Machine Learning

June 18, 2025

1 Types of Losses

A loss function is a mathematical formula that measures how far a model's predictions are from the actual values; it tells the model how wrong it is. Lower loss means better performance

1.1 Regression Losses

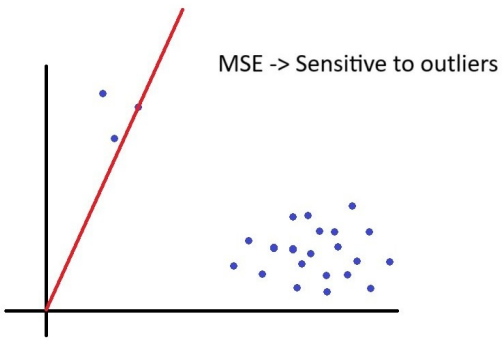
Regression losses are loss functions used in regression tasks (where the goal is to predict continuous values)

1.1.1 Mean Squared Error

$$L = (y_i - \hat{y}_i)^2$$

Disadvantages:

- **Sensitive to Outliers:** Squaring the errors gives more weight to large errors, which can distort the model if outliers are present.
- **Over-penalizes Large Errors:** A single big error can dominate the loss, possibly causing overfitting or poor model behavior.

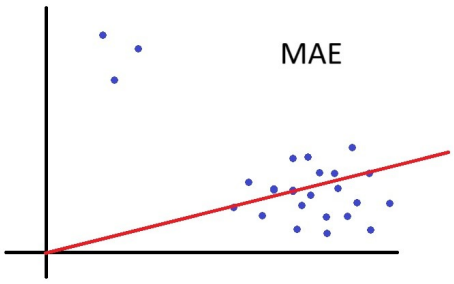


1.1.2 Mean Absolute Error

$$L = |y_i - \hat{y}_i|$$

It is robust to outliers.
Disadvantages:

- **Not Easily Differentiable** MAE's non-differentiability at zero can make optimization challenging for gradient-based methods, slowing down model training.



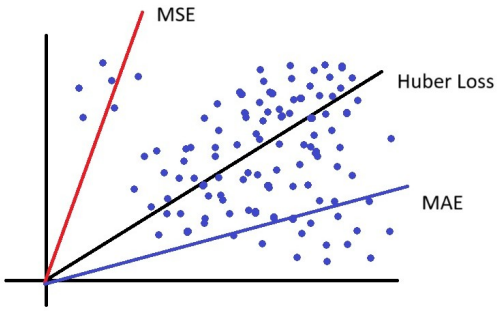
1.1.3 Huber Loss

$$L_\delta(a) = \begin{cases} \frac{1}{2}(y_i - \hat{y}_i)^2, & \text{for } |y_i - \hat{y}_i| \leq \delta \\ \delta\left(|y_i - \hat{y}_i| - \frac{1}{2}\delta\right), & \text{otherwise} \end{cases}$$

$\delta -> $ Hyperparameter

Disadvantages:

- A key disadvantage of Huber Loss is that it introduces a hyperparameter (delta) to control the transition between MSE and MAE, and choosing an optimal value for delta can be challenging and dataset-dependent.



1.2 Classification Losses

Classification losses are used in tasks where the goal is to predict categorical labels. They measure how well the model predictions match the true class labels.

1.2.1 Binary Cross Entropy

$$L = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y})$$

Disadvantages:

- **Multiple Local Minima** Multiple local minima in Binary Cross-Entropy Loss can cause optimization algorithms to get stuck in suboptimal solutions, slowing convergence.

1.2.2 Categorical Cross Entropy

$$L = \sum_{j=1}^{k} y_j \log(\hat{y}_j)$$

One hot encode the output classes.

Disadvantages:

- **Requirement for One-Hot Encoding** It increases memory usage and can be inefficient for tasks with many classes.

2 Linear Regression

Linear Regression is a statistical method used to model the relationship between a dependent variable and one or more independent variables by fitting a linear equation to observed data. It predicts outcomes by minimizing the difference between actual and predicted values using a best-fit line.

Distribution Model: We assume that the target variable y is generated from a linear model with Gaussian noise

$$y^i = \theta^t x^i + \epsilon^i, \quad \epsilon^i \ N(0, \sigma^2)$$

This implies that

$$p(y^{(i)} \mid x^{(i)}; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right).$$

$$\begin{aligned} L(\theta) &= \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right). \end{aligned}$$

$$\begin{aligned} \ell(\theta) &= \log L(\theta) \\ &= \log \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \\ &= \sum_{i=1}^{n} \log\left(\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right)\right) \\ &= n \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2. \end{aligned}$$

Hence, maximizing $\ell(\theta)$ gives the same answer as minimizing $\frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2$.

$$\frac{\partial}{\partial \theta}\left(\frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2\right) = -\sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)}) x^{(i)}.$$

Using gradient descent: $\theta := \theta - \alpha \nabla_\theta J(\theta)$,

where $\nabla_\theta J(\theta) = -\sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)}) x^{(i)}$.

Therefore, for a single training example,

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)}.$$

Algorithm 1 Linear Regression

Require: Feature matrix $X \in R^{m \times n}$, target vector $y \in R^m$, learning rate α, number of iterations N
Ensure: Parameters $\theta \in R^n$

```
Initialize θ := 0⃗
for iter = 1 to N do
    h := X · θ                                   // Hypothesis vector
    error := h − y                               // Error vector
    gradient := (y^(i) − h_θ(x^(i))) x_j^(i)
    θ := θ + α · gradient
end for
return θ =0
```

Batch Gradient Descent - We scan through the entire training dataset before taking a single step

$$\theta_j := \theta_j + \sum_{i=1}^{m} \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}.$$

Can lead to global optimum

Stochastic Gradient Descent - Just look at the current datapoint and take a single step

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}.$$

May end up oscillating

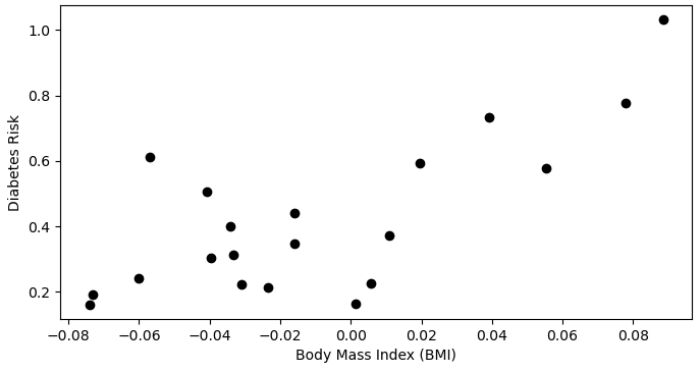
```
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from sklearn import datasets

# Load the diabetes dataset
X, y = datasets.load_diabetes(return_X_y=True, as_frame=True)

X['one'] = 1

# Collect 20 data points
X_train = X.iloc[-20:].loc[:, ['bmi','one']]
y_train = y.iloc[-20:] / 300

plt.scatter(X_train.loc[:, ['bmi']], y_train, color='black')
plt.xlabel('Body Mass Index')
plt.ylabel('Diabetes Risk')
```



Recall that a linear model has the form

$$y = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2 + \cdots + \theta_d \cdot x_d$$

where $\mathbf{x} \in R^d$ is a vector of features and y is the target. The θ_j are the *parameters* of the model.

