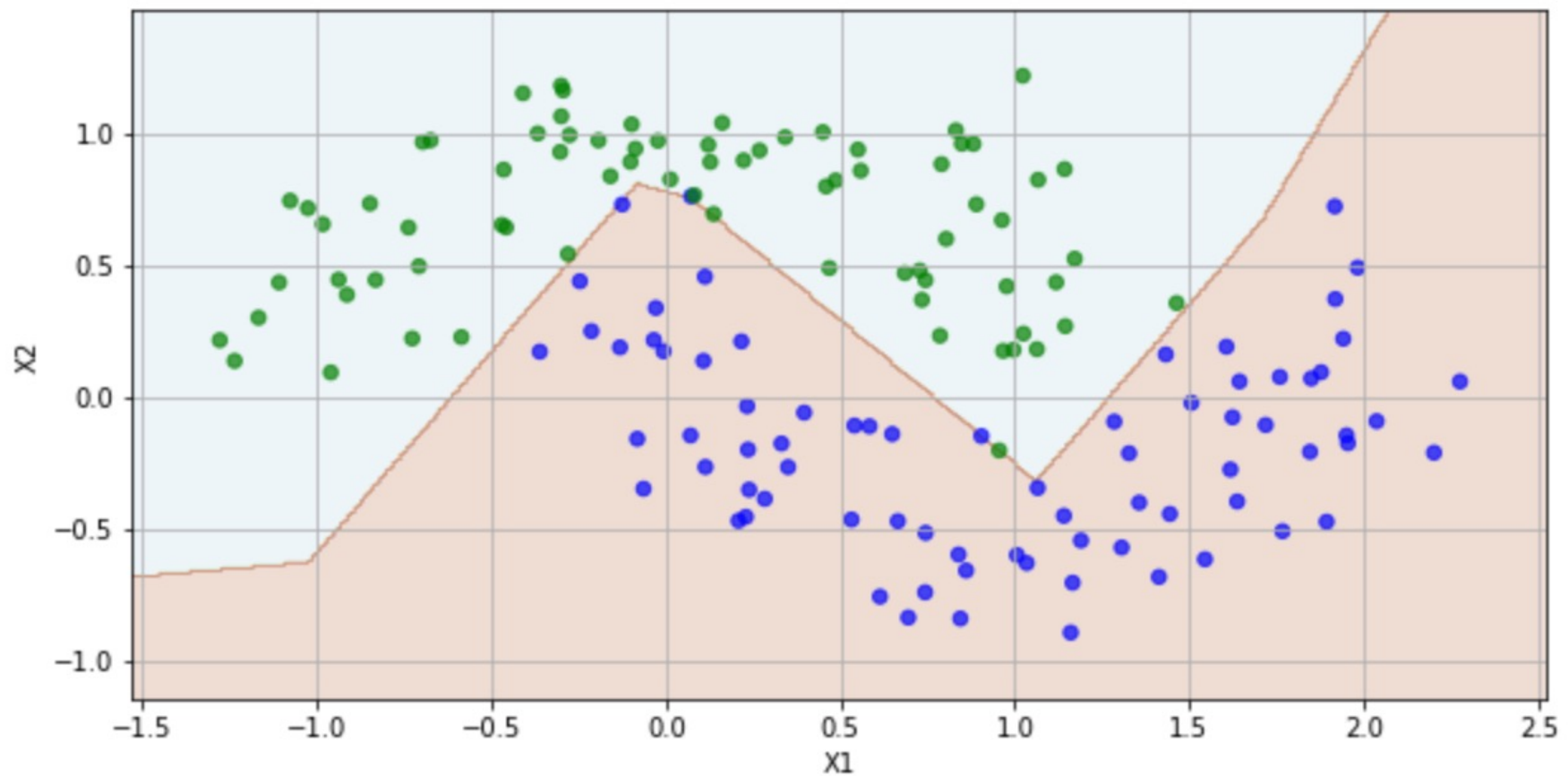
    Z = model.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)

