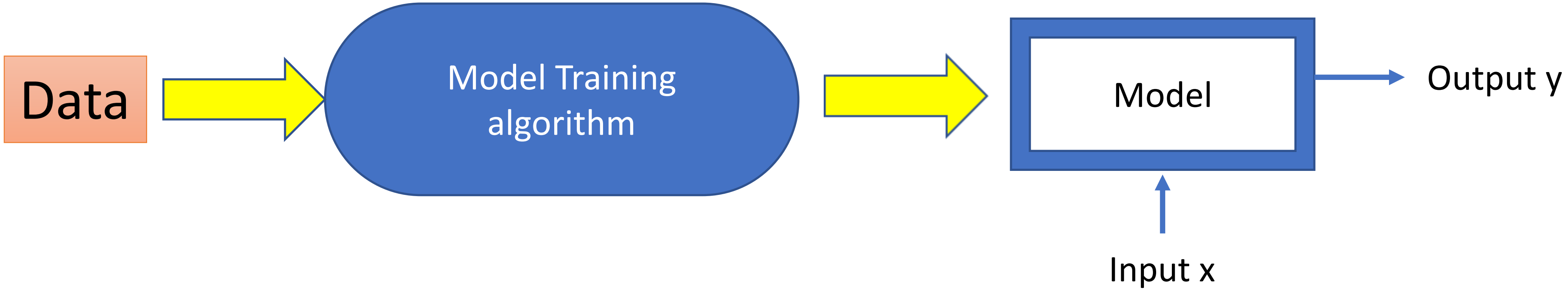
# Machine Learning basics

# Machine Learning

- It is a method that builds analytical model from data automatically.
- It is based on the idea that systems can learn from data, identify patterns and make decisions with minimal human intervention.



# Different Types of Machine Learning

| Unsupervised Learning | | Supervised Learning | | Reinforcement Learning |
|---|---|---|---|---|
| Clustering | Consumer segmentation | Classification | Fraud detection | Real-time decisions |
| | | | Image classification | Game AI |
| | Recommendation System | | | Robot Navigation |
| | | Regression | Price prediction | Skill acquisition |
| | | | Weather forecast | |

# Supervised Learning

- To learn a function that maps an input to an output based on a training data set that gives examples of input + label (which is the correct output) pairs
- Goal: From the training data set build a model that gives good prediction on the labels for the inputs in the dataset.
- Then, we can use this model to predict the outcome (i.e., the labels) of out-of-sample data.

Note: A model isn't necessarily a computer program, but rather, it's any mechanism that allows for a definite prediction given any input instance.

# Supervised Learning: Classification

- Every input x is associated with a label y where y is from some categorical data, i.e., data whose values can be divided into (a small number) of groups.

An example

| Item | Color | Shape | **Label** |
|---|---|---|---|
| Training data | | | |
| 1 | | small round | Apple |
| 2 | | big oval | Pear |
| 3 | | small round | Apple |
| 4 | | big round | Apple |
| : | : | : | : |
| | | | |
| | | | |

# Supervised Learning: Classification

- Every input x is associated with a label y where y is from some categorical data, i.e., data whose values can be divided into (a small number) of groups.
- We need to build a model from some training data for predicting the correct label of any given input.

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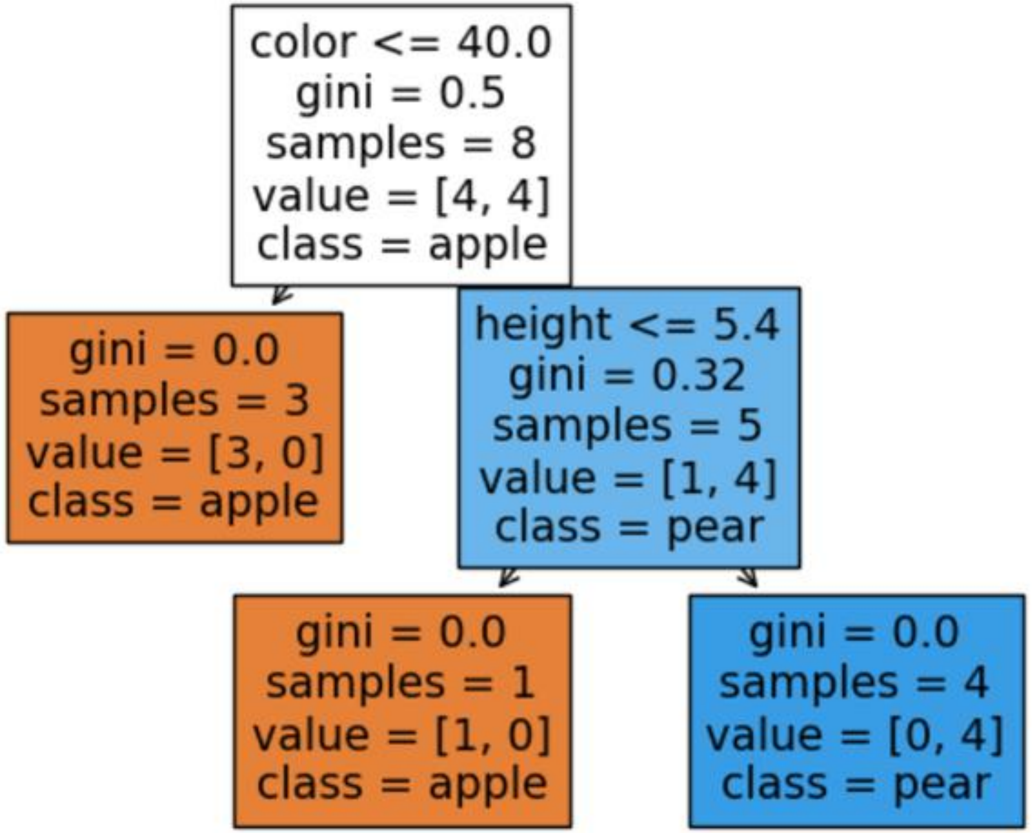
| : | : | : | : |
| New data | | | |
| | | big oval | ? |

# Supervised Learning: Classification




The model: Decision Tree model

## An example

| Item | Color | Shape | Label |
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| | | big oval | ? |

# Supervised learning: Regression

- Every input x is associated with a label y, where y is some numerical value (or some higher dimension numerical vector)

An example

| Temperature (°C)<br>**x** | Ice-cream Sales (No. of cones)<br>**y** |
|---|---|
| Training data | |
| 10 | 4 |
| 12 | 5 |
| 16 | 7 |
| 20 | 10 |
| … | |
| | |

# Supervised learning: Regression

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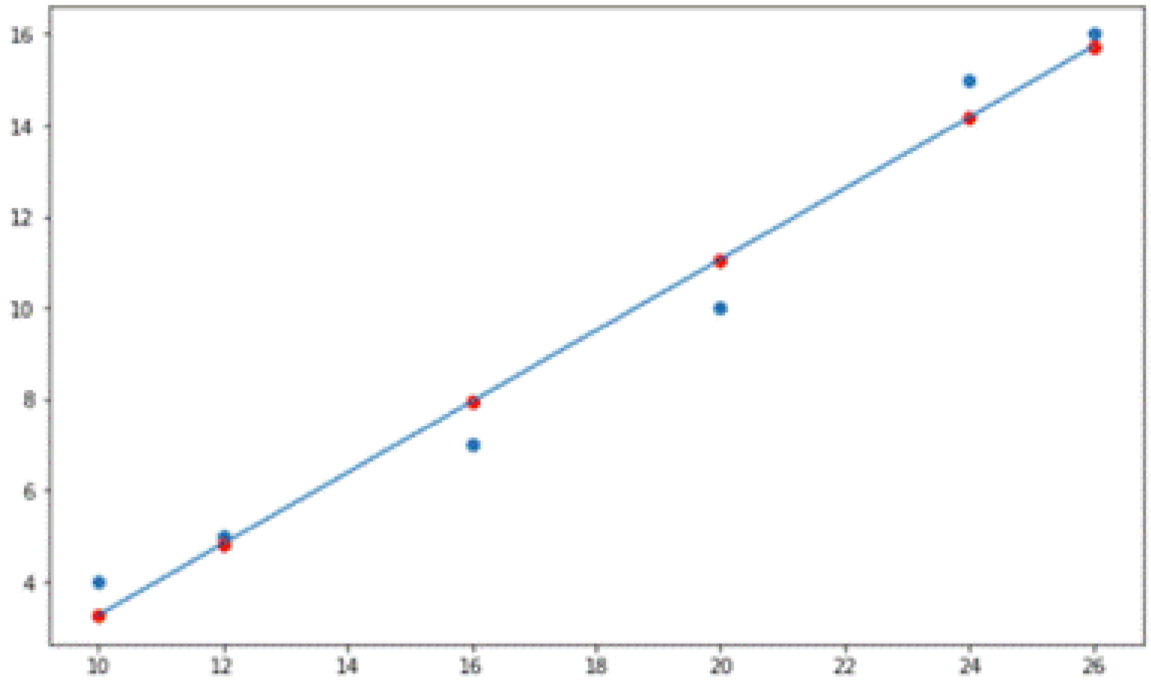
| new data | |
| 30 | **?** |

# Supervised learning: Regression




The model: Linear Regression $y = b + w \cdot x$

## An example

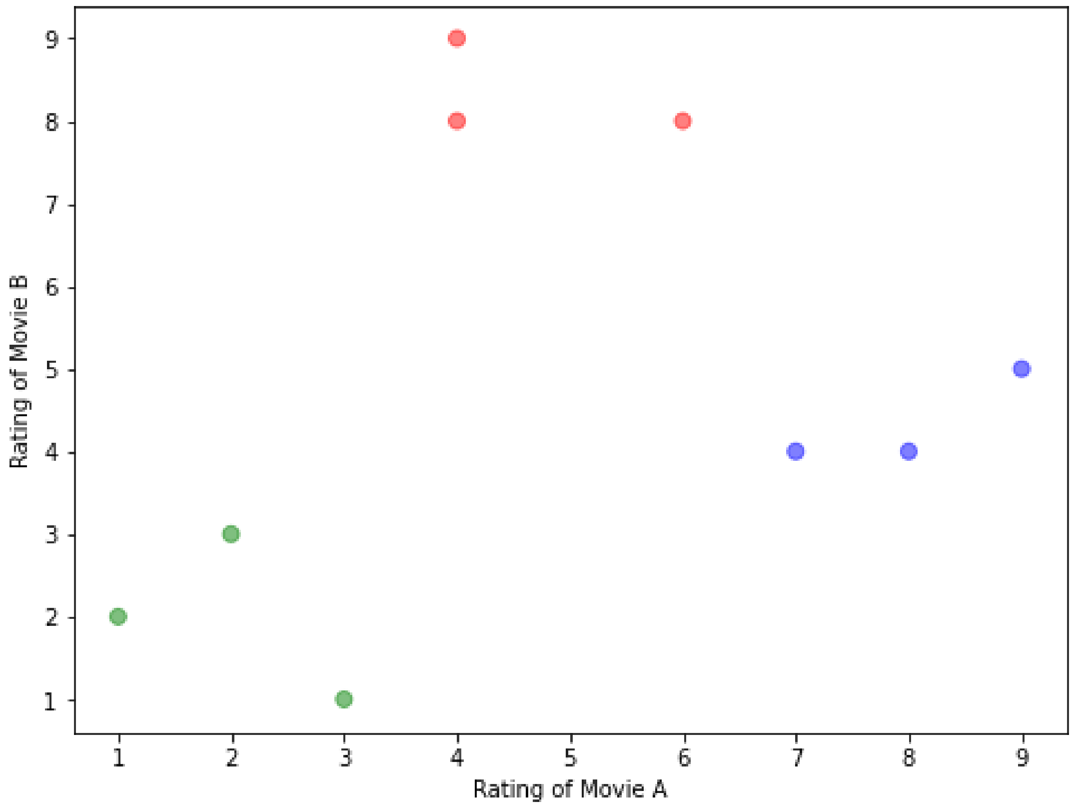
| Temperature (°C) x | Ice-cream Sales (No. of cones) y |
|---|---|
| Training data | |
| 10 | 4 |
| 12 | 5 |
| 16 | 7 |
| 20 | 10 |
| new data | |
| 30 | ? |

# Unsupervised Learning: Clustering

- To train and construct a model from which we can determine a natural grouping in data

| User | Rating of Movie A | Rating of Movie B |
|---|---|---|
| 1 | 1 | 2 |
| 2 | 7 | 4 |
| 3 | 2 | 3 |
| 4 | 6 | 8 |
| 5 | 4 | 8 |
| 6 | 8 | 4 |
| 7 | 9 | 5 |
| 8 | 3 | 1 |
| 9 | 4 | 9 |

# Unsupervised Learning: Clustering

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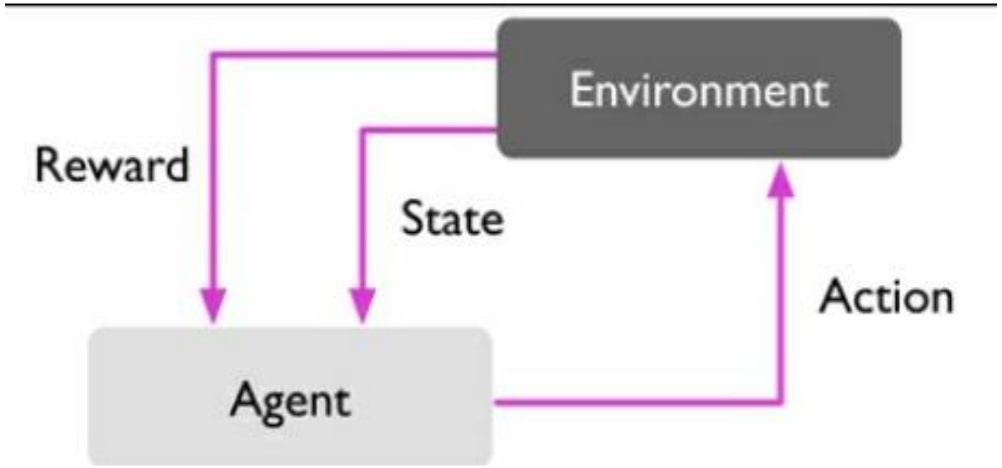
| 4 | 6 | 8 |
| 5 | 4 | 8 |
| 6 | 8 | 4 |
| 7 | 9 | 5 |
| 8 | 3 | 1 |
| 9 | 4 | 9 |