By using the notation $x_0 = 1$, we can represent the model in a vectorized form

$$f_\theta(x) = \sum_{j=0}^{d} \theta_j \cdot x_j = \theta^\top \mathbf{x}.$$

```
def f(X, theta):
    return X.dot(theta)

def mean_squared_error(theta, X, y):
    return 0.5 * np.mean((y - f(X, theta))**2)

def mse_gradient(theta, X, y):
```

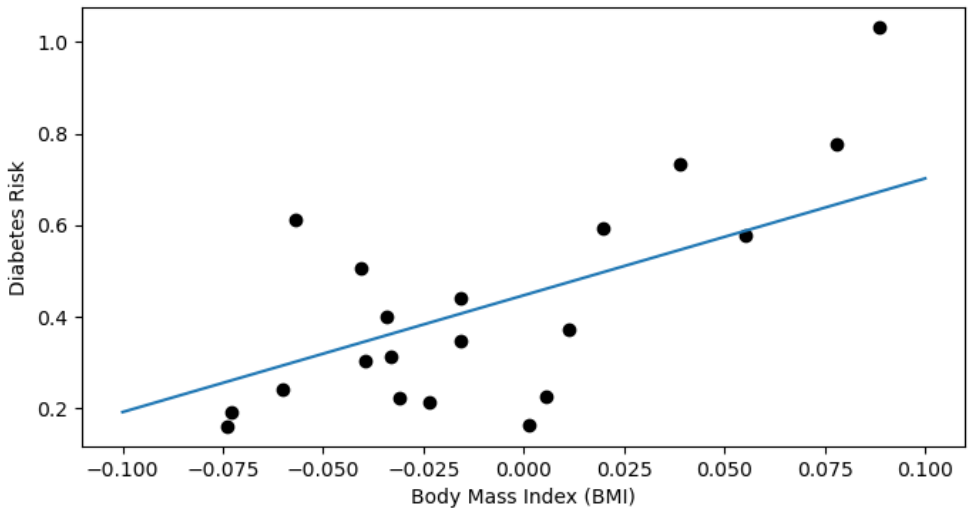
```
    return np.mean((f(X, theta) - y) * X.T, axis=1)

threshold = 1e-3
step_size = 4e-1
theta, theta_prev = np.array([2, 1]), np.ones(2,)
opt_pts = [theta]
opt_grads = []
iter = 0

while np.linalg.norm(theta - theta_prev) > threshold:
    if iter % 100 == 0:
        print('Iteration %d. MSE: %.6f' % (iter, mean_squared_error(theta, X_train, y_train))
            ↪ )
    theta_prev = theta
    gradient = mse_gradient(theta, X_train, y_train)
    theta = theta_prev - step_size * gradient
    opt_pts += [theta]
    opt_grads += [gradient]
    iter += 1

x_line = np.stack([np.linspace(-0.1, 0.1, 10), np.ones(10,)])
y_line = opt_pts[-1].dot(x_line)

plt.scatter(X_train.loc[:, ['bmi']], y_train, color='black')
plt.plot(x_line[0], y_line)
plt.xlabel('Body Mass Index (BMI)')
plt.ylabel('Diabetes Risk')
```



3 Logistic Regression

Logistic Regression is a statistical method used to model the probability that a given input belongs to a particular class (typically binary). It is used for classification tasks by modeling the probability of the output variable as a function of the input features using the logistic (sigmoid) function.

Distribution Model: We assume that the target variable y is generated from a Bernoulli distribution:

$$y^{(i)} \sim \text{Bernoulli}(p^{(i)}), \quad \text{where } p^{(i)} = \sigma(\theta^T x^{(i)}), \quad \sigma(z) = \frac{1}{1+e^{-z}}$$

This implies that

$$p(y^{(i)}|x^{(i)};\theta) = [\sigma(\theta^T x^{(i)})]^{y^{(i)}}[1-\sigma(\theta^T x^{(i)})]^{1-y^{(i)}}$$

$$L(\theta) = \prod_{i=1}^{n} p(y^{(i)}|x^{(i)};\theta) = \prod_{i=1}^{n}[\sigma(\theta^T x^{(i)})]^{y^{(i)}}[1-\sigma(\theta^T x^{(i)})]^{1-y^{(i)}}$$

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n}\left(y^{(i)}\log\sigma(\theta^T x^{(i)}) + (1-y^{(i)})\log(1-\sigma(\theta^T x^{(i)}))\right)$$

Hence, maximizing $\ell(\theta)$ is equivalent to minimizing the negative log-likelihood:

$$J(\theta) = -\ell(\theta) = -\sum_{i=1}^{n}\left(y^{(i)}\log\sigma(\theta^T x^{(i)}) + (1-y^{(i)})\log(1-\sigma(\theta^T x^{(i)}))\right)$$

$$\frac{\partial}{\partial\theta}J(\theta) = -\sum_{i=1}^{n}\left(y^{(i)} - \sigma(\theta^T x^{(i)})\right)x^{(i)}$$

Using gradient descent: $\theta := \theta - \alpha\nabla_\theta J(\theta)$,

where $\nabla_\theta J(\theta) = -\sum_{i=1}^{n}(y^{(i)} - \theta^T x^{(i)})x^{(i)}$.

Therefore, for a single training example,

$$\theta_j := \theta_j + \alpha\left(y^{(i)} - h_\theta(x^{(i)})\right)x_j^{(i)}.$$