    plt.figure(figsize=(10,5))
    plt.contourf(xx, yy, Z, cmap=plt.cm.Paired, alpha=0.2)

    my_dict = {-1:'r', 1:'b', 0:'g'}
    colors = np.vectorize(my_dict.get)(y)
    plt.scatter(X[:,0], X[:,1], s=30, c=colors, alpha=0.7)
    plt.xlim(x_min, x_max)
    plt.ylim(y_min, y_max)
    plt.xlabel('X1')
    plt.ylabel('X2')
    plt.grid()
```

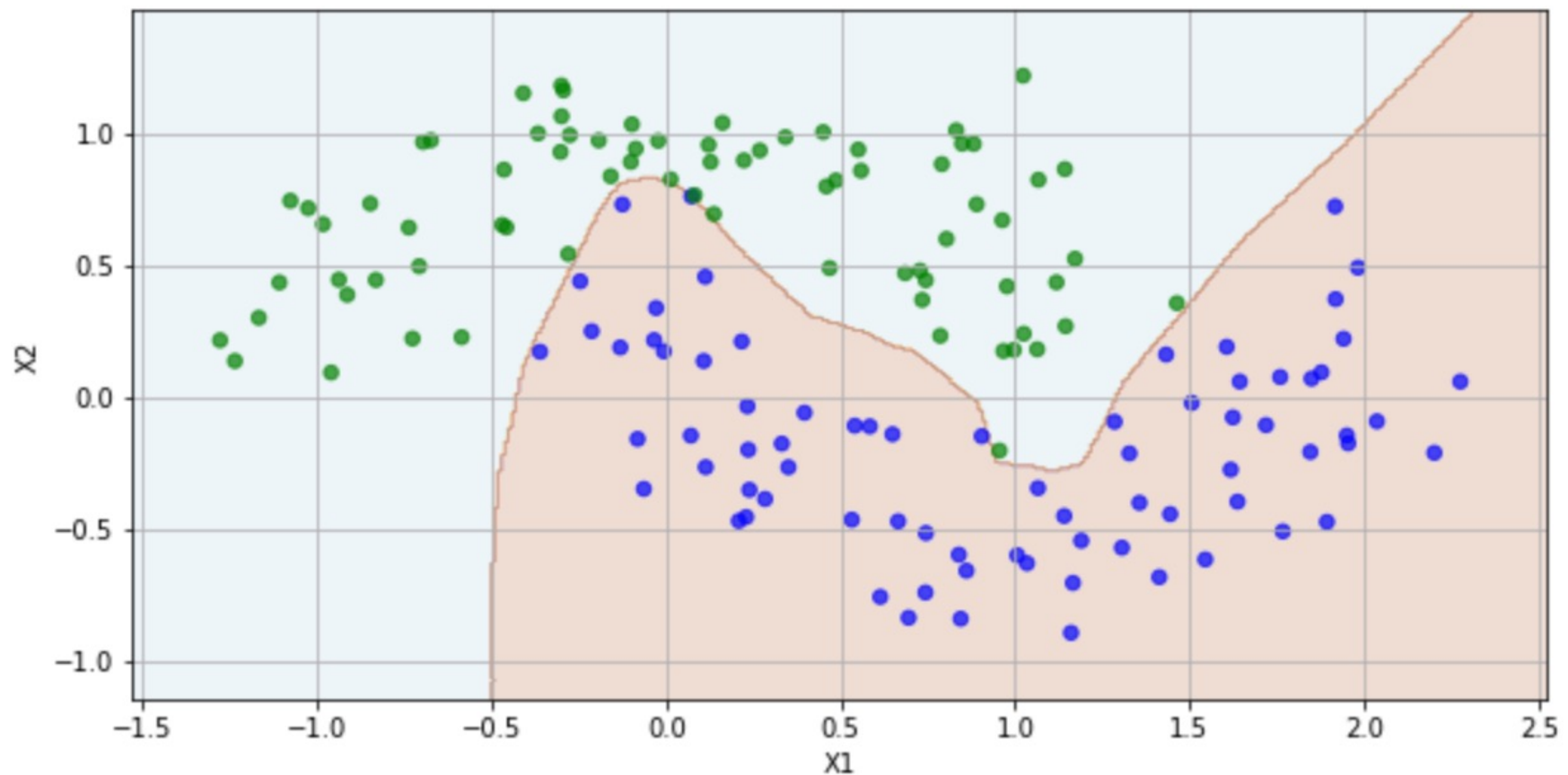

Example 1: 1 hidden layer with 10 nodes