The model: Partition the points into groups

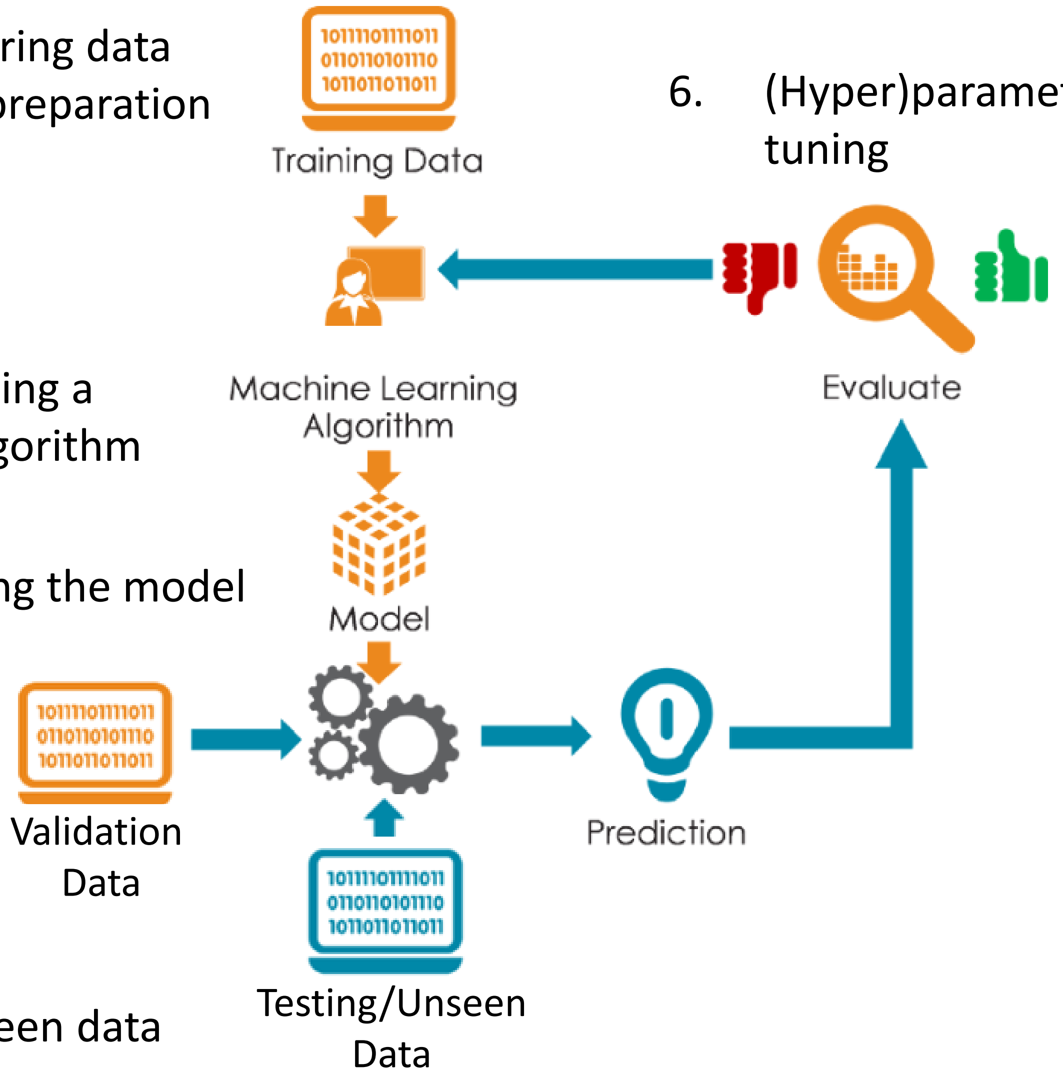
# Reinforcement Learning

- Reinforcement learning is learning what to do – how to map situations to actions – so as to maximize a numerical reward signal. The learner (agent) is not told which actions to take; instead, it must discover which actions yield the most reward by trying them.



# How to do Machine Learning?
# 7 steps of Machine Learning

1. Gathering data
2. Data preparation
3. Choosing a ML algorithm
4. Training the model
5. Evaluation
6. (Hyper)parameter tuning
7. Predicting unseen data



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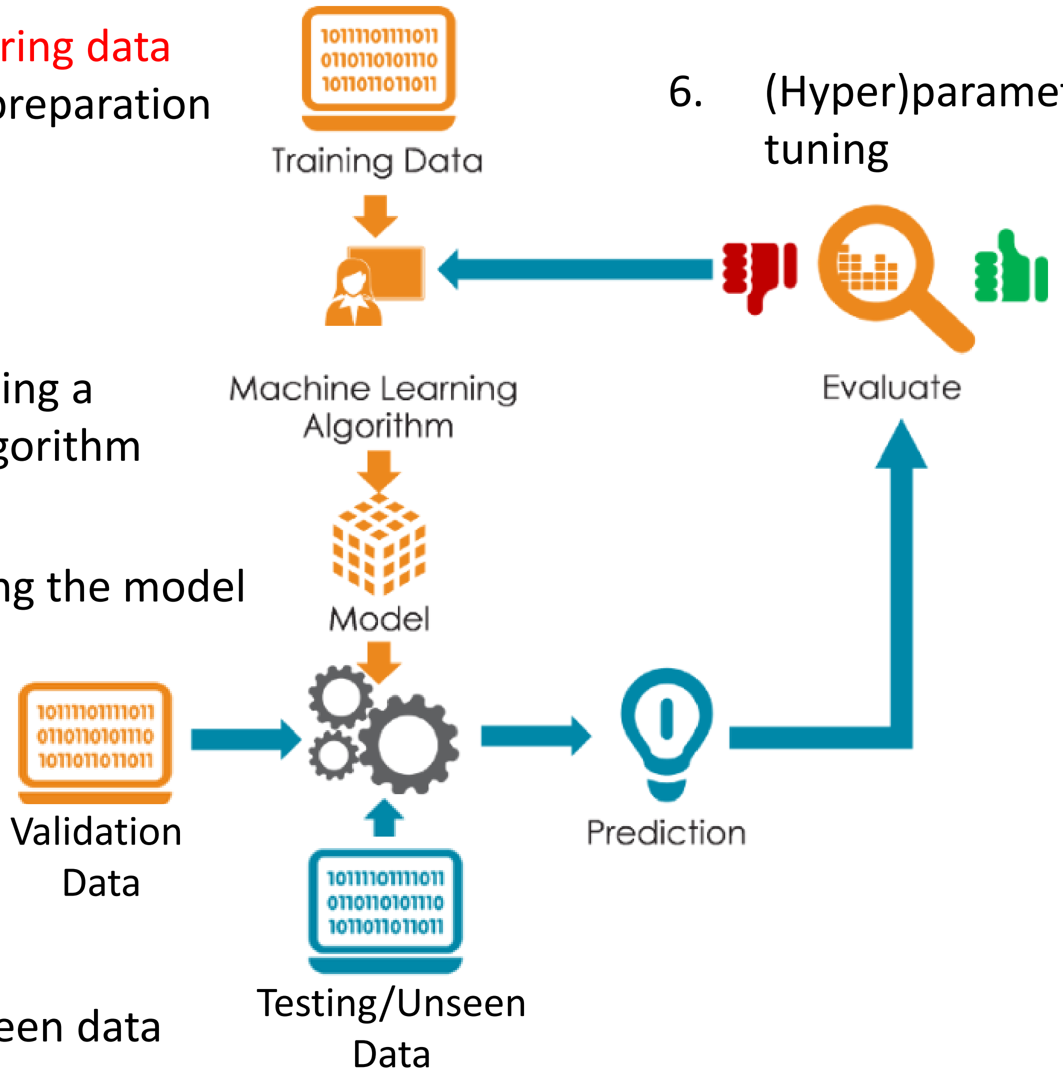

# How to do Machine Learning?
# 7 steps of M

Handling missing values and outliers
Feature scaling
Feature selection
Feature extraction: dimensionality reduction

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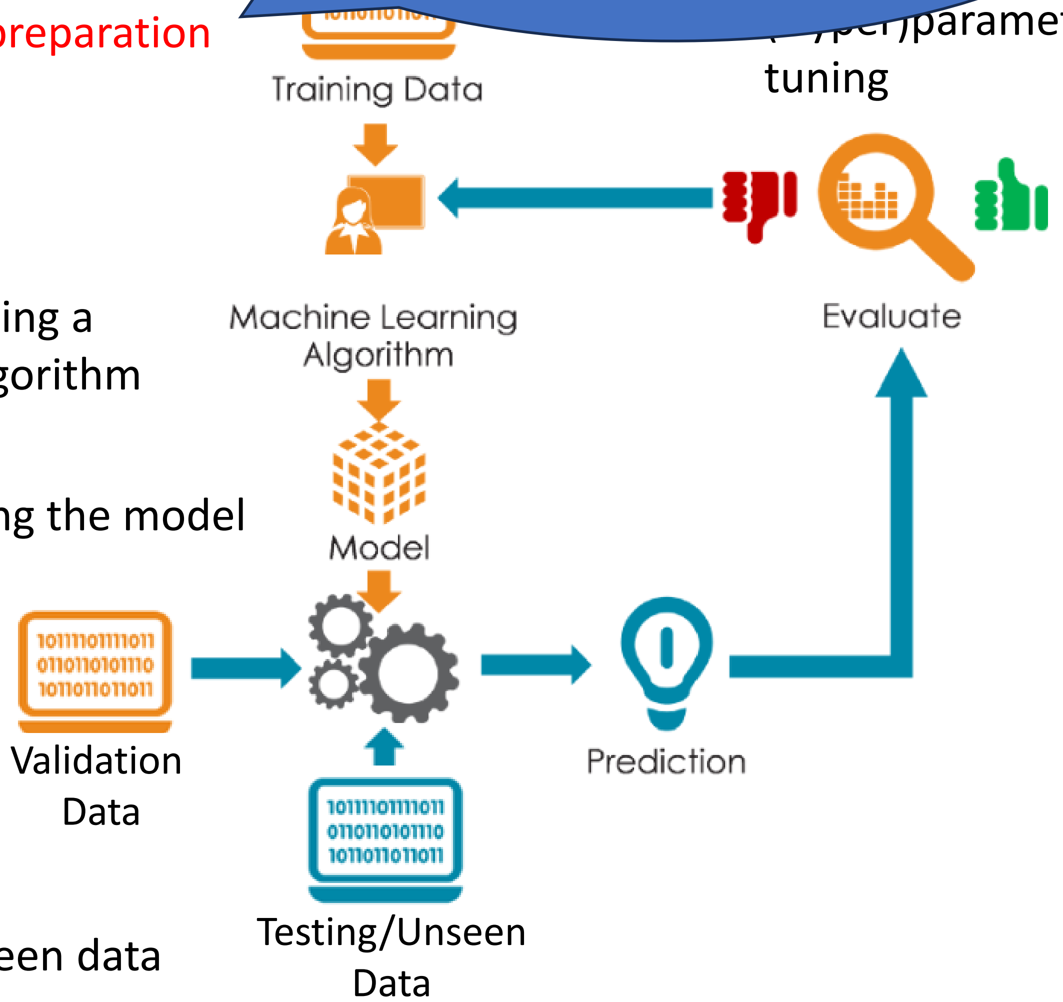
per)parameter tuning



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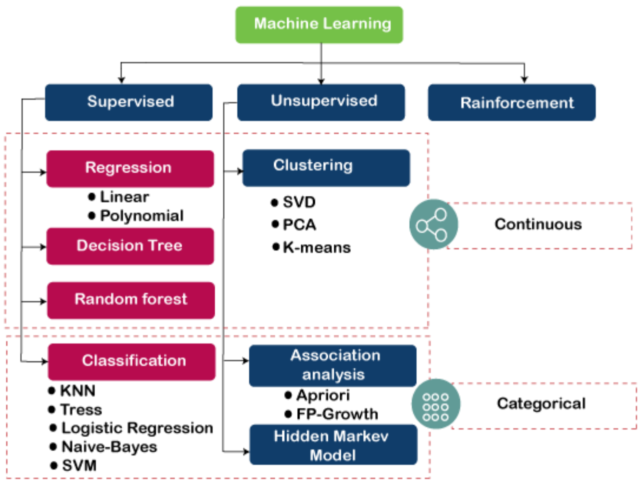
# 7 steps of Machine Learning

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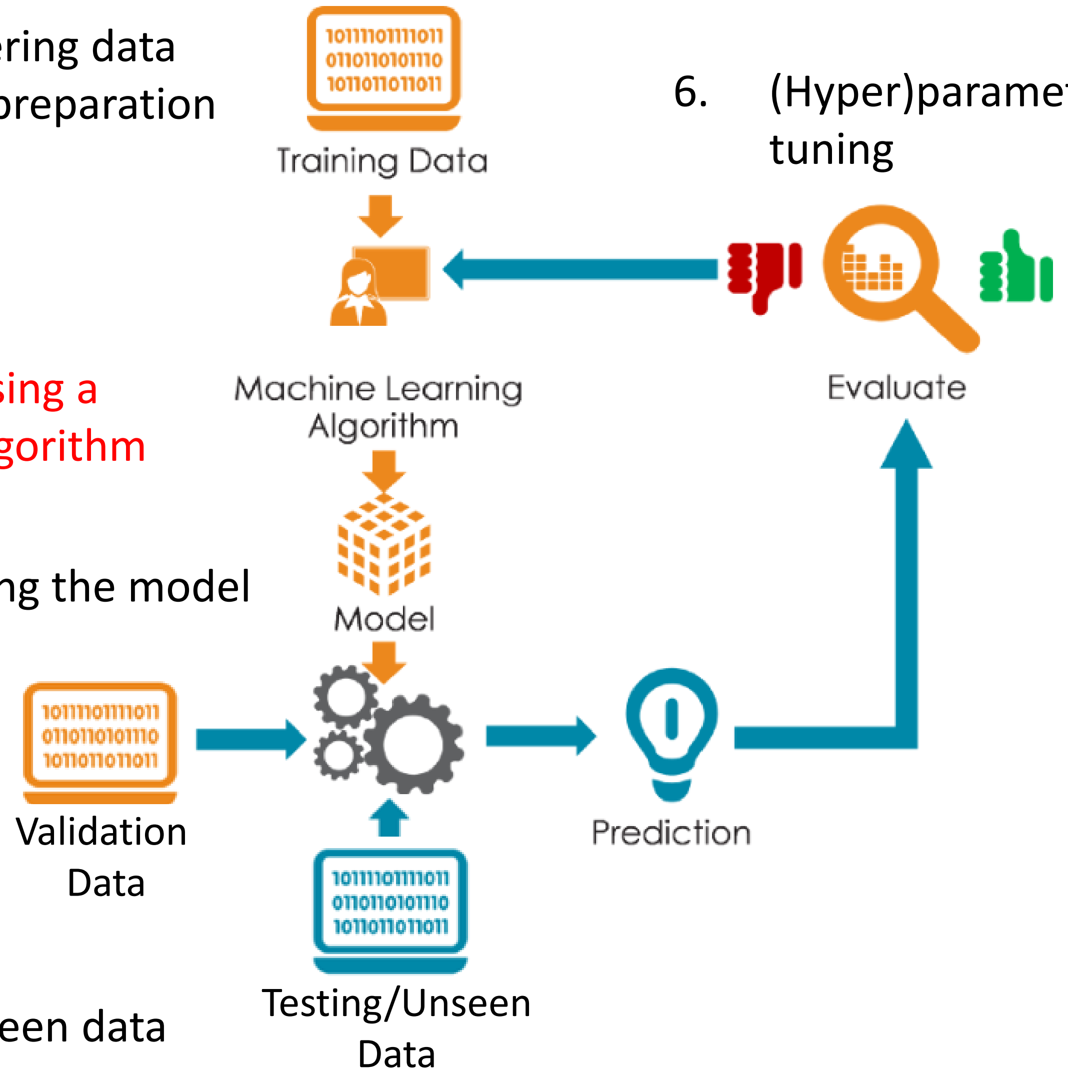