Algorithm 2 Logistic Regression

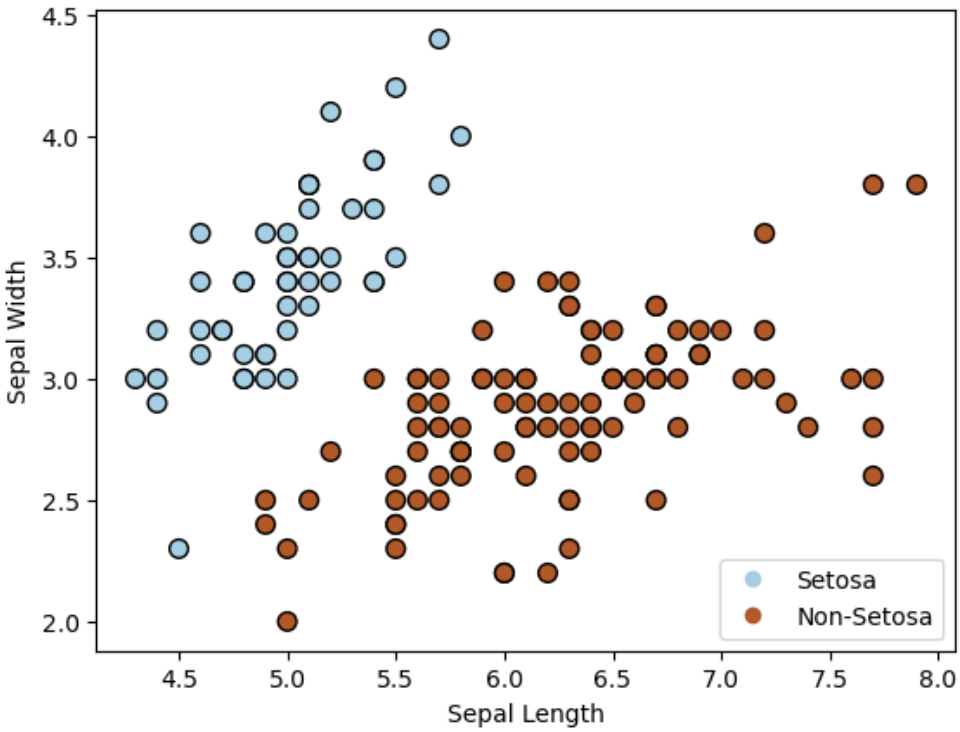
Require: Feature matrix $X \in R^{m\times n}$, target vector $y \in R^m$, learning rate α, number of iterations N
Ensure: Parameters $\theta \in R^n$
0: Initialize $\theta := \vec{0}$
0: **for** iter = 1 to N **do**
0: $z := X \cdot \theta$ {Linear combination}
0: $h := \sigma(z)$ {Sigmoid hypothesis}
0: $error := h - y$ {Error vector}
0: $gradient := X^T \cdot error$
0: $\theta := \theta - \alpha \cdot gradient$
0: **end for**
0: **return** θ =0

```
import numpy as np
import pandas as pd
from sklearn import datasets
import warnings
warnings.filterwarnings('ignore')

# Load the Iris dataset
iris = datasets.load_iris(as_frame=True)
iris_X, iris_y = iris.data, iris.target
```

```
iris_y2 = iris_y.copy()
iris_y2[iris_y2==2] = 1

# Plot also the training points
p1 = plt.scatter(iris_X.iloc[:, 0], iris_X.iloc[:, 1], c=iris_y2,
            edgecolor='k', s=60, cmap=plt.cm.Paired)
plt.xlabel('Sepal Length')
plt.ylabel('Sepal Width')
plt.legend(handles=p1.legend_elements()[0], labels=['Setosa', 'Non-Setosa'], loc='lower right
    ↪ ')
```




```
import numpy as np
from matplotlib import pyplot as plt

def sigmoid(z):
    return 1/(1+np.exp(-z))

def f(X, theta):
    return sigmoid(X.dot(theta))

def log_likelihood(theta, X, y):
    return (y*np.log(f(X, theta) + 1e-6) + (1-y)*np.log(1-f(X, theta) + 1e-6)).mean()

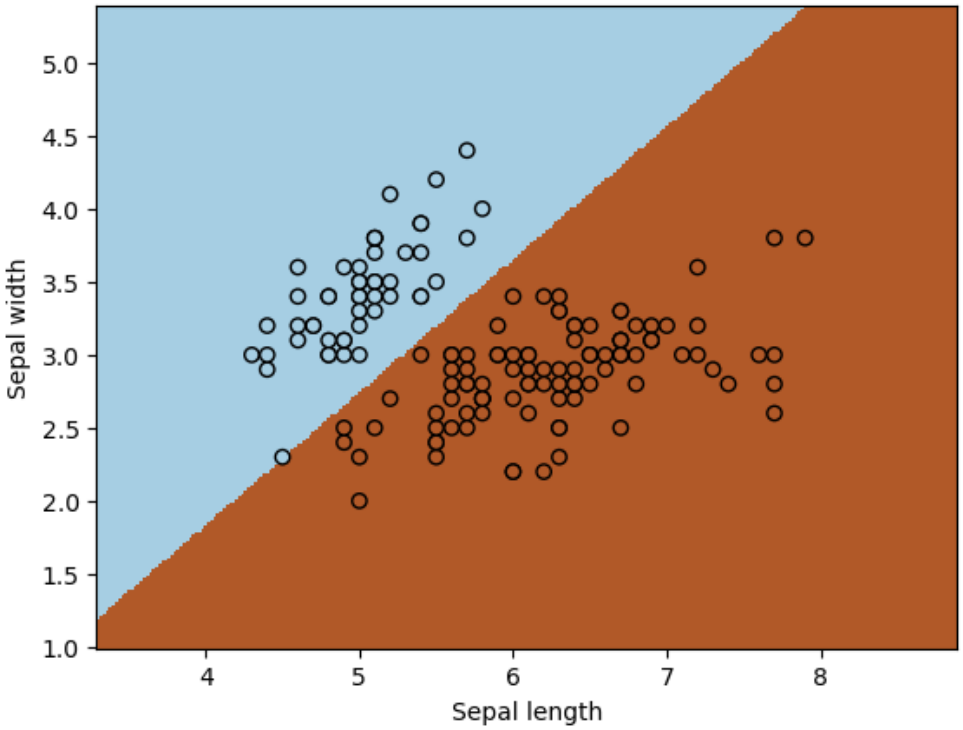
def loglik_gradient(theta, X, y):
    return np.mean((y - f(X, theta)) * X.T, axis=1)

threshold = 5e-5
step_size = 1e-1

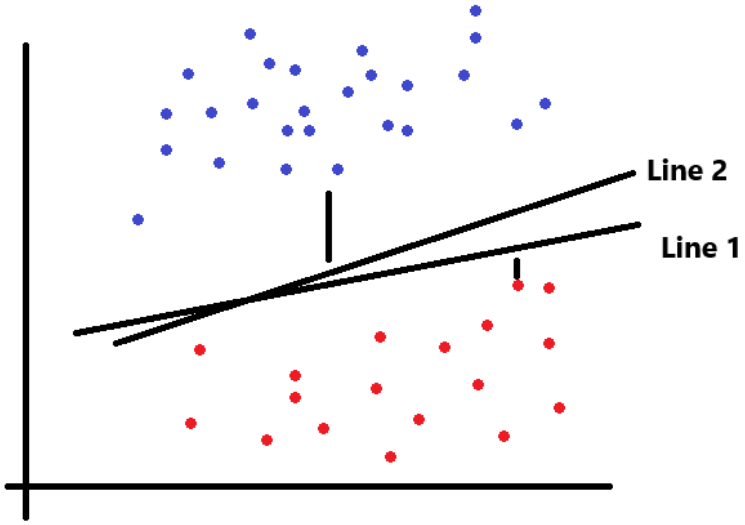
theta, theta_prev = np.zeros((3,)), np.ones((3,))
opt_pts = [theta]
opt_grads = []
iter = 0
iris_X['one'] = 1
X_train = iris_X.iloc[:,[0,1,-1]].to_numpy()
```

```
y_train = iris_y2.to_numpy()

while np.linalg.norm(theta - theta_prev) > threshold:
# while True:
    if iter % 50000 == 0:
        print('Iteration %d. Log-likelihood: %.6f' % (iter, log_likelihood(theta, X_train,
            ↪ y_train)))
    theta_prev = theta
    gradient = loglik_gradient(theta, X_train, y_train)
    theta = theta_prev + step_size * gradient
    opt_pts += [theta]
    opt_grads += [gradient]
    iter += 1
```