```
mlp = MLPClassifier(solver='lbfgs', random_state=0, hidden_layer_sizes=[10])  
mlp.fit(X_train, y_train)  
plot1(mlp, X_train, y_train)
```



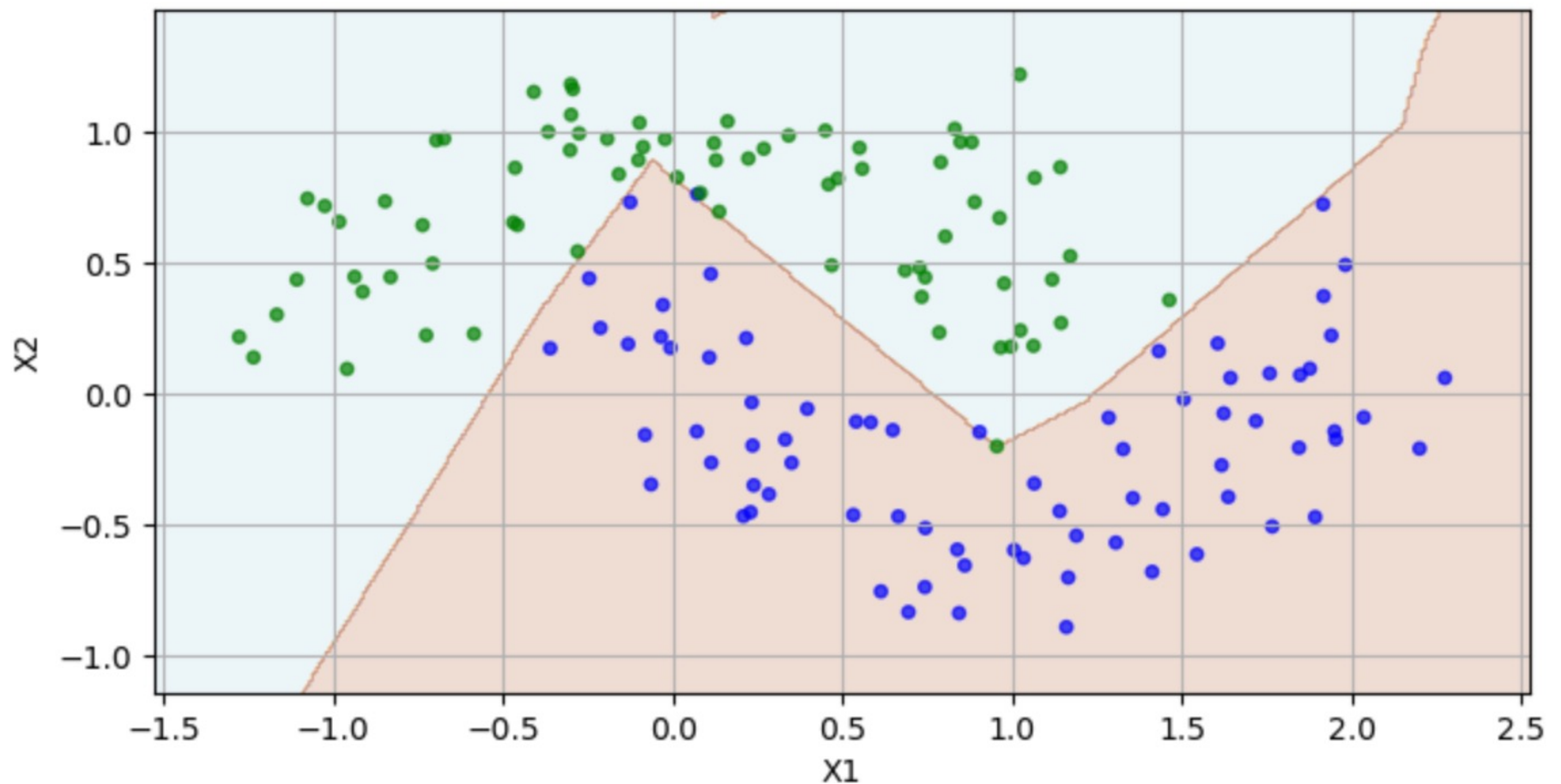
Example 1: 1 hidden layer with 100 nodes