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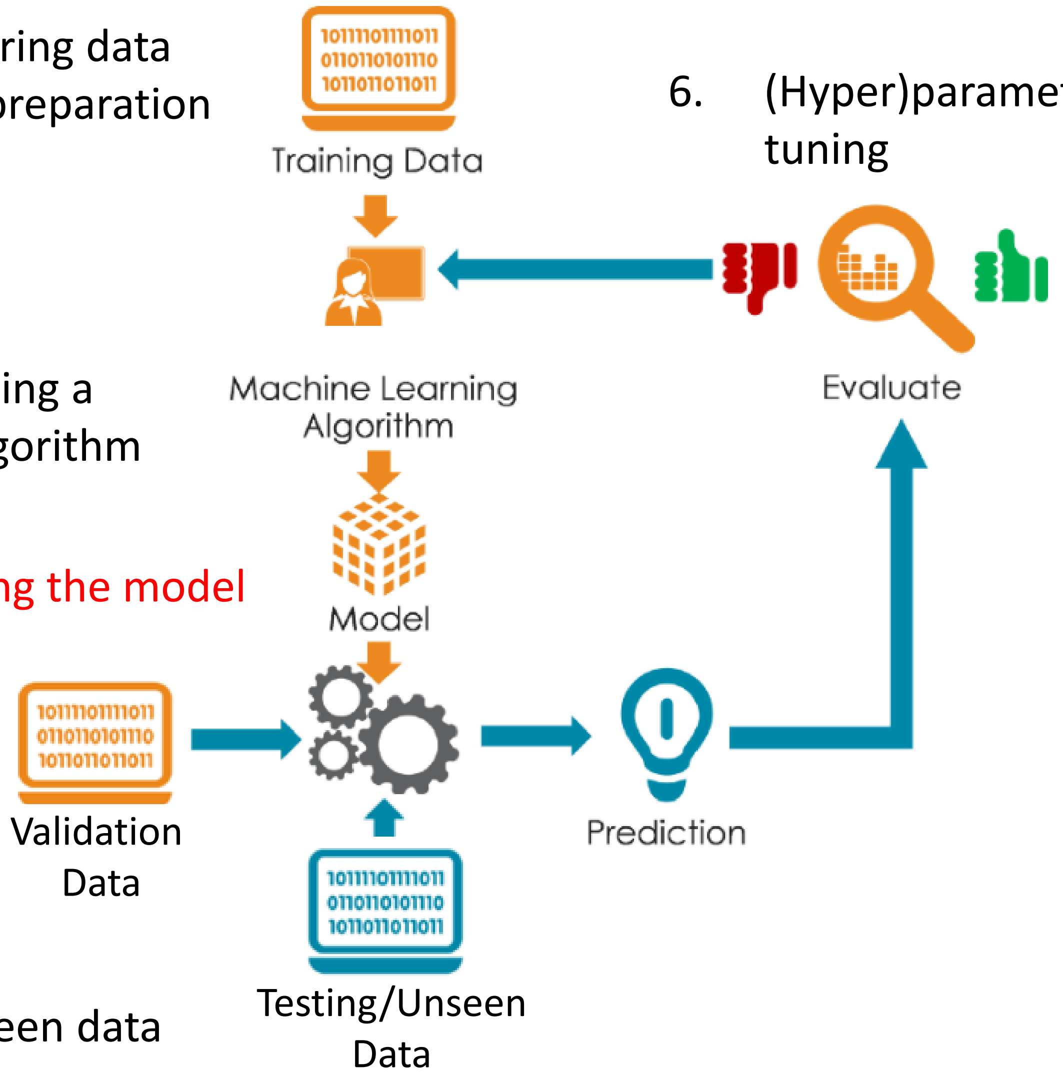

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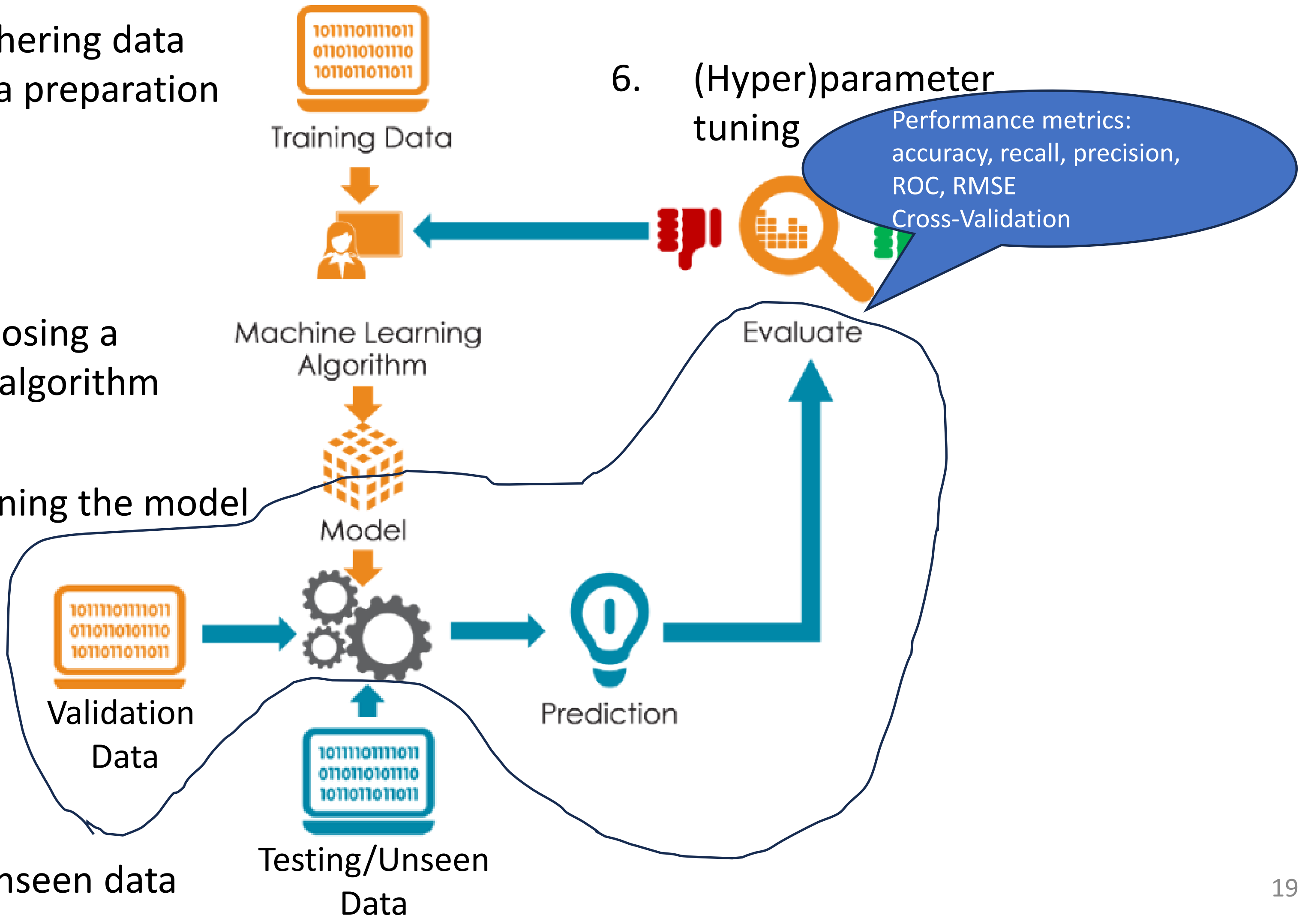

# How to do Machine Learning?
# 7 steps of Machine Learning

Hyperparameter Optimization: Grid-Search

1. Gather
2. Data preparation
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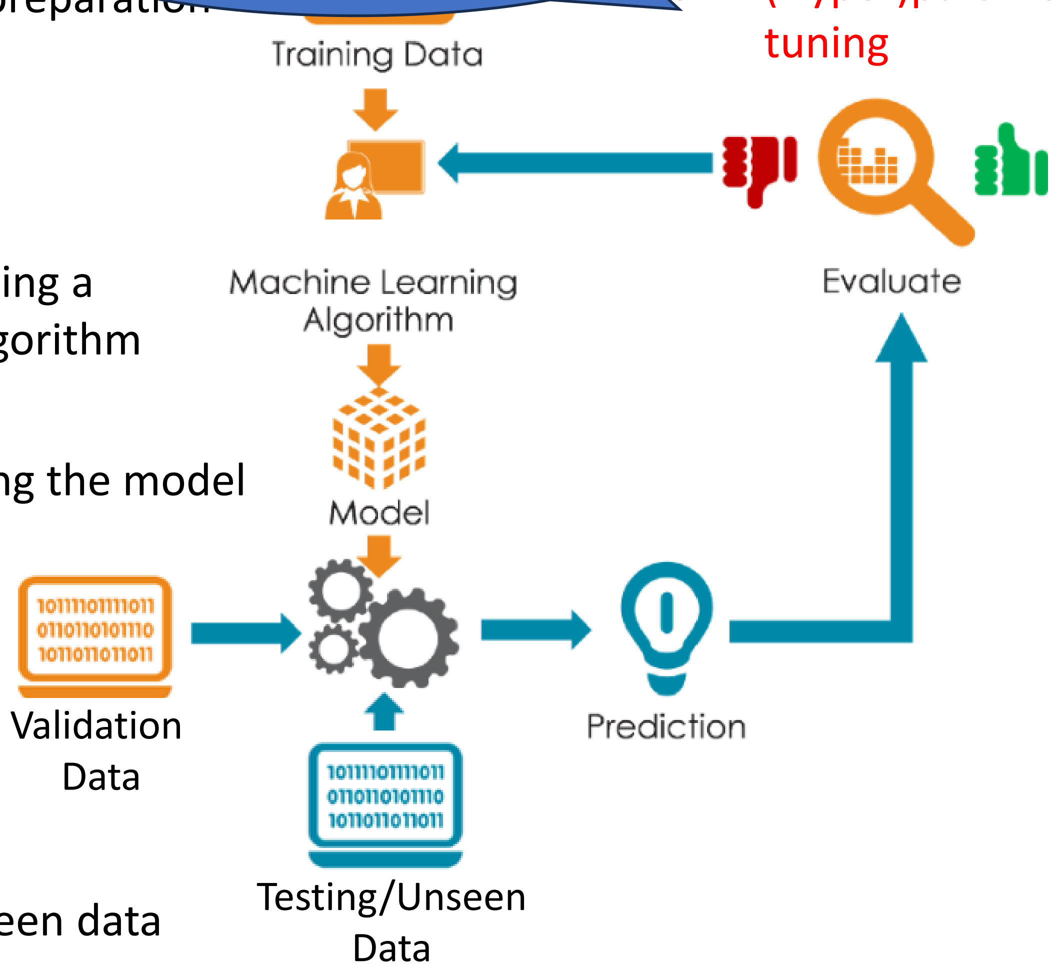


# Performance measurement for classification

- The accuracy of a trained ML model for classification: The number of correct predictions (i.e., predicted outcome = correct outcome, or according to our notation, $\hat{y} = y$)
- Accuracy is a good metric for balanced classification task. But not necessarily for imbalanced ones.
  - E.g. Fraud detection in bank transactions:
    - It is no un-common that > 99% of transactions are normal, and < 1% fraud
    - If ML model does nothing but keep saying no (i.e., the transaction is not frauded), its accuracy is 99%. But it is of no use!

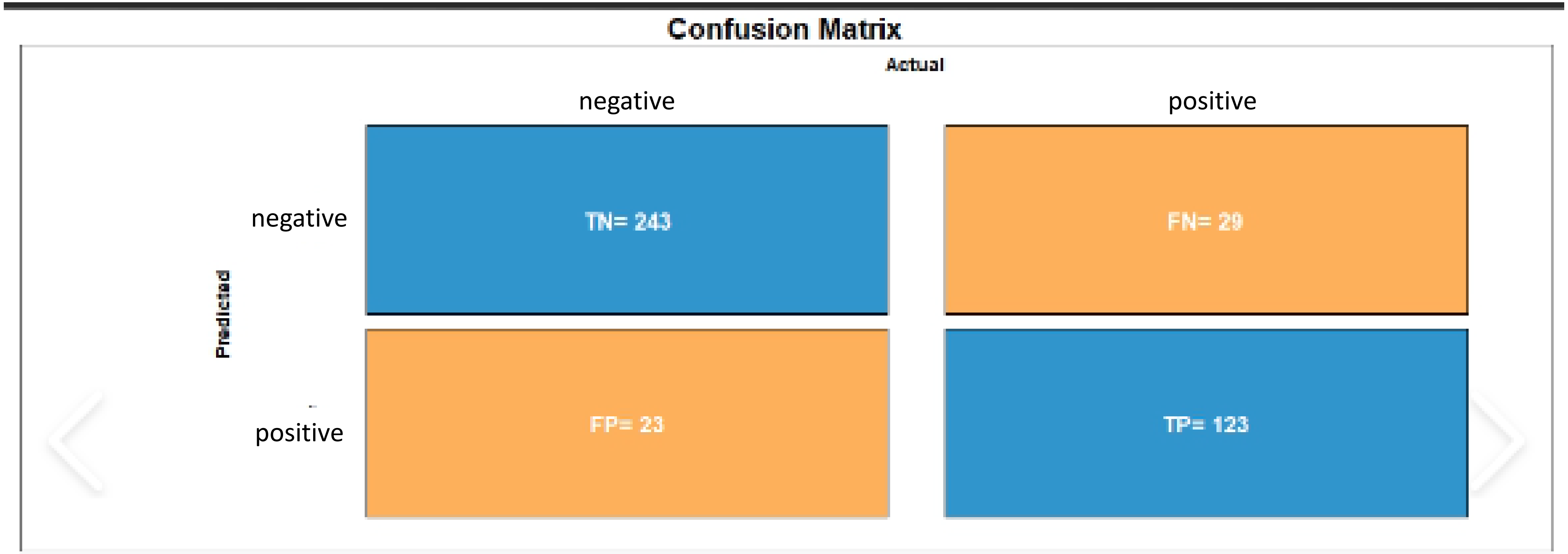
# Better measure (for binary classification)

- Binary classification
  - Given any input, the ML algorithm predicts Positive / Negative.

    E.g., Positive if the transaction is frauded; Negative it is not frauded.
- There are four possibilities
  - True Positive: actual is positive, and ML predicts a positive.
  - True Negative: actual is negative, and ML predicts a negative.
  - False Negative: actual is positive, but ML predicts a negative.
  - False Positive: actual is negative, but the test predicts a positive.