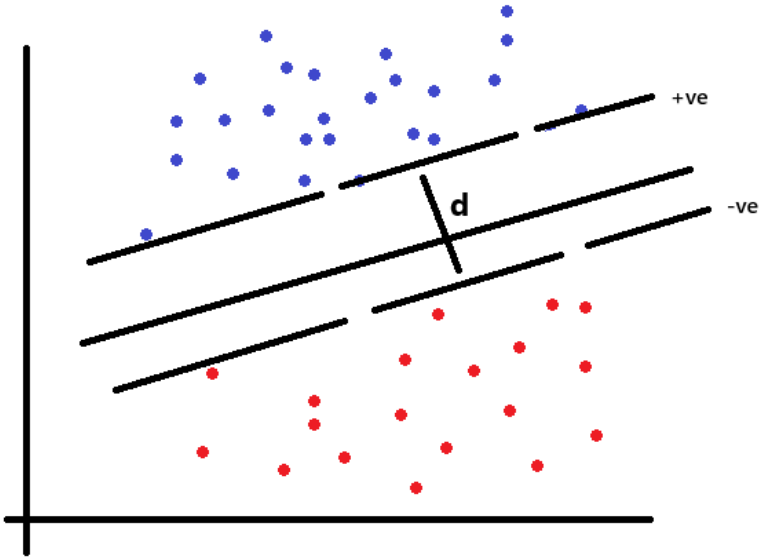


4 Support Vector Machines



The whole idea of SVM lies in the fact that it wants to select that hyperplane that classifies these points, as widely as possible. In this case it is Line 2.

4.1 Mathematics of SVM



Decision Rule:

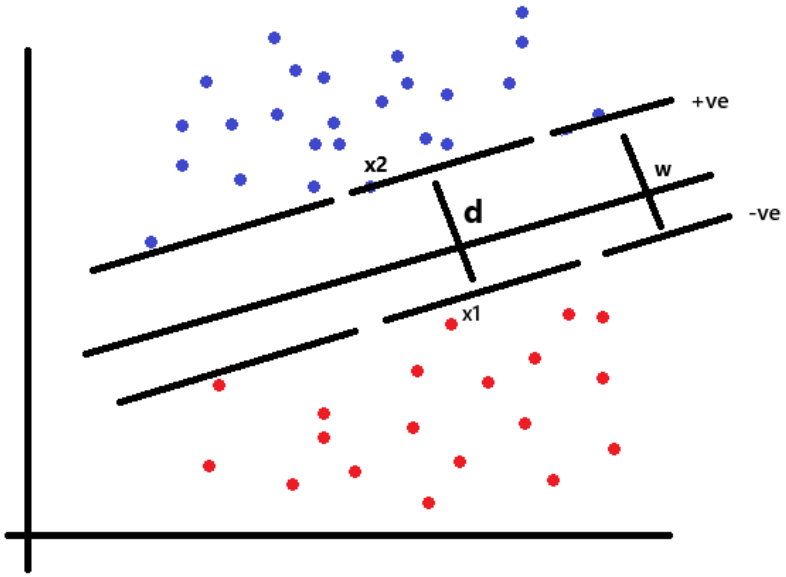
$$\hat{y} = \begin{cases} +1 & \text{if } \vec{w} \cdot \vec{x}_i + b \geq 0 \\ -1 & \text{if } \vec{w} \cdot \vec{x}_i + b < 0 \end{cases}$$

Therefore, by combining both the equations of the constraint, we get:

$$y_i.(\vec{w}.\vec{x_i} + b) \geq 1$$

For support vectors,

$$y_i.(\vec{w}.\vec{x_i} + b) = 1$$



$$d = \frac{(\vec{x}_2 - \vec{x}) \cdot \vec{\omega}}{\|\vec{\omega}\|} = \frac{\vec{x}_2 \cdot \vec{\omega} - \vec{x} \cdot \vec{\omega}}{\|\vec{\omega}\|}$$

$$y_i(\vec{\omega} \cdot \vec{x}_i + b) = 1$$

$$1 \cdot (\vec{\omega} \cdot \vec{x}_2 + b) = 1$$

$$d = \frac{(1 - b) - (-1 - b)}{\|\vec{\omega}\|}$$

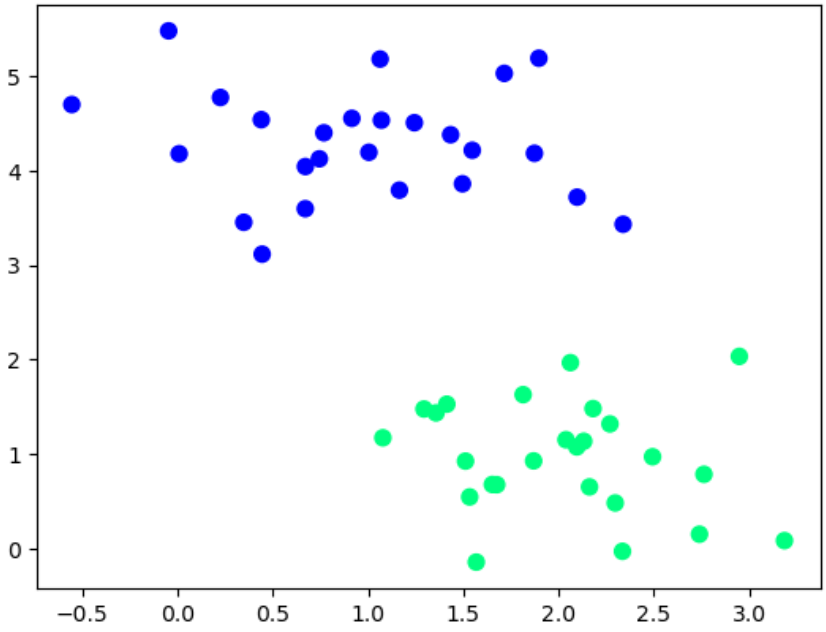
$$d = \frac{2}{\|\vec{\omega}\|}$$

$$\arg \max_{(\vec{\omega}^*, b^*)} \frac{2}{\|\vec{\omega}\|} \quad \text{subject to} \quad y_i(\vec{\omega} \cdot \vec{x}_i + b) \geq 1$$

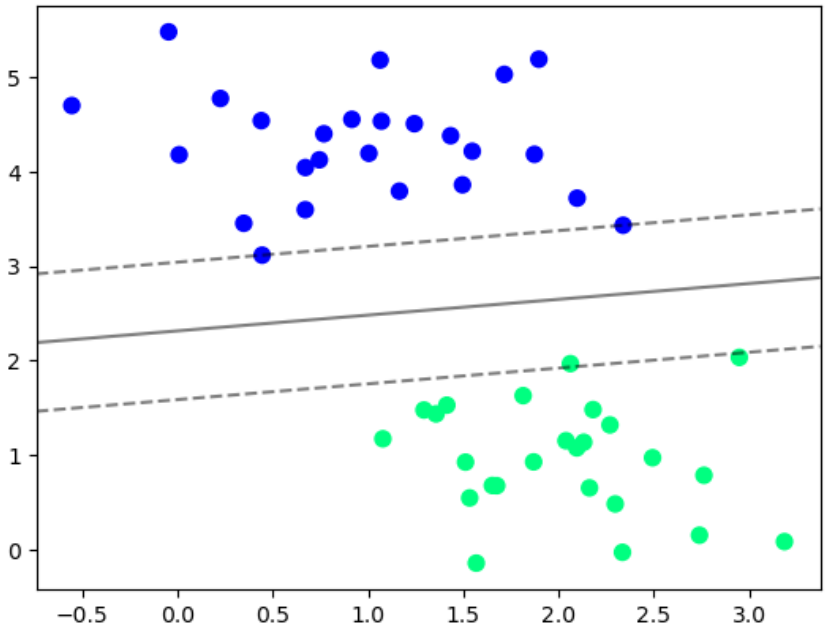
It is Hard Margin SVM for linearly separable data

```
import numpy as np
import matplotlib.pyplot as plt
from scipy import stats
import seaborn as sns
from sklearn.datasets._samples_generator import make_blobs

X, y = make_blobs(n_samples = 50, centers = 2,
                  random_state= 0, cluster_std= 0.60)
plt.scatter(X[:,0], X[:, 1], c = y, s= 50, cmap='winter')
```




```
from sklearn.svm import SVC    # Support Vector Classifier
model = SVC(kernel='linear', C = 1)
model.fit(X,y)
```