```
mlp = MLPClassifier(solver='lbfgs', random_state=0, hidden_layer_sizes=[100])  
mlp.fit(X_train, y_train);  
plot1(mlp, X_train.values, y_train)
```



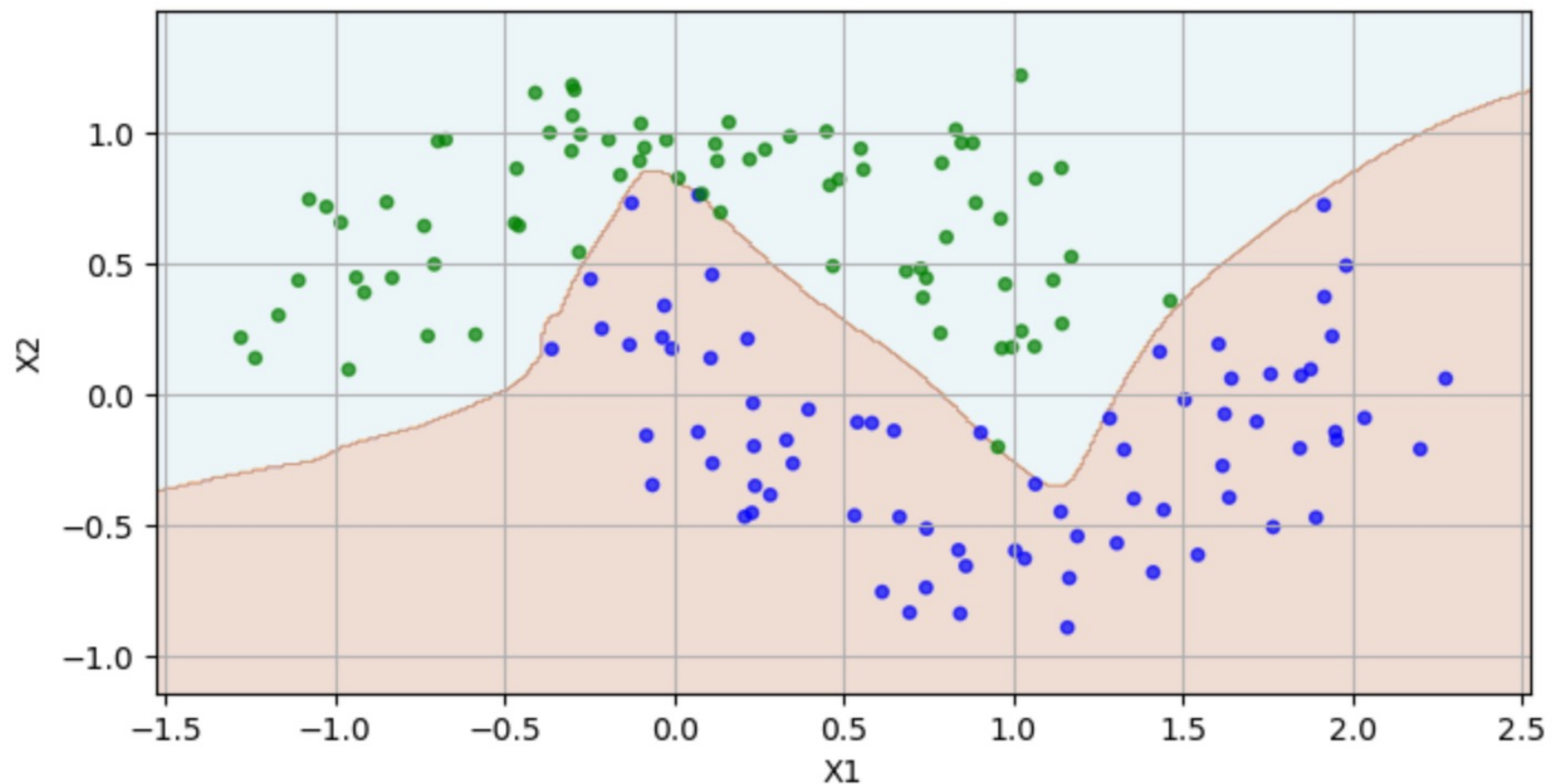
Example 1: 2 hidden layers with 10 nodes each