# Confusion matrix

## An example (which can be constructed by the confusion_matrix(y_actual, y_pred) method from sklearn)



# Performance measures for binary classification

| Name 1 | Name 2 | Definition |
|---|---|---|
| TPR | Recall | $\frac{\mathrm{TP}}{\mathrm{TP+FN}}$ |
| TNR | 1-FPR | $\frac{\mathrm{TN}}{\mathrm{TN+FP}}$ |
| PPV | Precision | $\frac{\mathrm{TP}}{\mathrm{TP+FP}}$ |

# Performance measures for binary classification

True positive rate: measures the % of positive instances that ML can detect.

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# Performance measures for binary classification

True positive rate: measures the % of positive instances that ML can detect.

True negative rate: measures the % of negative instances that ML can detect.

Positive predictive values: measures the % of correct instances that ML reports positive

| Name 1 | Name 2 | |
|---|---|---|
| TPR | Recall | $\frac{TP}{TP+FN}$ |
| TNR | 1-FPR | $\frac{TN}{TN+FP}$ |
| PPV | Precision | $\frac{TP}{TP+FP}$ |

# Performance measures for binary classification

Other names you may find in the literature.

| Name 1 | Name 2 | Definition |
| --- | --- | --- |
| TPR | Recall | $\frac{\mathrm{TP}}{\mathrm{TP+FN}}$ |
| TNR | 1-FPR | $\frac{\mathrm{TN}}{\mathrm{TN+FP}}$ |
| PPV | Precision | $\frac{\mathrm{TP}}{\mathrm{TP+FP}}$ |

# F1-score: Another measure for binary classification

- Combine recall and precision
- Definition

$$\text{F1 Score} = \frac{2}{\frac{1}{\text{Precision}} + \frac{1}{\text{Recall}}}$$

To have a good (high) F1-score, both recall and precision have to be good.

# Performance measure of regression

- Sum of Square Errors $$\mathrm{SSE} = \sum_{\mathrm{i}=1}^{\mathrm{n}} (\mathrm{y_i} - \hat{\mathrm{y}}_\mathrm{i})^2$$

  where $y_i$ and $\hat{y}_i$ are the true output and the model prediction for the $ith$ data point.

- Mean Square Error $$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$$

- Root Mean Square Error

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$$

# Software libraries for ML

# Traditional ML methods: scikit-learn

- Scikit-learn (also known as sklearn) is a free software library for Python. It includes various numerous machine learning algorithms for classification, regression and clustering.
- It was initially developed as a Google summer of code project in 2007. Later, the French institute INRIA got involved and the first public release was published in 2010.

# scikit-learn

*Machine Learning in Python*

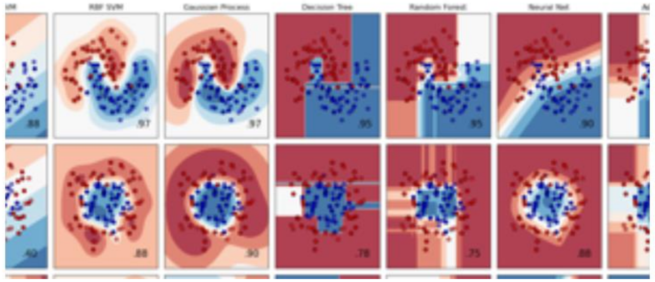
Getting Started | Release Highlights for 1.6

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

## Classification

Identifying which category an object belongs to.

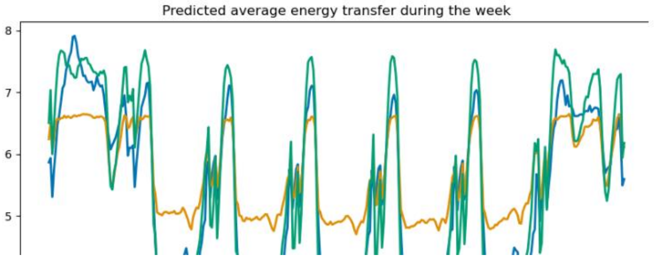
**Applications:** Spam detection, image recognition.
**Algorithms:** Gradient boosting, nearest neighbors, random forest, logistic regression, and more...



## Regression

Predicting a continuous-valued attribute associated with an object.

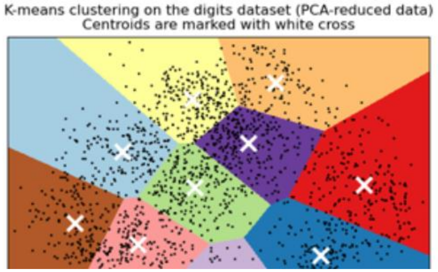
**Applications:** Drug response, stock prices.
**Algorithms:** Gradient boosting, nearest neighbors, random forest, ridge, and more...




## Clustering

Automatic grouping of similar objects into sets.

**Applications:** Customer segmentation, grouping experiment outcomes.
**Algorithms:** k-Means, HDBSCAN, hierarchical clustering, and more...



https://scikit-learn.org/stable/supervised_learning.html





# 1. Supervised learning

# 1. Supervised learning

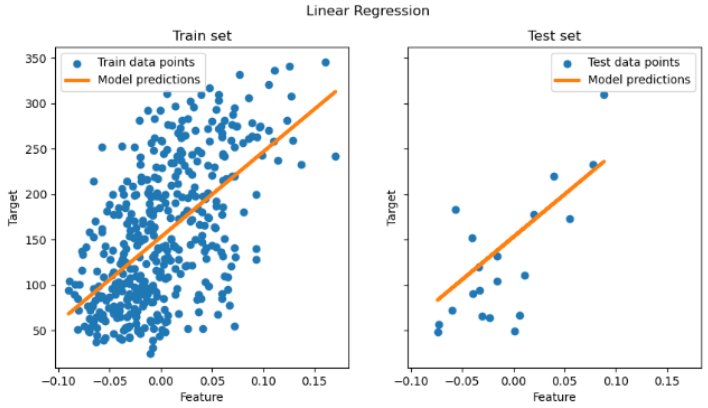
## 1.1. Linear Models



### 1.1.1. Ordinary Least Squares

`LinearRegression` fits a linear model with coefficients $w = (w_1, \ldots, w_p)$ to minimize the residual sum of squares between the observed targets in the dataset, and the targets predicted by the linear approximation. Mathematically it solves a problem of the form:

$$\min_{w} ||Xw - y||_2^2$$




`LinearRegression` will take in its `fit` method arrays `X`, `y` and will store the coefficients $w$ of the linear model in its `coef_` member:

```
>>> from sklearn import linear_model
>>> reg = linear_model.LinearRegression()
>>> reg.fit([[0, 0], [1, 1], [2, 2]], [0, 1, 2])
LinearRegression()
>>> reg.coef_
array([0.5, 0.5])
```

# Some examples

# Supervised learning: Linear Regression model for predicting ice cream sales

```
[1] import matplotlib.pyplot as plt
    import numpy as np
    from sklearn.linear_model import LinearRegression
```

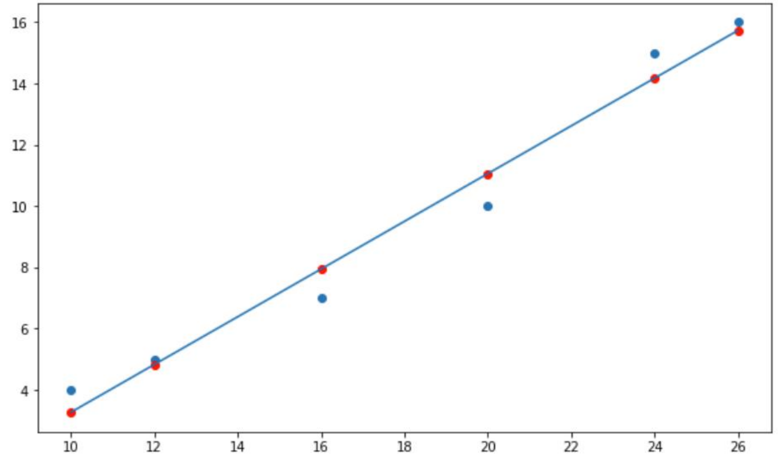
```
x = np.array([10,12,16,20,24,26]).reshape((-1,1))
y = np.array([4,5,7,10,15, 16])
```

```
[3] model = LinearRegression()
    model.fit(x, y)
```

```
[4] y_pred = model.predict(x)

    plt.figure(figsize=(10,6))
    plt.scatter(x,y)
    plt.scatter(x,y_pred,color='r')
    x_seq = np.linspace(x.min(),x.max(),15).reshape((-1,1))
    plt.plot(x_seq, model.predict(x_seq))
    plt.show()
```

| Temperature (°C) x | Ice-cream Sales (No. of cones) y |
|---|---|
| 10 | 4 |
| 12 | 5 |
| 16 | 7 |
| 20 | 10 |
| 24 | 15 |
| 30 | ? |



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```

Why reshape() here?

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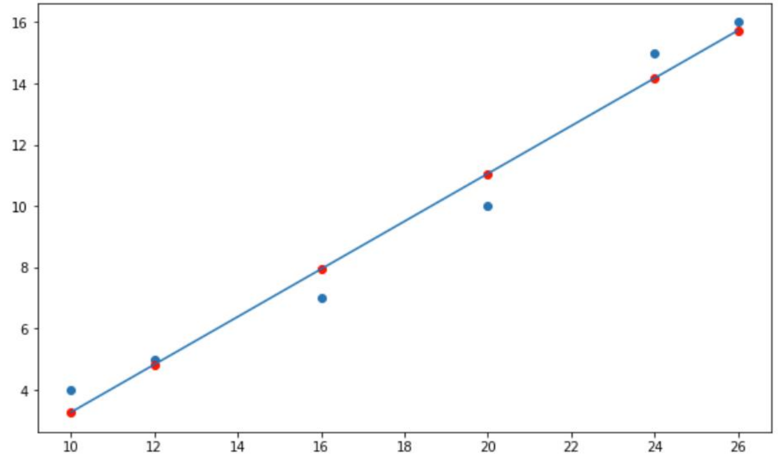

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     plt.plot(x_seq, model.predict(x_seq))
     plt.show()
```

```
model.predict([[30]])
```

```
array([18.84615385])
```

| Temperature (°C) x | Ice-cream Sales (No. of cones) y |
|---|---|
| 10 | 4 |
| 12 | 5 |
| 16 | 7 |
| 20 | 10 |
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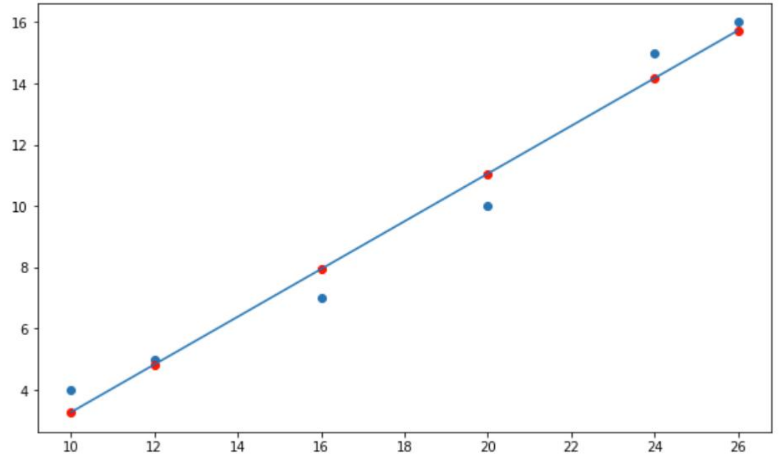
| 30 | ? |



# Supervised learning: Classifying Apple vs Pear

```
from sklearn import tree
import numpy as np
```

```
features = ['color', 'width', 'height']
fruitnames=['apple', 'pear']

data =np.array( [[10, 5.3, 4.8], [62, 5.5, 7.8], [85, 5.7, 4.9], [58, 6.8, 5.9],
        [15, 8.6, 7.7], [100, 5.4, 8.2], [22, 5.8, 5.6], [71, 4.5, 6.3]])
labels = np.array([0, 1, 0, 1, 0, 1, 0, 1])
```

```
[3] fruit_classifier = tree.DecisionTreeClassifier()
```

```
[4] fruit_classifier = fruit_classifier.fit(data, labels)
```

```
[5] predit = fruit_classifier.predict(np.array([[101, 6.3, 7.9],[25, 4.5, 3.8],[85, 5.2, 4.0]]))
    predit

    array([1, 0, 0])
```

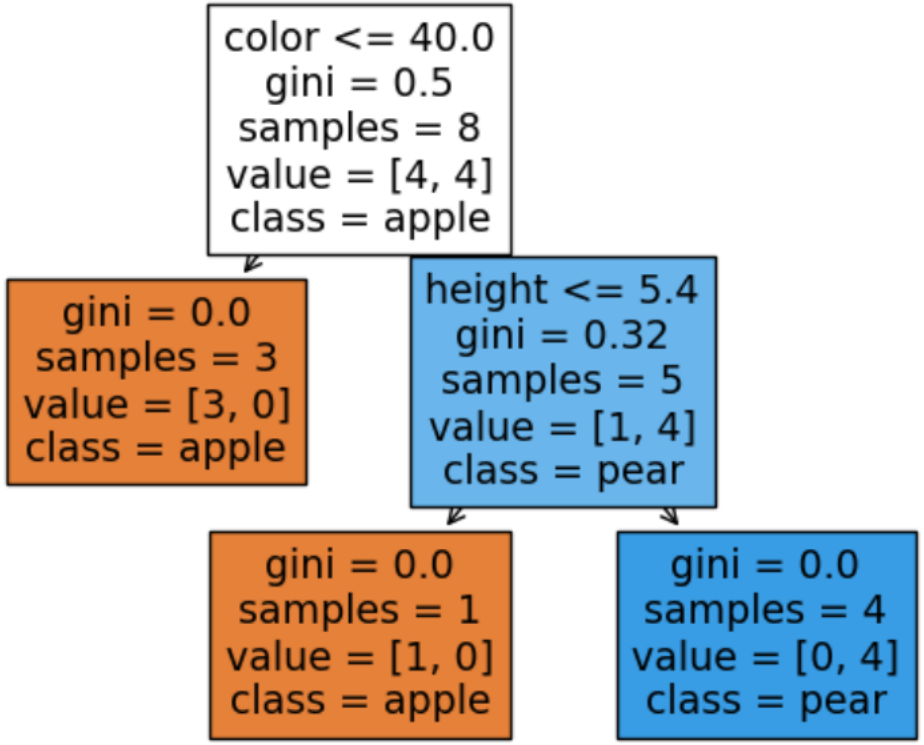
```
[9] print(fruitnames[int(fruit_classifier.predict([[101,6.3,7.9]]))])

    pear
```

# Supervised learning: Classifying Apple vs Pear

```
tree.plot_tree(fruit_classifier, feature_names = features, class_names = fruit_names,
               filled = True)
```