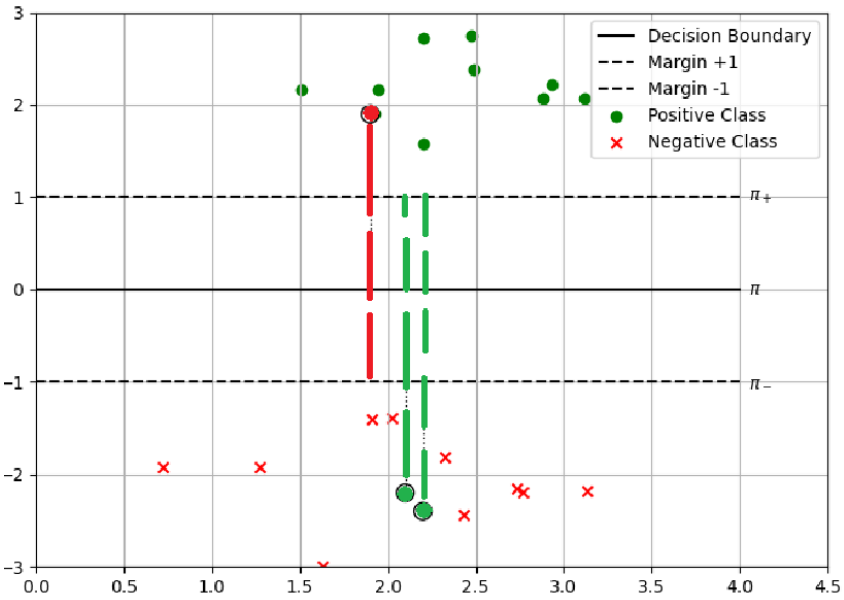
4.2 Non Linear Separable Data

We have

$$\arg\min_{\vec{\omega},b}\left(\frac{1}{2}\|\vec{\omega}\|^2 + C\sum_{i=1}^{n}\zeta_i\right)$$

C is a hyperparameter.

If all the points are correctly classified then $\zeta = 0$ It shows how much a data point breaks the margin rule, helping the SVM allow some mistakes while still trying to keep the margin as wide as possible, basically it's the distance as indicated in the figure.



Thus, we have to minimize this distance.

If C value is increased then we are forcing the algorithm to **not** misclassify any point.

If we are making the C's value small, then we are insisting the algo to maximize the margin irrespective of the misclassifications that it will be making.

4.3 Kernel

A *kernel* is a function that helps Support Vector Machines (SVM) work in higher dimensions without actually converting the data. It calculates the similarity between data points in a way that makes complex patterns easier to separate.

Types of Kernels:

- **Linear Kernel:**

$$K(x, x') = x \cdot x'$$

  Works well when the data is linearly separable.

- **Polynomial Kernel:**

$$K(x, x') = (x \cdot x' + c)^d$$

  Can model curved boundaries. c is a constant and d is the degree of the polynomial.

- **RBF (Gaussian) Kernel:**

$$K(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$$

  Good for non-linear data. It focuses more on nearby points.

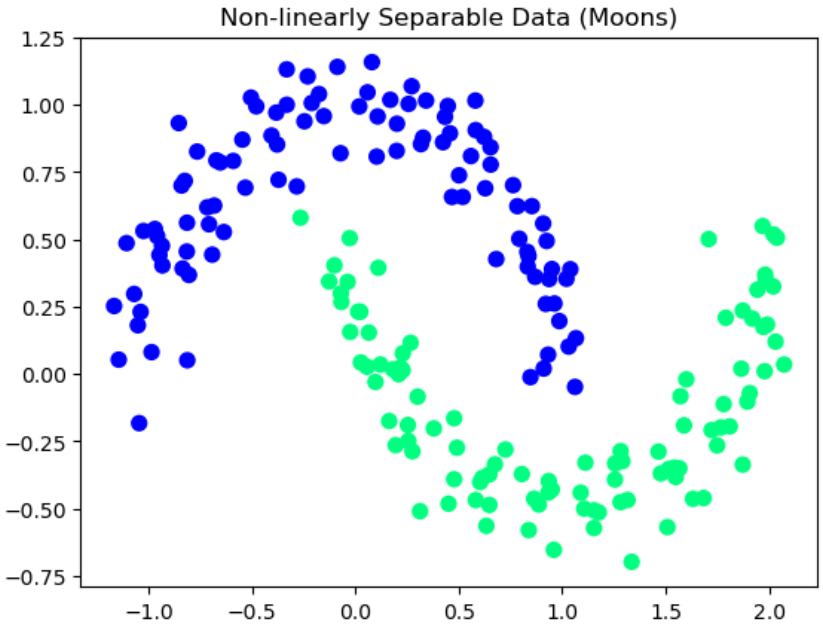
- **Sigmoid Kernel:**

$$K(x, x') = \tanh(a \cdot x \cdot x' + b)$$

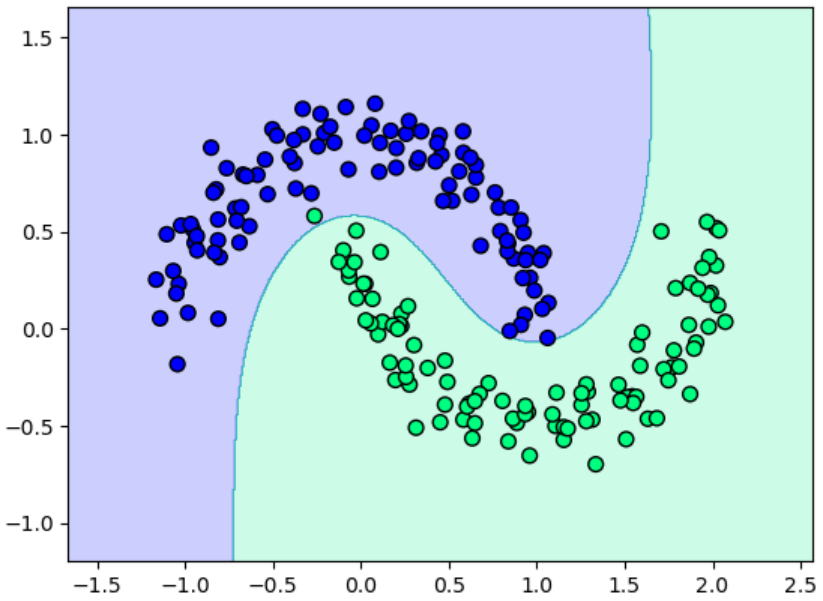
  Similar to what neural networks do. Not used often in practice.

```
from sklearn.datasets import make_moons

X, y = make_moons(n_samples=200, noise=0.1, random_state=0)
# Plot the data
plt.scatter(X[:, 0], X[:, 1], c=y, s=50, cmap='winter')
plt.title("Non-linearly Separable Data (Moons)")
plt.show()
```