```
mlp = MLPClassifier(solver='lbfgs', random_state=0, hidden_layer_sizes=[10, 10])  
mlp.fit(X_train, y_train)  
plot1(mlp, X_train, y_train)
```



Example 1: Two 10-node hidden layers with **tanh**

```
mlp = MLPClassifier(solver='lbfgs', activation='tanh', max_iter = 1000,  
                    random_state=0, hidden_layer_sizes=[10, 10])  
mlp.fit(X_train, y_train)  
plot1(mlp, X_train, y_train)
```



Example 1: Two 10-node hidden layers with **tanh**

```
# Test accuracy rate
```

```
mlp.fit(X_train, y_train)
y_pred = mlp.predict(X_test)
accuracy_score(y_test, y_pred)
```

```
0.98
```

```
pd.crosstab(y_test, y_pred, rownames = ['y_test'], colnames=['predictions'])
```

y_test	predictions	
	0	1
0	24	1
1	0	25

test set 25%

Example 2 – MLP Cancer dataset

Cancer Data

Cancer Data

Example 2 – MLP on Cancer data

```
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split

from sklearn.neural_network import MLPClassifier
from sklearn.datasets import load_breast_cancer
```

```
cancer = load_breast_cancer()
cancer.keys()
```

```
dict_keys(['data', 'target', 'frame', 'target_names', 'DESCR', 'feature_names'])
```

```
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)
```

```
mlp = MLPClassifier(random_state=42)
mlp.fit(X_train, y_train);
```


Example 2 – MLP on Cancer data

```
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split

from sklearn.neural_network import MLPClassifier
from sklearn.datasets import load_breast_cancer
```

```
cancer = load_breast_cancer()
cancer.keys()
```

```
dict_keys(['data', 'target', 'frame', 'target_names', 'DESCR', 'feature_names'])
```

```
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)
```

```
mlp = MLPClassifier(random_state=42)
mlp.fit(X_train, y_train);
```

sklearn.neural_network.MLPClassifier

```
class sklearn.neural_network.MLPClassifier(hidden_layer_sizes=(100,), activation='relu', *, solver='adam', alpha=0.0001,
batch_size='auto', learning_rate='constant', learning_rate_init=0.001, power_t=0.5, max_iter=200, shuffle=True,
random_state=None, tol=0.0001, verbose=False, warm_start=False, momentum=0.9, nesterovs_momentum=True,
early_stopping=False, validation_fraction=0.1, beta_1=0.9, beta_2=0.999, epsilon=1e-08, n_iter_no_change=10,
```

Example 2 – MLP on Cancer data

```
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split

from sklearn.neural_network import MLPClassifier
from sklearn.datasets import load_breast_cancer
```

```
cancer = load_breast_cancer()
cancer.keys()
```

```
dict_keys(['data', 'target', 'frame', 'target_names', 'DESCR', 'feature_names'])
```