```
[Text(0.4, 0.8333333333333334, 'color <= 40.0\ngini = 0.5\nsamples = 8\nvalue = [4, 4]\nclass = apple')
 Text(0.2, 0.5, 'gini = 0.0\nsamples = 3\nvalue = [3, 0]\nclass = apple'),
 Text(0.6, 0.5, 'height <= 5.4\ngini = 0.32\nsamples = 5\nvalue = [1, 4]\nclass = pear'),
 Text(0.4, 0.16666666666666666, 'gini = 0.0\nsamples = 1\nvalue = [1, 0]\nclass = apple'),
 Text(0.8, 0.16666666666666666, 'gini = 0.0\nsamples = 4\nvalue = [0, 4]\nclass = pear')]
```



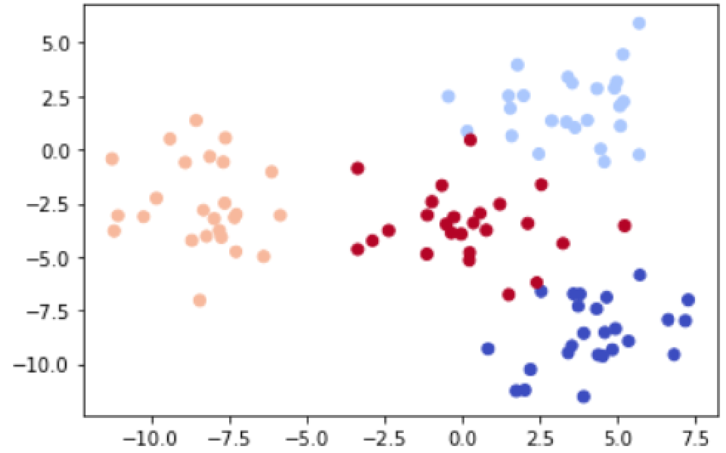
# Unsupervised learning: clustering points on 2D plane

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

```
from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs

x, y = make_blobs(n_samples=100, centers=4, random_state=500, cluster_std=1.75)
```

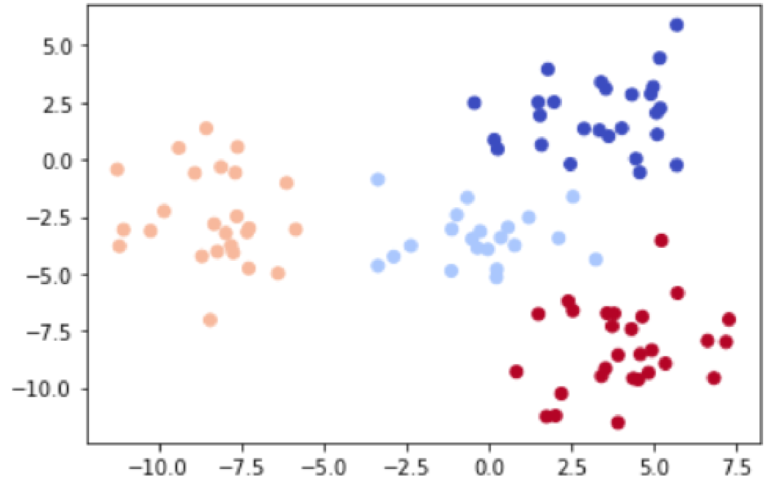
```
plt.scatter(x[:,0],x[:,1], c=y, cmap='coolwarm')
plt.show()
```



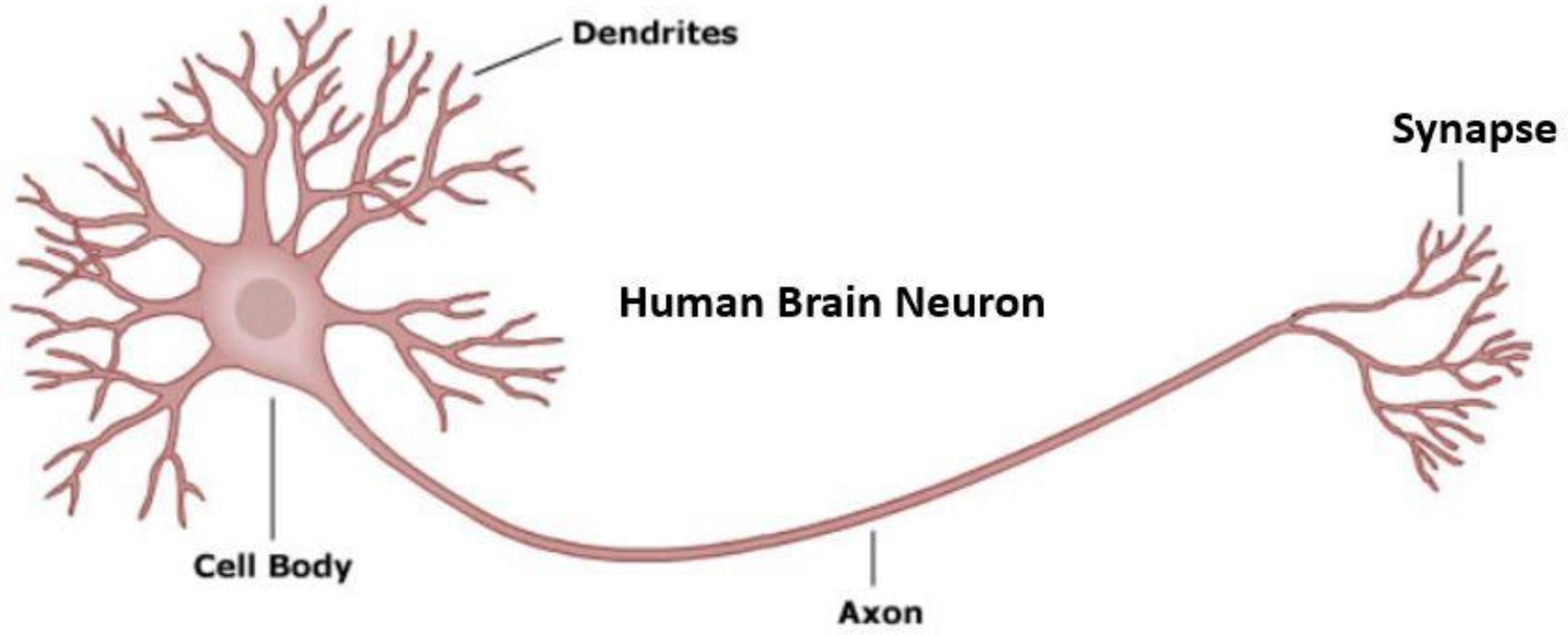

```
model = KMeans(n_clusters=4, random_state = 0)
model.fit(x)