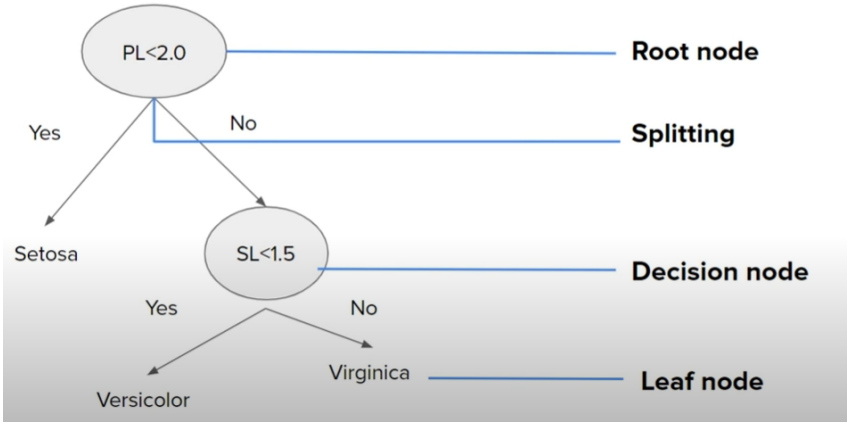

```
from sklearn.svm import SVC    # Support Vector Classifier
model = SVC(kernel='rbf', C = 1)
model.fit(X,y)
```



5 Decision Trees

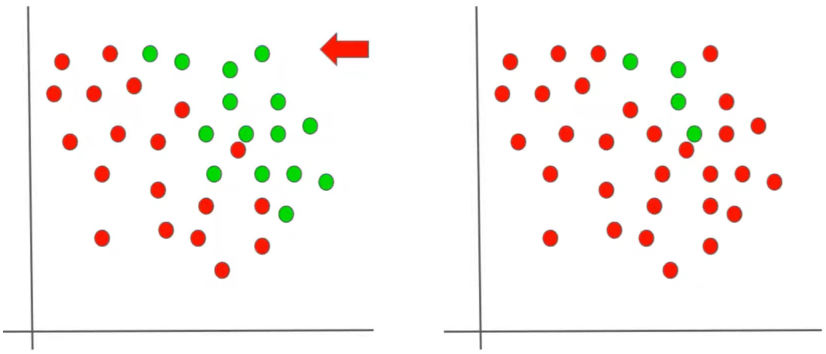
A **Decision Tree** is a supervised machine learning algorithm used for both *classification* and *regression* tasks. It models decisions and their possible consequences using a tree-like structure.

- Begin with your training dataset, which should have some feature variables and classification or regression output.
- Determine the "best feature" in the dataset to split the data on;
- Split the data into subsets that contain the correct values for this best feature. This splitting basically defines a node on the tree, i.e., each node is a splitting point based on a certain feature from our data.



5.1 Entropy

Entropy is a measure of disorder.
More Knowledge ⇒ Less Entropy



The mathematical formula for entropy is:

$$E(S) = \sum_{i=1}^{c} -p_i \log_2 p_i$$

Where p_i is simply the frequentist probability of an element/class i in our data.
For example, if our data has only 2 class labels Yes and No, then:

$$E(D) = -p_{\text{yes}} \log_2(p_{\textbf{yes}}) - p_{\textbf{no}} \log_2(p_{\text{no}})$$

Salary	Age	Purchase
20000	21	Yes
10000	45	No
60000	27	Yes
15000	31	No
12000	18	No

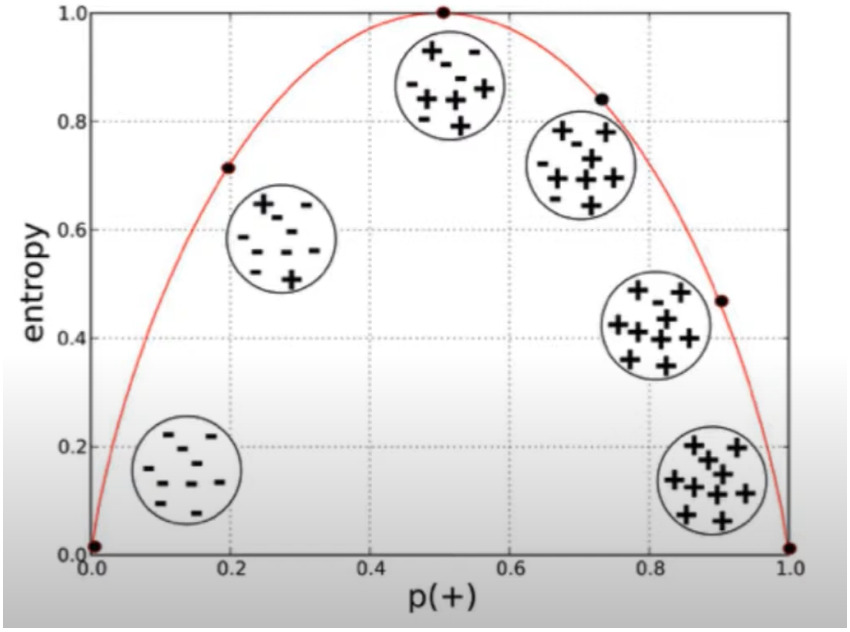
Let:

- P_y = probability of Yes = $\frac{2}{5}$
- P_n = probability of No = $\frac{3}{5}$

$$H(D) = -P_y \log_2(P_y) - P_n \log_2(P_n)$$

$$H(D) = -\frac{2}{5} \log_2\left(\frac{2}{5}\right) - \frac{3}{5} \log_2\left(\frac{3}{5}\right)$$

$$H(D) \approx 0.97$$



5.2 Information Gain

Information Gain is a metric used to train Decision Trees. Specifically, this metric measures the quality of a split in a Decision Tree

Information Gain = E(Parent) − {Weighted Average} × E(Children)

Outlook	**Temperature**	**Humidity**	**Windy**	**PlayTennis**
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