```
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)
```

```
mlp = MLPClassifier(random_state=42)
mlp.fit(X_train, y_train);
```

```
# Accuracy rate
mlp.score(X_test, y_test)
```

```
0.916083916083916
```

Example 2 – Standardize the data

```
scaler = StandardScaler()  
scaler.fit(X_train)  
X_train_scaled = scaler.transform(X_train)  
X_test_scaled = scaler.transform(X_test)
```

Example 2 – Standardize the data

```
scaler = StandardScaler()  
scaler.fit(X_train)  
X_train_scaled = scaler.transform(X_train)  
X_test_scaled = scaler.transform(X_test)
```

```
mlp = MLPClassifier(random_state=0)  
mlp.fit(X_train_scaled, y_train);
```

```
/opt/anaconda3/lib/python3.7/site-packages/sklearn/neural_network/_multilayer_perceptron.py:696:  
Stochastic Optimizer: Maximum iterations (200) reached and the optimization hasn't converged yet.  
ConvergenceWarning,
```

```
mlp.score(X_test_scaled, y_test)
```

```
0.965034965034965
```

Example 2

Increase max_iter

```
mlp = MLPClassifier(max_iter=1000, random_state=0)
mlp.fit(X_train_scaled, y_train)
mlp.score(X_test_scaled, y_test)
```

0.972027972027972

No Convergence
Warning

Regularization on MLP

```
mlp = MLPClassifier(max_iter=1000, alpha=0.9, random_state=0)
mlp.fit(X_train_scaled, y_train)
mlp.score(X_test_scaled, y_test)
```

0.9790209790209791

search for the
best alpha

```
y_pred = mlp.predict(X_test_scaled)
accuracy_score(y_test, y_pred)
```

0.9790209790209791

Example 2 - weights

Weights

```
len(mlp.coefs_)
```

```
2
```

list of 2 arrays

```
# weights from 30 inputs to 100 hidden nodes
```

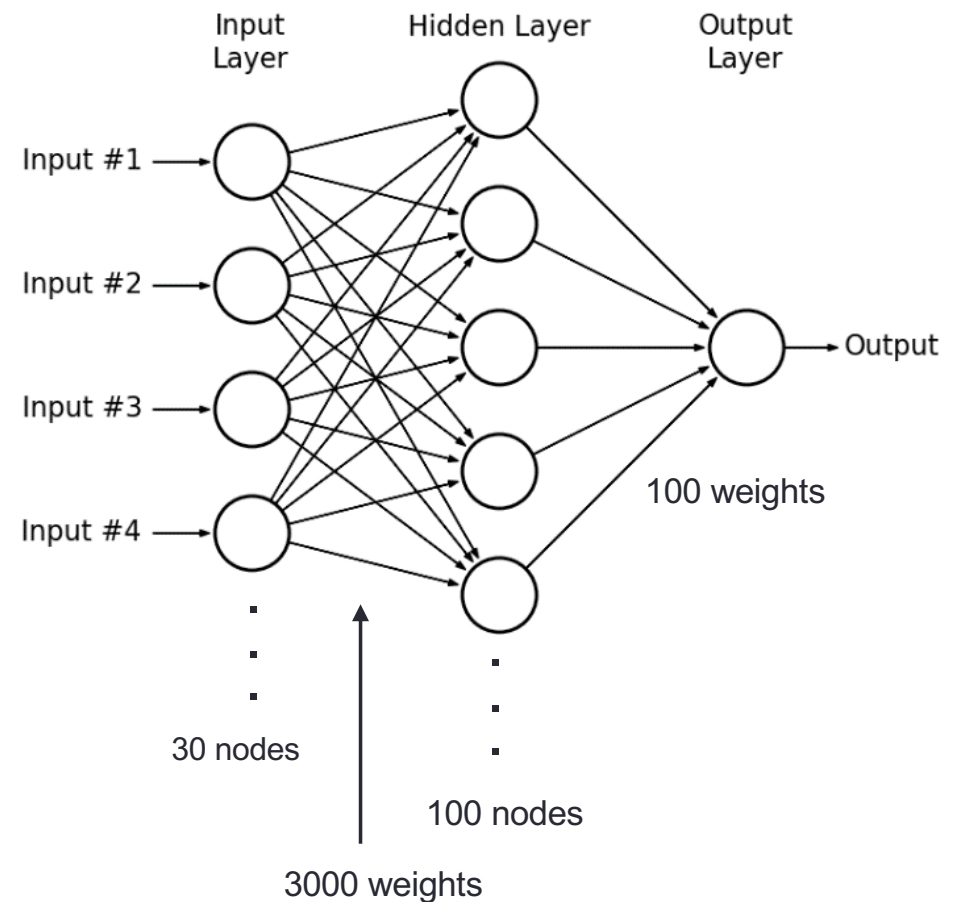
```
mlp.coefs_[0].shape
```