y_ = model.predict(x)
```

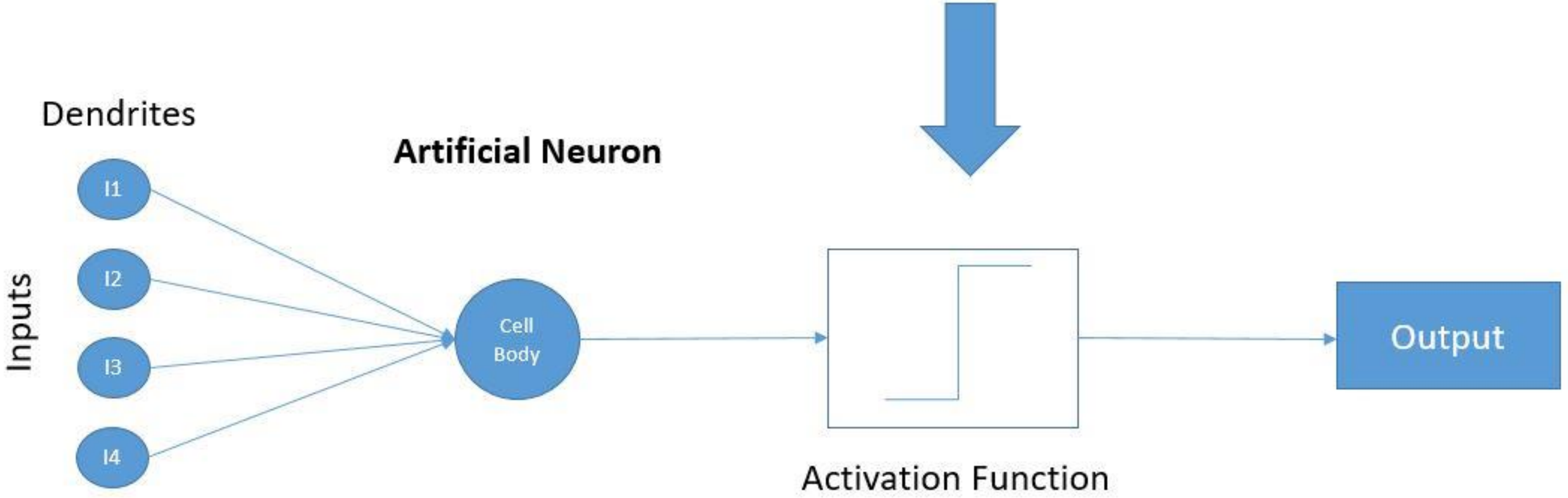
```
plt.scatter(x[:,0],x[:,1], c = y_, cmap='coolwarm')
plt.show()
```



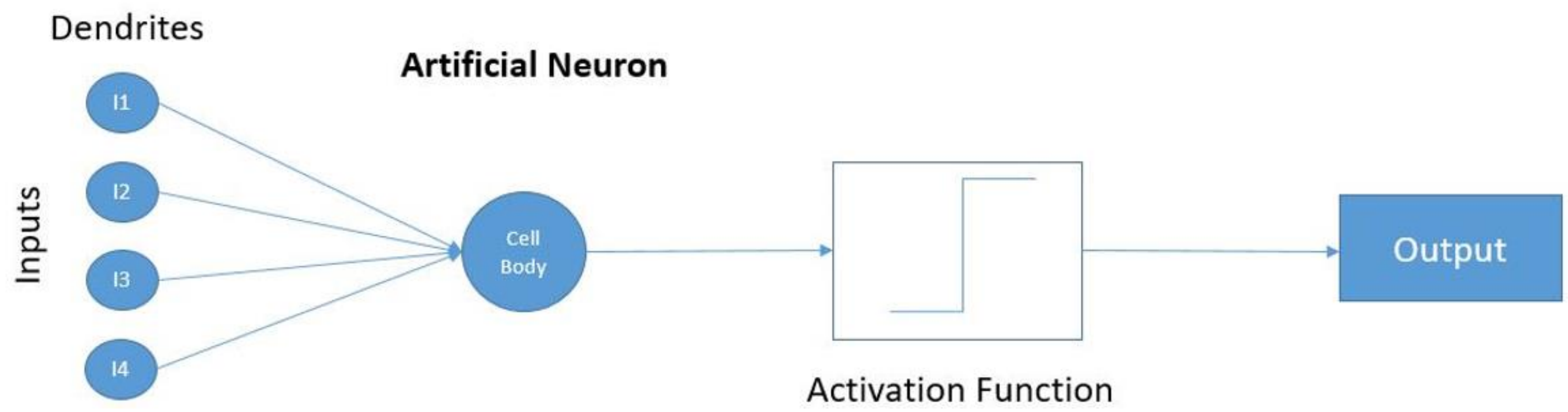
# Artificial neural network and deep learning

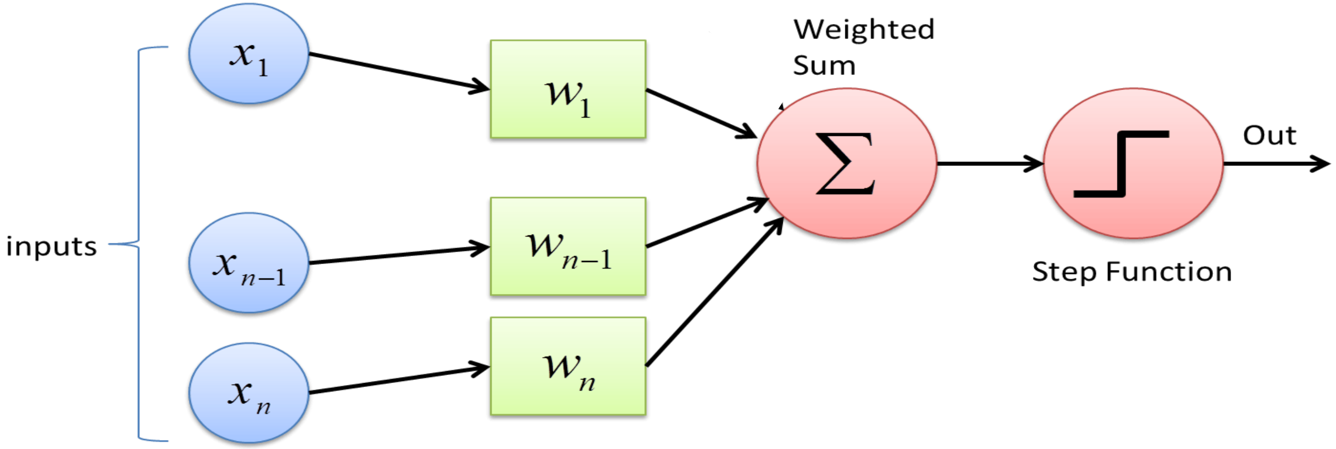



A neuron



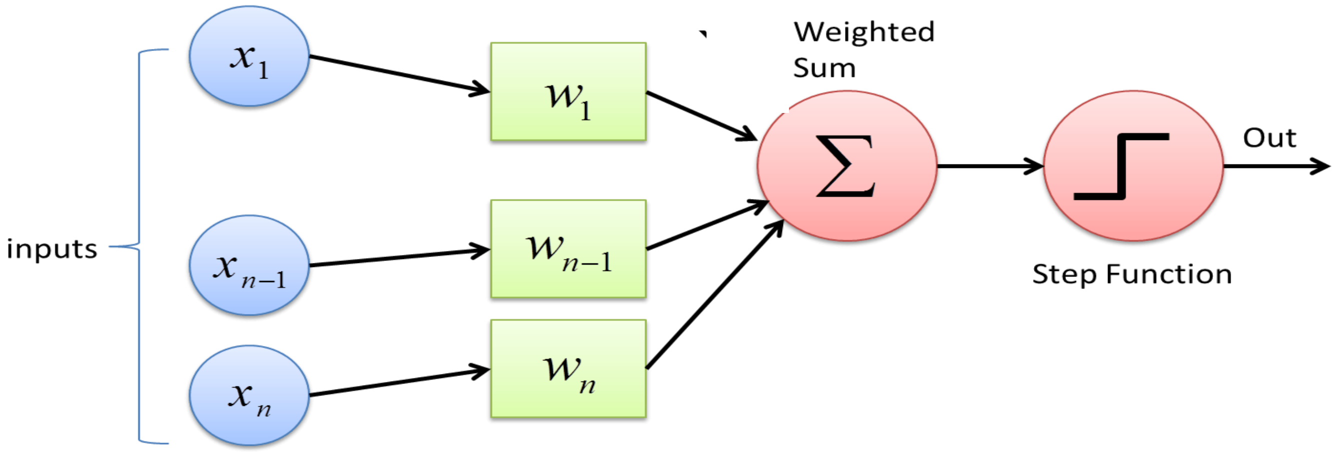

An
artificial
neuron




Perceptron:
Final model for an artificial neuron

# The Perceptron




We now introduce a simple aritifical neural network called Perceptron and explain how to apply it to the *binary classification* task where we refer to our two classes as 1 (positive class) and -1 (negative class). Given a certain input $x = (x_1, x_2, \ldots, x_m)$, and a correspoinding weights $(w_1, w_2, \ldots, w_m)$, we predict $x$ is in class 1 if the *net input*

$$z = w_1x_1 + w_2x_2 + \cdots + w_mx_m$$

is greater than or equal to some threshold $\theta$, and predict -1 otherwise.

# The Perceptron

To be more concrete, we define the decision function $\phi(z)$ where

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

We use $\phi(z)$ to help us classify a data point $x = (x_1, x_2, \ldots, x_m)$ as follows:

we compute the *net input* $z = w_1x_1 + w_2x_2 + \cdots + w_mx_m$ and classify $x$ into the class $\hat{y} = \phi(z) \in \{1, -1\}$.

To train a set of $n$ data points

$$\left\{x^{(i)} = [x_1^{(i)}, x_2^{(i)}, \ldots, x_m^{(i)}] \text{ for } 1 \leq i \leq n\right\},$$

with the set of their class label

$$\left\{y^{(i)} \in \{1, -1\} \text{ for } 1 \leq i \leq n\right\},$$

we need to decide the best weights $w_1, w_2, \ldots, w_m$ and threshold $\theta$ such that our prediction

$$\left\{\hat{y}^{(i)} = \phi(w_1 x_1^{(i)} + w_2 x_2^{(i)} + \cdots + w_m x_m^{(i)}) \text{ for } 1 \leq i \leq n\right\}$$

has the smallest number of mis-classifications $y^{(i)} \neq \hat{y}^{(i)}$, or equivalently, the sum

$$\sum_{1 \leq i \leq n} \left|y^{(i)} - \hat{y}^{(i)}\right|$$

is as small as possible.

# The Perceptron

A simple trick for simplication. Instead of determining two sets of values, namely the weights $w_i$'s and the threshold $\theta$, we can redefine the net input from

$$z = w_1x_1 + w_2x_2 + \cdots + w_mx_m$$

to

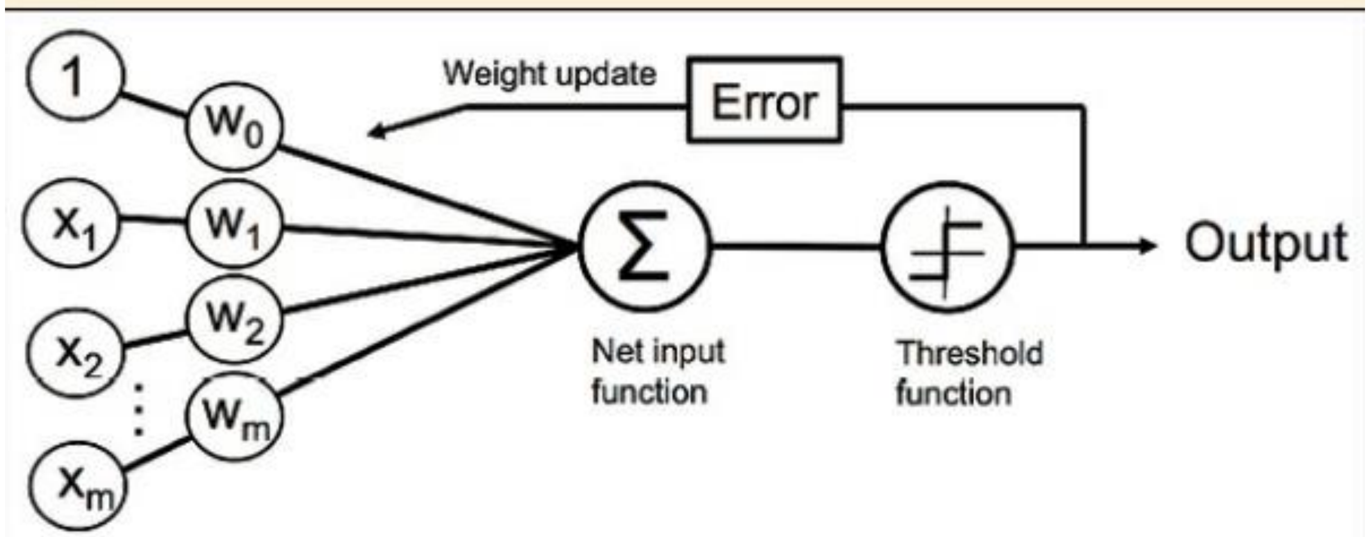
$$z = w_0x_0 + w_1x_1 + w_2x_2 + \cdots + w_mx_m$$

where $w_0 = -\theta$ and $x_0 = 1$. Then, we classify $x = (x_1, x_2, \ldots, x_m)$ into the class 1 if $z \geq 0$, and -1 otherwise, i.e., we classify $x$ into class $\phi(z)$ where $\phi$ is redefined as follows:

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

The weight $w_0 = -\theta$ is usually called the *bias unit.*

# How to train a perceptron?



# How to train a perceptron?

The idea:

- Initialize the weights to some small random numbers.
- For each training example $x^{(i)}$:

  a. Compute the output value $\hat{y}^{(i)}$ (based on the current weights).

  b. Update the weights $w_j = w_j + \Delta w_j$.

# How to train a perceptron?

What we want:

- If $y^{(i)} = \hat{y}^{(i)}$: We don't want any change, i.e., $\Delta w_j = 0$ for all $1 \leq j \leq m$.
- If $y^{(i)} = 1$ and $\hat{y}^{(i)} = -1$: We want that with the new weights $w_j'$'s, the value net input
$$z' = w_0'x_0 + w_1'x_1 + \cdots + w_m'x_m$$
will increase, i.e., $z' > z$ so that we'd have a better chance to get $z' > 0$ and thus $\hat{y}^{(i)} = \phi(z')$ becomes 1.
- If $y^{(i)} = -1$ and $\hat{y}^{(i)} = 1$: We want that with the new weights $w_j'$'s, the value net input
$$z' = w_0'x_0 + w_1'x_1 + \cdots + w_m'x_m$$
will decrease, i.e., $z' < z$ so that we'd have a better chance to get $z' < 0$ and thus $\hat{y}^{(i)} = \phi(z')$ becomes $-1$.

# How to train a perceptron?

Rosenblatt's proposed the following rule for $\Delta w_j$:

$$\Delta w_j = \eta(y^{(i)} - \hat{y}^{(i)})x_j^{(i)}$$

Here, $\eta$ is the learning rate (typically a small constant between 0.0 and 1.0) for avoiding over-shooting. It is not difficult to verify that Rosenblatt's rule satisfies the above three conditions.

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A very important hyper-parameter, especially for a training data set with million of examples.

# Deep learning: TensorFlow and Keras

- TensorFlow is a free software library for machine learning and AI. It can be used across a range of tasks but focuses on training and inference of deep neural networks.
- TensorFlow was developed by the Google Brain team.
- Keras is a free software library that provides a Python interface for neural network. It is commonly used as an interface for the TensorFlow library.

# Why not Pytorch?

It is "*an open source machine learning framework that accelerates the path from research prototyping to production deployment.*"[22]

22 https://pytorch.org/

# Why not Pytorch?

Written by Vihar Kurama

## PyTorch vs. TensorFlow: My Recommendation

TensorFlow is a very powerful and mature deep learning library with strong visualization capabilities and several options to use for high-level model development. It has production-ready deployment options and support for mobile platforms. PyTorch, on the other hand, is still a relatively young framework with stronger community movement and it's more Python-friendly.

What I would recommend is if you want to make things faster and build AI-related products, TensorFlow is a good choice. PyTorch is mostly recommended for research-oriented developers as it supports fast and dynamic training.