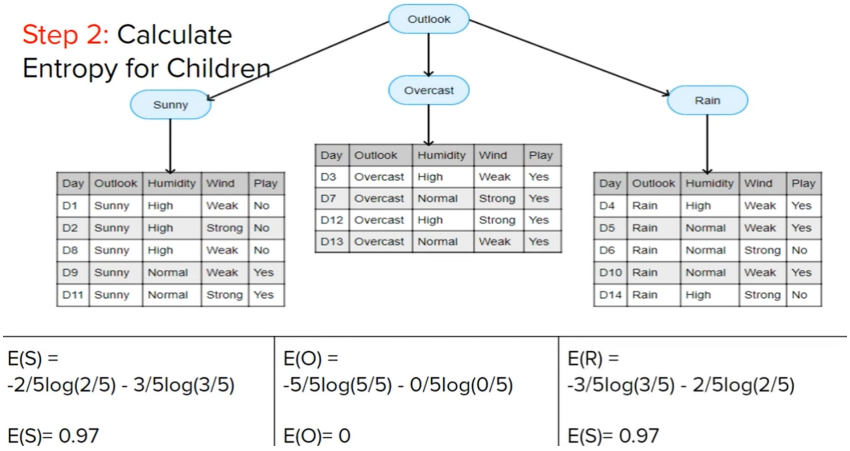
Entropy of Parent Dataset:

$$E(P) = -p_y \log_2(p_y) - p_n \log_2(p_n)$$

$$= -\frac{9}{14} \log_2\left(\frac{9}{14}\right) - \frac{5}{14} \log_2\left(\frac{5}{14}\right)$$

$$E(P) = \mathbf{0.94}$$

On the basis of *'Outlook'* column, let's divide it. We will group by



Day	Outlook	Humidity	Wind	Play
D1	Sunny	High	Weak	No
D2	Sunny	High	Strong	No
D8	Sunny	High	Weak	No
D9	Sunny	Normal	Weak	Yes
D11	Sunny	Normal	Strong	Yes

Day	Outlook	Humidity	Wind	Play
D3	Overcast	High	Weak	Yes
D7	Overcast	Normal	Strong	Yes
D12	Overcast	High	Strong	Yes
D13	Overcast	Normal	Weak	Yes

Day	Outlook	Humidity	Wind	Play
D4	Rain	High	Weak	Yes
D5	Rain	Normal	Weak	Yes
D6	Rain	Normal	Strong	No
D10	Rain	Normal	Weak	Yes
D14	Rain	High	Strong	No

$$\text{Weighted Entropy} = \frac{5}{14} \times 0.97 + \frac{4}{14} \times 0 + \frac{5}{14} \times 0.97$$

$$W.E(\text{Children}) = \mathbf{0.69}$$

$$\text{Information Gain} = E(\text{Parent}) - \{\text{Weighted Average}\} \times E(\text{Children})$$

$$\text{IG} = \mathbf{0.97 - 0.69 = 0.28}$$

So the information gain (or the decrease in entropy/impurity) when you split this data on the basis of **Outlook** condition/column is **0.28**.

To determine the best split, the algorithm calculates the **Information Gain** for all the columns. The column that has the **highest Information Gain** (i.e., the maximum decrease in entropy) is selected to split the data.

After selecting the best column, the decision tree **recursively** repeats this process. It uses a **greedy search** strategy from top to bottom, finding Information Gain at every level of the tree until the data is perfectly classified or a stopping condition is met.

5.3 Gini Impurity

Gini Impurity is a metric used to measure how often a randomly chosen element from the dataset would be incorrectly classified if it was randomly labeled according to the distribution of labels in the subset.

It is mainly used in the CART (Classification and Regression Tree) algorithm.

$$Gini = 1 - \sum_{i=1}^{c} p_i^2$$

Where p_i is the probability of an element being classified to class i.

A Gini value of 0 means perfect purity (all elements belong to a single class), and higher values indicate more impurity.

- **Gini Impurity** is **computationally faster**, making it a preferred choice when speed is important.

- **Entropy** tends to produce a **more balanced tree** in some cases, as it considers the distribution of class probabilities more precisely.

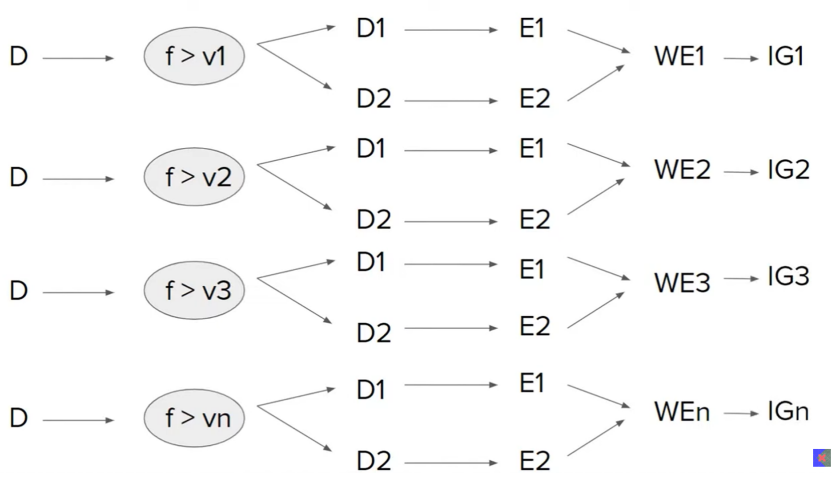
Solution: Perform **hyperparameter tuning** to choose between Gini and Entropy based on the performance of your specific dataset.

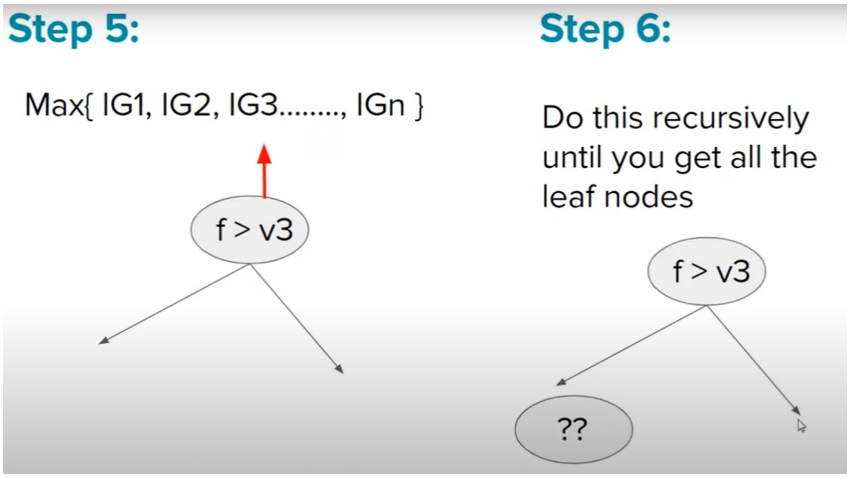
5.4 Handling Numerical values in Decision Trees

S No	User Rating	Downloaded
1	3.5	Yes
2	4.6	Yes
3	2.2	No
4	1.6	Yes
5	4.1	No
6	3.9	No
7	3.2	No
9	2.9	Yes
10	4.8	Yes
11	3.3	No
12	2.5	Yes
13	1.9	Yes

Sort the Data on the Basis of Numerical Column

S No	User Rating	Downloaded
1	1.6	Yes
2	1.9	Yes
3	2.2	No
4	2.5	Yes
5	2.9	Yes
6	3.2	No
7	3.3	No
9	3.5	Yes
10	3.9	No
11	4.1	No
12	4.6	Yes
13	4.8	Yes





5.5 Role of `max_depth` in Overfitting and Underfitting

In a Decision Tree, the parameter `max_depth` controls the maximum depth the tree is allowed to grow.