```
(30, 100)
```

```
# weights from 100 hidden nodes to the output node
```

```
mlp.coefs_[1].shape
```

```
(100, 1)
```



Example 2 - weights

```
# weights from 30 inputs to 100 hidden nodes
```

```
dfc = pd.DataFrame(mlp.coefs_[0])  
dfc.columns = ['x' + str(x) for x in range(1,101)]  
dfc.index = cancer.feature_names  
np.round(dfc,4)
```

← store weights in a dataframe
← set column names
← set row names
← round coefs values

Example 2 - weights

weights from 30 inputs to 100 hidden nodes

```
dfc = pd.DataFrame(mlp.coefs_[0])
dfc.columns = ['x' + str(x) for x in range(1,101)]
dfc.index = cancer.feature_names
np.round(dfc,4)
```

100 hidden nodes

	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	...	x91	x92	x93
mean radius	-0.0666	0.2167	0.0002	0.0000	-0.1716	-0.1724	-0.0144	0.1295	0.0000	0.0017	...	-0.1856	0.0001	0.0423
mean texture	-0.2148	0.0662	-0.0000	-0.0000	0.1667	-0.1189	-0.0000	0.0777	-0.0009	-0.0777	...	-0.1800	0.0088	0.0941
mean perimeter	0.0522	-0.1585	-0.0037	0.0089	0.0247	-0.2331	-0.0089	0.0432	-0.0229	-0.0521	...	-0.2212	-0.0175	0.0645
mean area	-0.1934	0.0265	0.0000	0.0000	0.0830	0.1879	0.0000	-0.0991	0.0016	-0.0243	...	0.1973	-0.0000	-0.0175
mean smoothness	-0.1693	0.1882	-0.0000	0.0030	-0.0931	0.1523	0.0000	-0.2373	0.0097	-0.0407	...	-0.0334	-0.0000	-0.0427
mean compactness	0.1589	-0.0196	-0.0000	0.0024	0.1134	-0.1178	0.0103	0.1277	0.0155	0.0006	...	-0.1209	0.0000	-0.0754
mean concavity	-0.0126	-0.1817	-0.0028	-0.0104	-0.0735	0.0677	-0.0015	-0.0542	-0.0000	-0.0035	...	0.0121	0.0000	-0.0091
mean concave points	0.1279	-0.2572	-0.0000	-0.0058	-0.1201	0.2725	-0.0000	0.1377	-0.0004	-0.0022	...	-0.0830	0.0000	-0.0099
mean symmetry	0.0892	-0.1357	-0.0000	-0.0000	-0.0468	0.0855	0.0133	0.1542	0.0000	-0.0480	...	0.0836	0.0050	0.0609

30
input
nodes

3000 weight coeffs

Example 2 – weights to Output node

weights from 100 hidden nodes to the output node

```
dfc = pd.DataFrame(mlp.coefs_[1])
dfc.index = ['x' + str(x) for x in range(1,101)]
dfc.columns = ['y']
np.round(dfc,4)
```

	y
x1	-0.1964
x2	0.1213
x3	0.0187
x4	0.0000
x5	-0.1035
...	...
x96	0.0111
x97	0.1944
x98	0.0123
x99	-0.1806
x100	-0.0408