# Example: classifying digits

# Deep Learning: Train a neural network for digit classification

The MNIST (Modified National Institute of Standards and Technology) dataset for training.

- It is a large dataset of handwritten digits created in 1998.
- Over the years, researchers used this dataset to test the accuracy of different ML methods.

Sample images from MNIST test dataset

| Type | Classifier | Error rate (%) |
|---|---|---|
| Linear classifier | Pairwise linear classifier | 7.6[10] |
| Decision stream with Extremely randomized trees | Single model (depth > 400 levels) | 2.7[23] |
| K-Nearest Neighbors | K-NN with non-linear deformation (P2DHMDM) | 0.52[24] |
| Boosted Stumps | Product of stumps on Haar features | 0.87[25] |
| Non-linear classifier | 40 PCA + quadratic classifier | 3.3[10] |
| Random Forest | Fast Unified Random Forests for Survival, Regression, and Cla | 2.8[27] |
| Support-vector machine (SVM) | Virtual SVM, deg-9 poly, 2-pixel jittered | 0.56[28] |
| Deep neural network (DNN) | 2-layer 784-800-10 | 1.6[29] |
| Deep neural network | 2-layer 784-800-10 | 0.7[29] |
| Deep neural network | 6-layer 784-2500-2000-1500-1000-500-10 | 0.35[30] |
| Convolutional neural network (CNN) | 6-layer 784-40-80-500-1000-2000-10 | 0.31[31] |
| Convolutional neural network | 6-layer 784-50-100-500-1000-10-10 | 0.27[32] |
| Convolutional neural network (CNN) | 13-layer 64-128(5x)-256(3x)-512-2048-256-256-10 | 0.25[17] |
| Convolutional neural network | Committee of 35 CNNs, 1-20-P-40-P-150-10 | 0.23[12] |
| Convolutional neural network | Committee of 5 CNNs, 6-layer 784-50-100-500-1000-10-10 | 0.21[19][20] |
| Random Multimodel Deep Learning (RMDL) | 10 NN-10 RNN - 10 CNN | 0.18[22] |
| Convolutional neural network | Committee of 20 CNNS with Squeeze-and-Excitation Networks | 0.17[34] |

# Deep Learning: Train a neural network for digit classification

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[2]  (train_images, train_labels), (test_images, test_labels) = mnist.load_data()
     train_images.shape, train_labels.shape, test_images.shape, test_labels.shape
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[3]  train_images = train_images.reshape((60000, 28*28))/255
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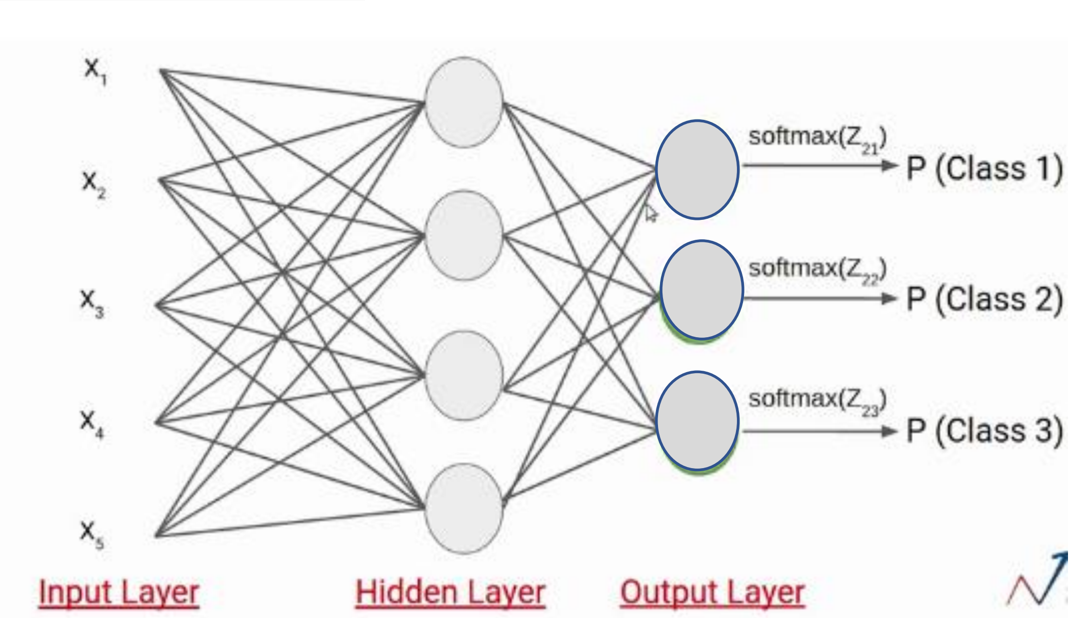


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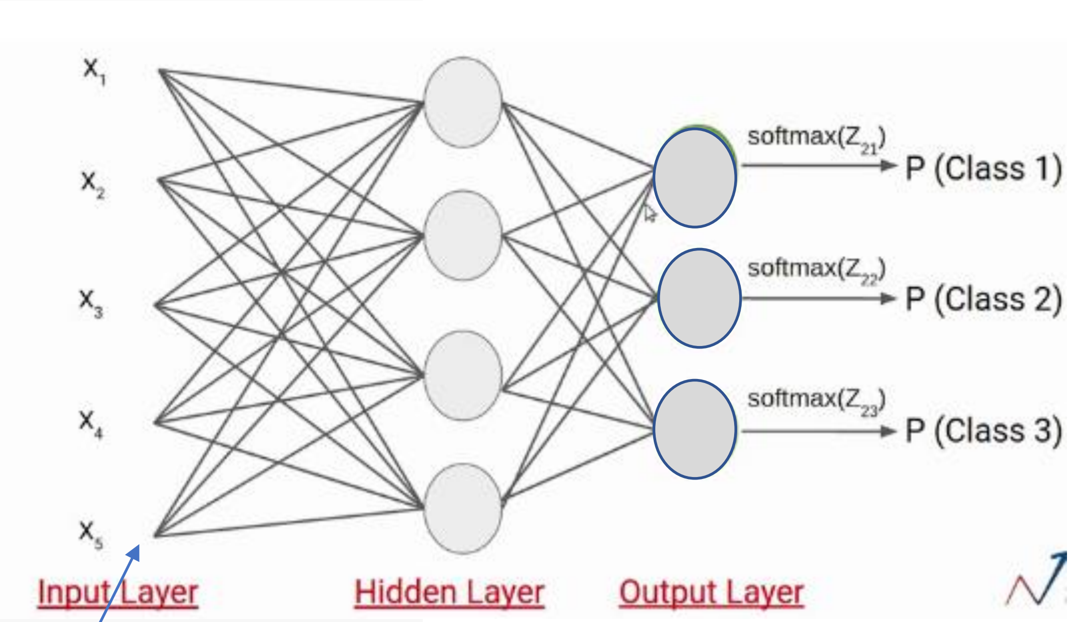


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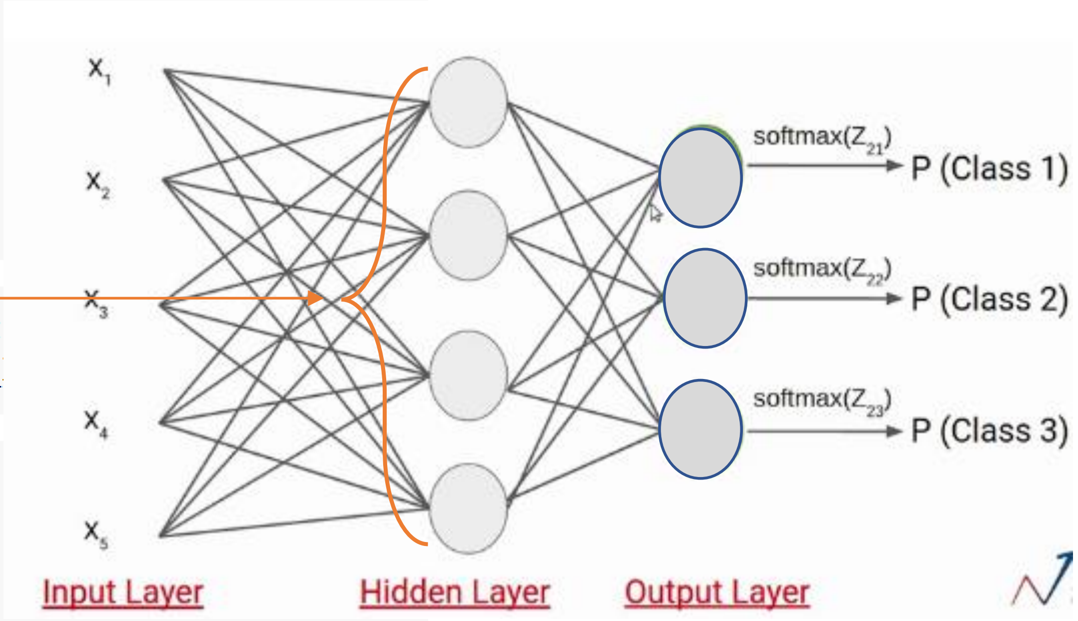

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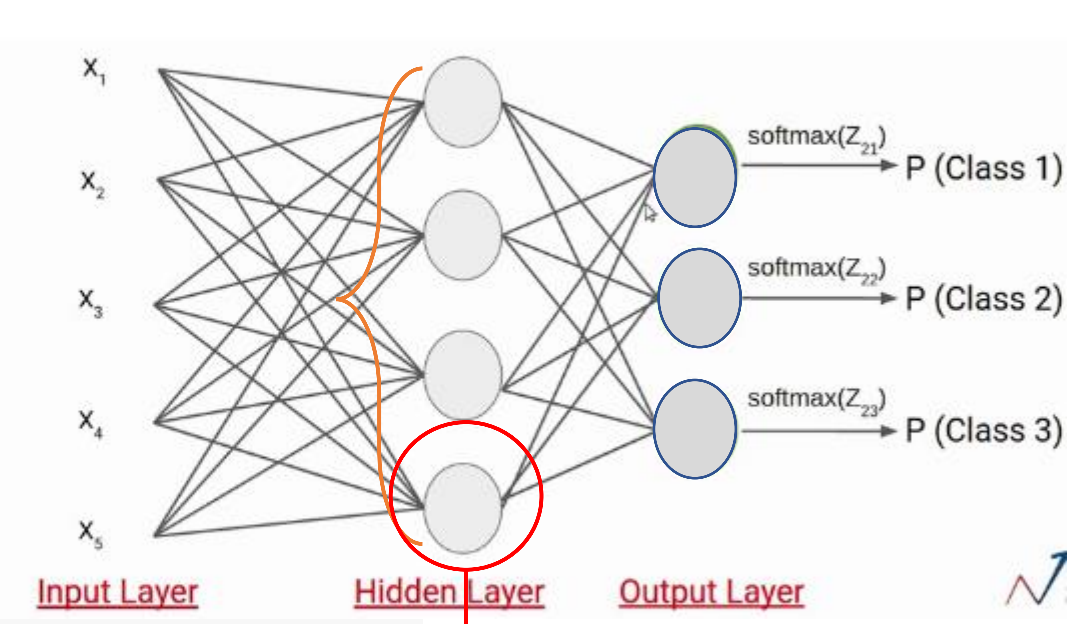


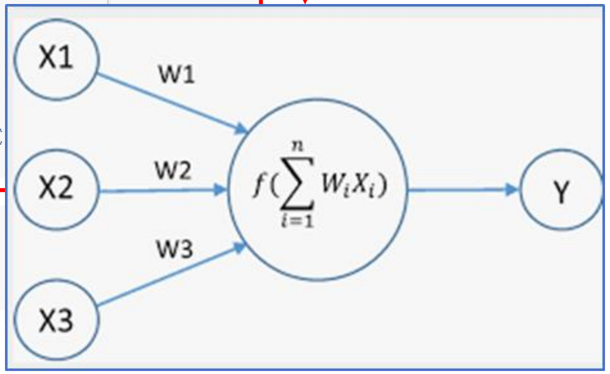

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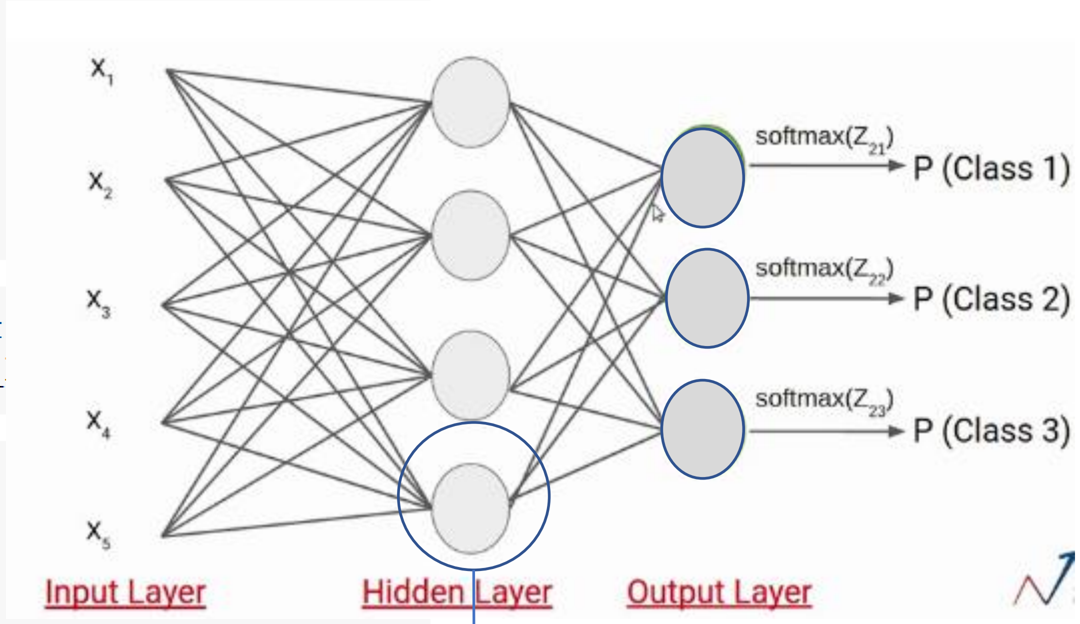


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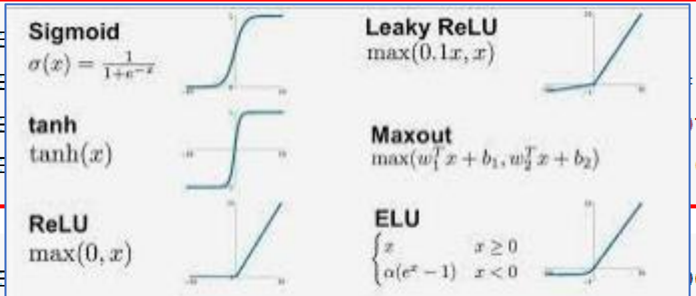


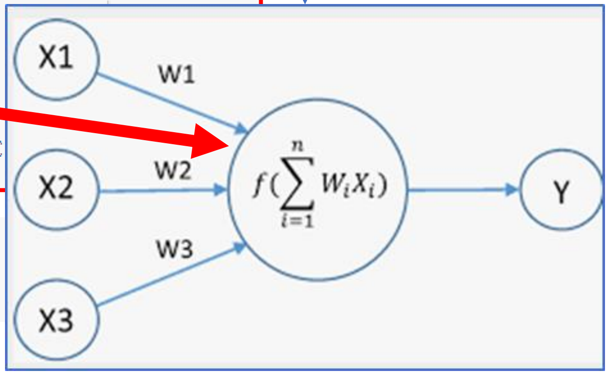


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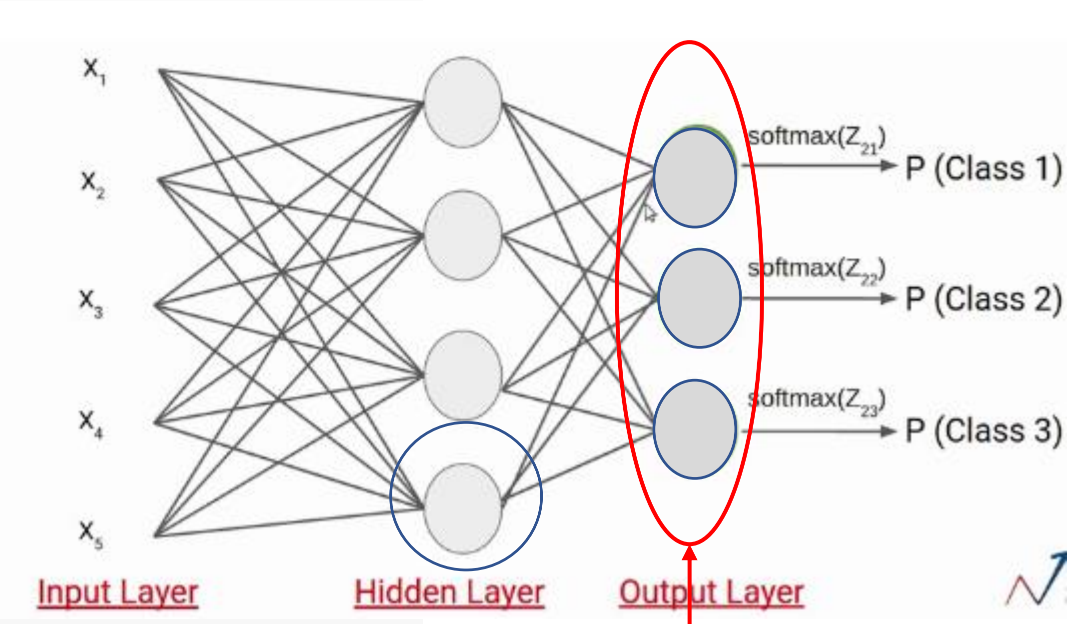


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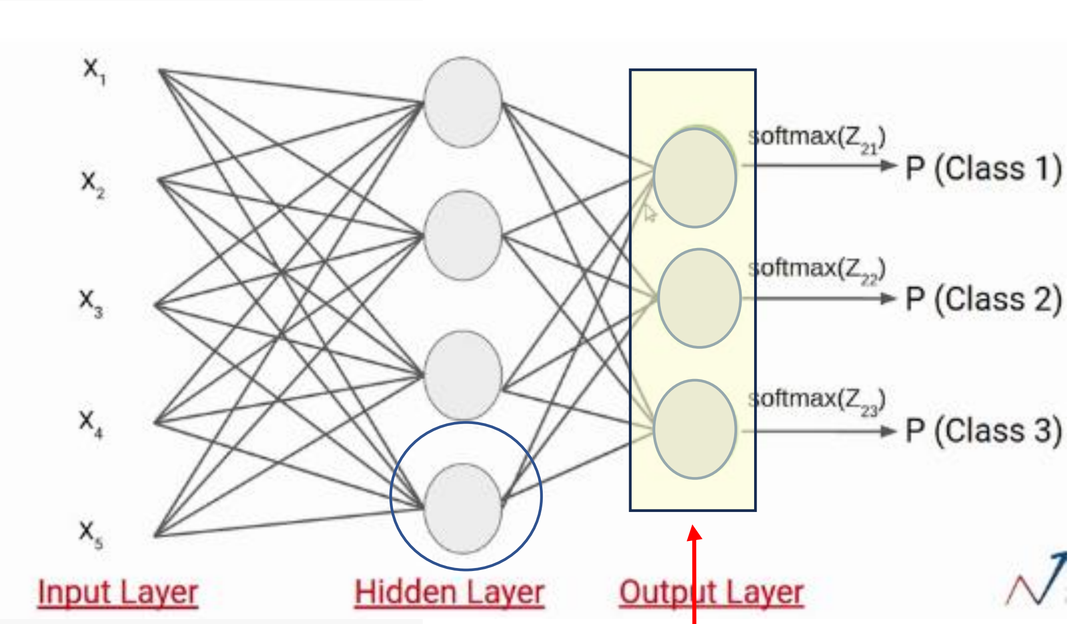


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softmax function

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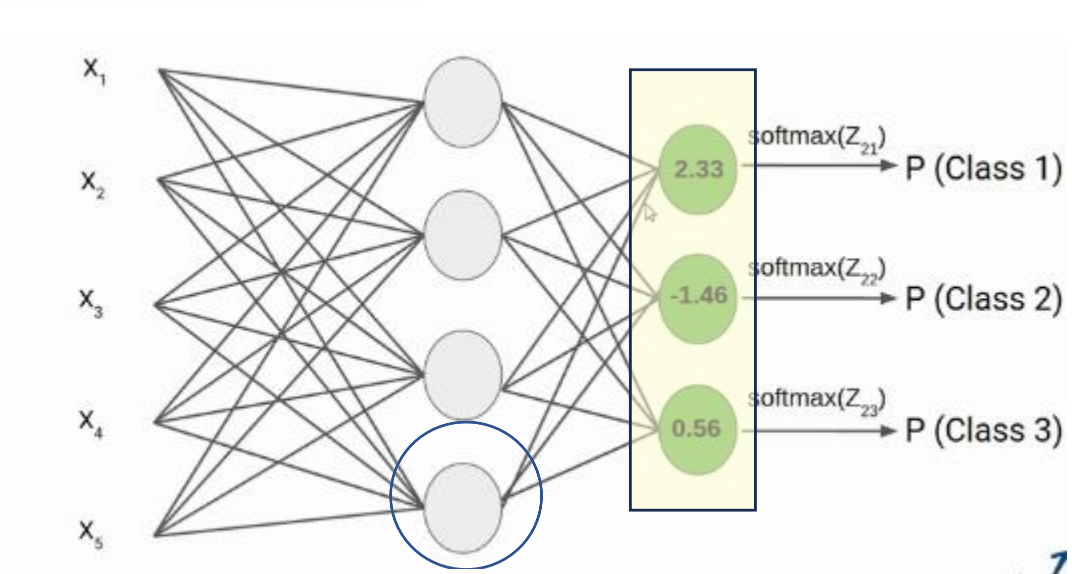


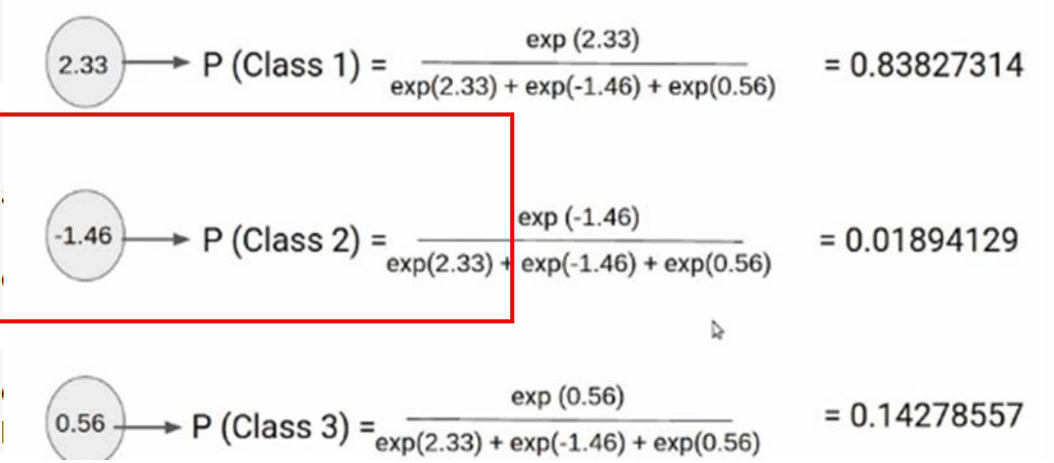

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The probability that the input is in class 2.

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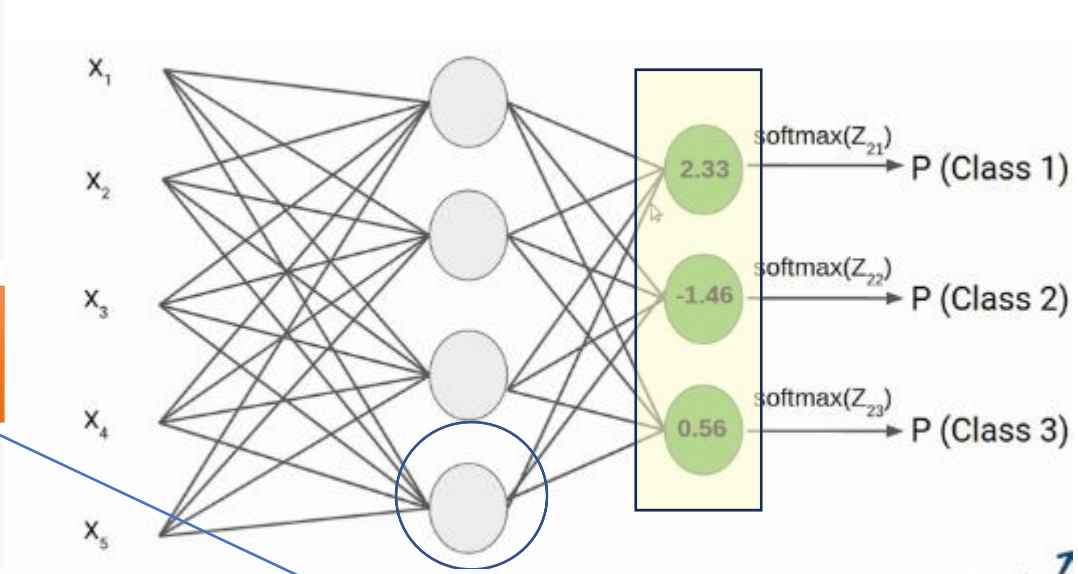


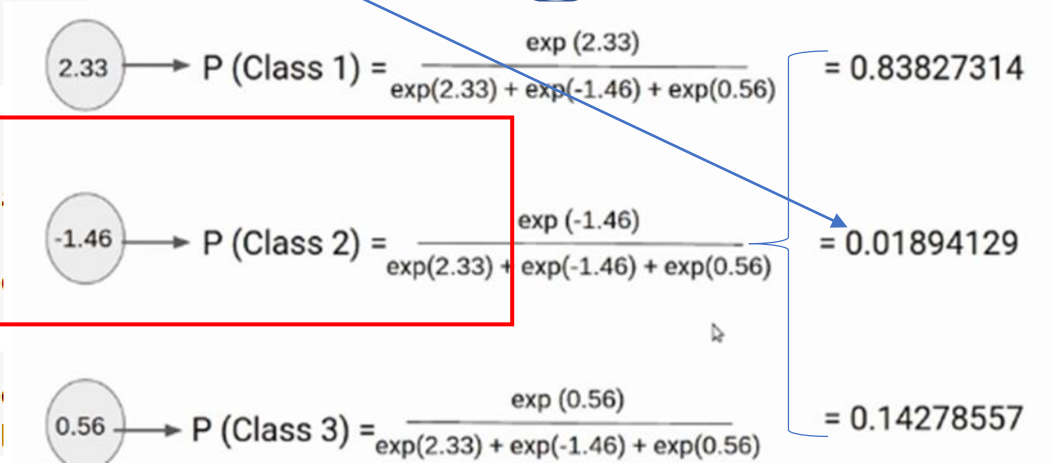

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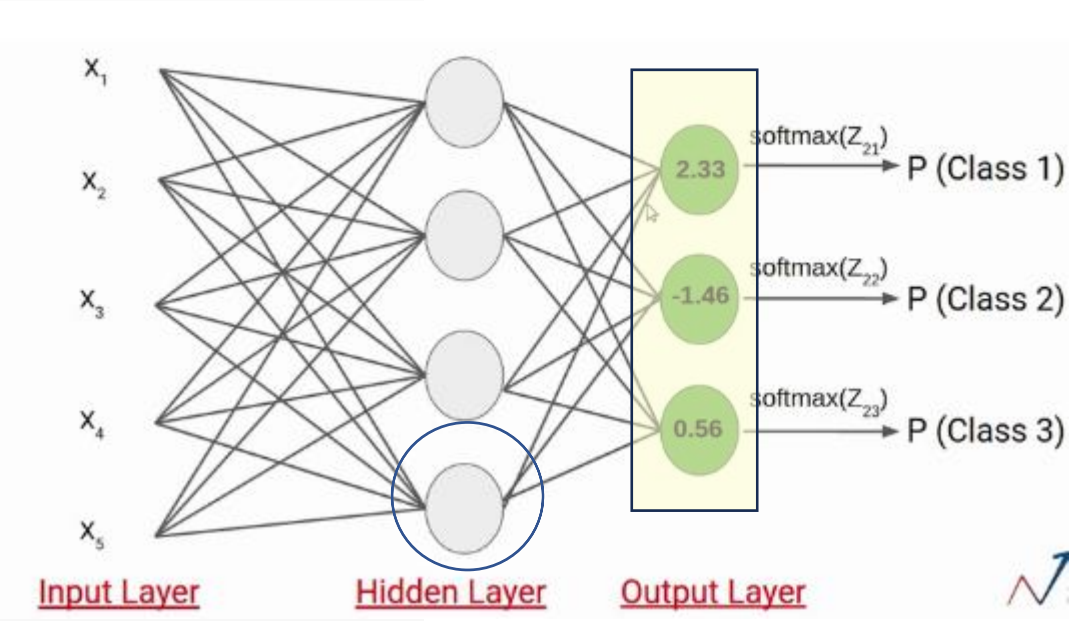


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# Deep Learning: Train a neural network for digit classification

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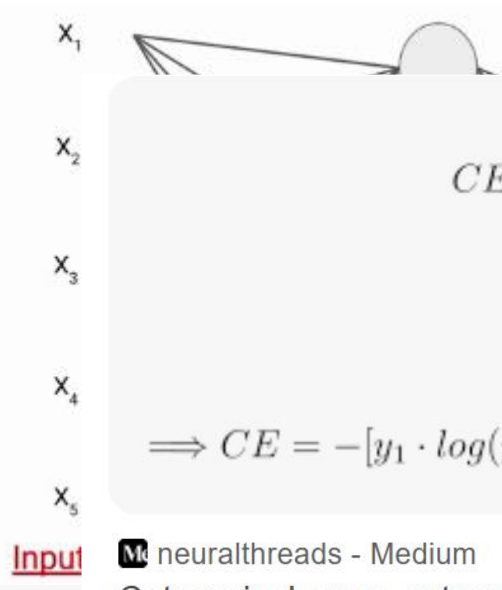


$$CE = -\sum_{i=1}^{i=N} y\_true_i \cdot log(y\_pred_i)$$

$$CE = -\sum_{i=1}^{i=N} y_i \cdot log(\hat{y}_i)$$

$$\Longrightarrow CE = -[y_1 \cdot log(\hat{y}_1) + y_2 \cdot log(\hat{y}_2) + y_3 \cdot log(\hat{y}_3)]$$

neuralthreads - Medium

Categorical cross-entropy loss - ?????

You don’t need to remember it. All you need to know is the optimizer will set the weights appropriately to make CE as small as possible (over the training data set).

# Deep Learning: Train a neural network for digit classification

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The algorithm we choose to minimize the loss functions. There are many choices:

- SGD
- RMSprop
- Adam
- AdamW
- Adadelta
- Adagrad
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Behaviour of different optimizer: [CS231n Convolutional Neural Networks for Visual Recognition]

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One epoch is one complete pass of the training dataset through the algorithm

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The number of data points used for an update of the weights

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batch_size = 1: Each update is fast, but the path to the minimum is not smooth: there are ups and down

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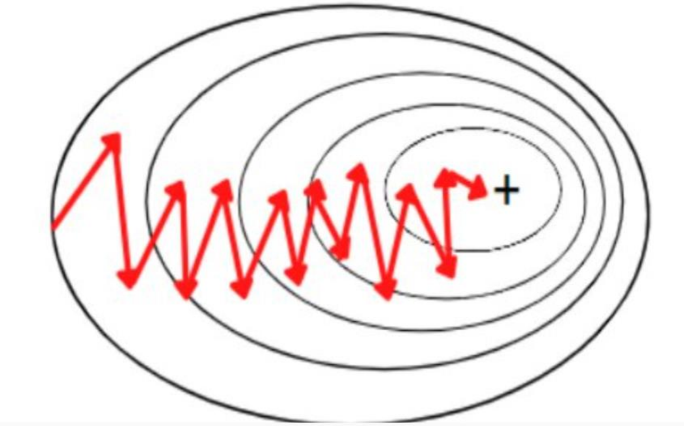

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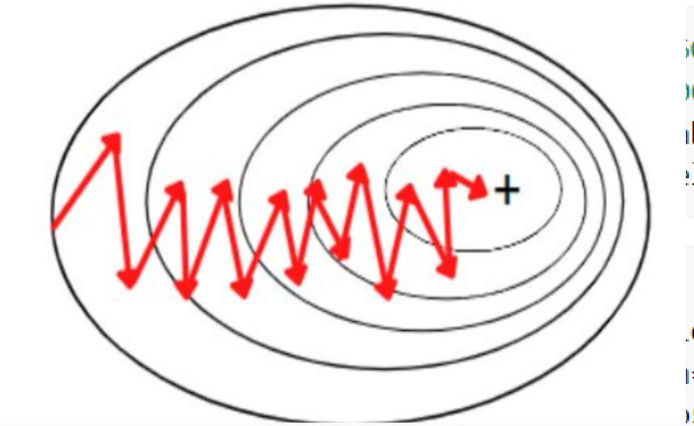
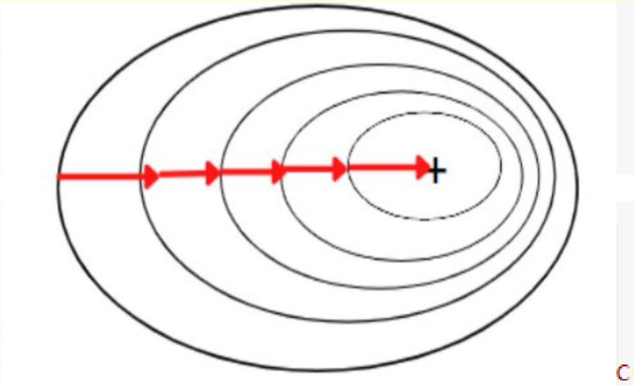


batch_size = the size of the whole data set: Each update is very slow, but the path to the minimum is very smooth



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batch_size = somewhere between 1 and dataset's size

```
[2 ... ,
   ... s
[3 ... 0000,
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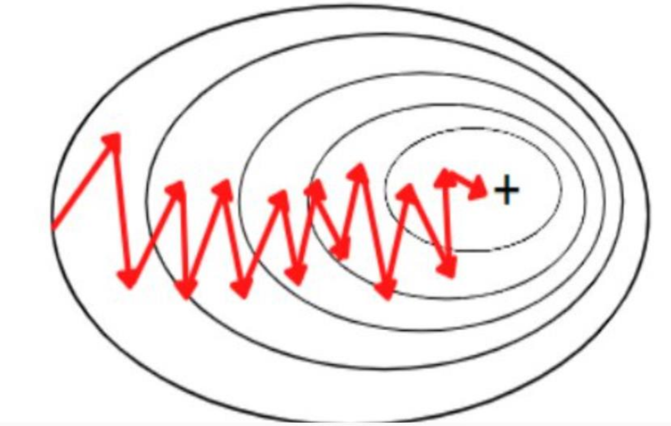

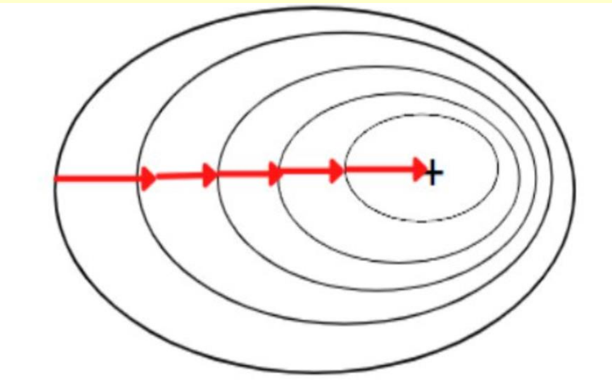

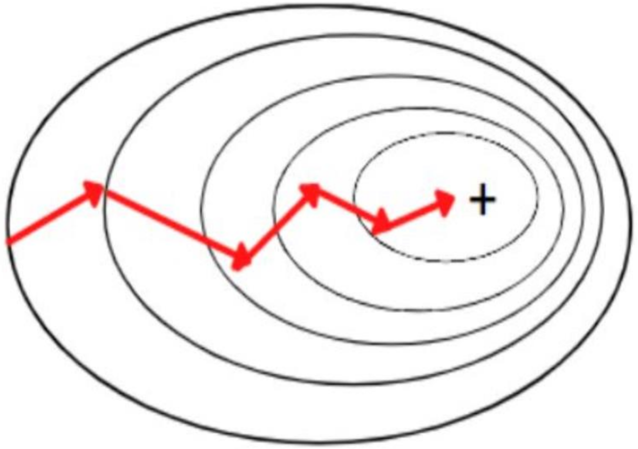

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