- **max_depth=None** means the tree will grow until all leaves are pure or contain fewer samples than the minimum required to split.
- This can lead to a **very deep tree**, capturing all the patterns, including noise in the training data.
- As a result, it often causes **overfitting**, where the model performs well on training data but poorly on unseen data.
- Conversely, setting `max_depth` to a very small value may result in a **shallow tree**, unable to capture sufficient structure in the data, leading to **underfitting**.

Conclusion: Proper tuning of `max_depth` is crucial to balance the bias-variance tradeoff and prevent overfitting or underfitting.

6 Key Hyperparameters of Decision Trees in `scikit-learn`

The following are the most important hyperparameters for tuning the performance of a `DecisionTreeClassifier`:

- `criterion` **(default = "gini")**
  Function to measure the quality of a split:
  - `"gini"` — Gini Impurity
  - `"entropy"` or `"log_loss"` — Information Gain
- `max_depth = None`
  The maximum depth of the tree. If set to `None`, the tree expands until all leaves are pure, which can lead to overfitting.
- `min_samples_split = 2`
  The minimum number of samples required to split an internal node. If a node has fewer than this number of samples, it will not be split and becomes a leaf.

  Setting a higher value helps control overfitting by preventing the model from learning overly specific or noisy patterns.

  Example:

  Consider the following dataset:

Feature (X)	Target (Y)
3.0	Yes
4.5	Yes
5.2	No
6.1	Yes
7.4	No

If `min_samples_split = 3`, a node must contain at least 3 samples to be split.

Suppose after the first split, one child node receives only 2 samples (e.g., {5.2, 7.4}). Even if it's impure, the split will be stopped because it doesn't meet the `min_samples_split` threshold. That node will become a leaf, helping prevent overfitting to tiny sample groups.

- `min_samples_leaf = 1`
  The minimum number of samples required to be at a **leaf node**. This parameter ensures that no split will create a child node with fewer than the specified number of training samples.

  Setting a higher value helps smooth the model and reduces overfitting by avoiding splits that result in very small, highly specific leaves.

  Example:

  Consider the dataset:

Feature (X)	Target (Y)
2.0	No
3.5	Yes
4.2	Yes
5.1	No
6.8	Yes

  If `min_samples_leaf = 2`, then every **leaf** must have at least 2 data points.

  Suppose a split divides the data such that one resulting leaf has only 1 sample (e.g., {6.8, Yes}). This split will be rejected, even if it improves purity, because it violates the minimum leaf size constraint. The algorithm will look for alternative splits that leave at least 2 samples in every leaf.

  This helps reduce model complexity and improve generalization on unseen data.

- `max_features = None`
  The number of features to consider when looking for the best split. Can be set to:
  - `"sqrt"` — useful for classification tasks
  - `"log2"` — for logarithmic feature scaling
  - `None` — use all features

- `max_leaf_nodes = None`
  Grows tree with the specified maximum number of leaf nodes using best-first search.

- `min_impurity_decrease = 0.0`
  A node will split only if this condition is met: the decrease in impurity must be at least this value.

- `ccp_alpha = 0.0`
  Complexity parameter used for Minimal Cost-Complexity Pruning. A higher value will prune more of the tree.

Interactive Decision Tree Visualizer:
https://dt-visualise.herokuapp.com/

6.1 Splitting in Regression Trees

In Regression Trees, unlike classification trees, the goal is to predict a continuous output variable. The tree splits the dataset into regions such that the **variance (or squared error)** within each region is minimized.

6.2 Splitting Criterion

At each node, the algorithm chooses a split that minimizes the following cost function:

$$\text{MSE}(t) = \frac{1}{|D_t|} \sum_{i \in D_t} (y_i - \bar{y}_t)^2$$

Where:

- D_t is the set of data points at node t
- y_i is the true value for sample i
- $\bar{y}_t$ is the mean target value at node t

The best split is the one that minimizes the **weighted sum of mean squared errors (MSE)** for the two resulting child nodes.

6.3 Illustrative Example

Consider the following simple dataset:

Feature (X)	**Target (Y)**
2.0	10
3.0	12
4.0	14
5.0	16
6.0	18

Let us consider a possible split at $X = 4.5$. This results in two subsets:

- Left node: $\{(2.0, 10), (3.0, 12), (4.0, 14)\}$ with mean $\bar{y}_L = 12$
- Right node: $\{(5.0, 16), (6.0, 18)\}$ with mean $\bar{y}_R = 17$

Calculate MSE for both:

$$\text{MSE}_L = \frac{1}{3}\left[(10-12)^2 + (12-12)^2 + (14-12)^2\right] = \frac{1}{3}(4+0+4) = \frac{8}{3}$$

$$\text{MSE}_R = \frac{1}{2}\left[(16-17)^2 + (18-17)^2\right] = \frac{1}{2}(1+1) = 1$$

$$\text{Total Weighted MSE} = \frac{3}{5}\cdot\frac{8}{3} + \frac{2}{5}\cdot 1 = \frac{8}{5} + \frac{2}{5} = 2$$

This score is then compared with other possible splits (e.g., $X = 3.5$, $X = 5.5$), and the split with the **lowest total MSE** is chosen.

Summary

Regression Trees aim to create splits that minimize the variance within the resulting nodes. This is achieved using a greedy approach where, at each step, the split that leads to the lowest total MSE is selected. As more splits are added, the model becomes more complex and capable of capturing finer patterns — at the risk of overfitting.

7 Random Forest

Random Forest is a machine learning algorithm that combines **many decision trees** to make better predictions.

Each tree gives a result, and the forest **votes** for the best answer:

- For classification: it picks the class with the most votes.
- For regression: it takes the average of all trees.

It is more accurate and stable than using a single decision tree, and it helps avoid overfitting.

7.1 Difference Between Bagging and Random Forest

Bagging (Bootstrap Aggregating) involves training multiple base models (typically Decision Trees) on different bootstrapped subsets of the dataset. However, each base model receives all the features (columns), and the randomness comes only from **row sampling**.

Random Forest, on the other hand, extends Bagging by introducing an additional layer of randomness: **feature (column) sampling**. In Random Forest:

- Each Decision Tree is trained not just on a random subset of the data rows, but also on a random subset of the features.
- Moreover, **column sampling happens at every node split**, not just at the start of tree training.

Key Differences:

- In **Bagging**, all trees see all features — randomness is introduced only via row sampling.
- In **Random Forest**, each split in every tree considers a randomly selected subset of features, leading to more diversity among trees.

This additional randomness in Random Forest often leads to **better generalization performance** compared to standard Bagging, because it reduces correlation among the trees in the ensemble.

7.2 Hyperparameters in Random Forest

RandomForestClassifier has several hyperparameters that affect model performance. Below are the key ones with simple explanations and examples.

- `n_estimators` — Number of decision trees in the forest. More trees usually improve performance but increase computation time.
  Example: `RandomForestClassifier(n_estimators=100)` creates a forest with 100 trees.
- `max_depth` — Controls the maximum depth of each tree. Prevents overfitting if set properly.
  Example: `RandomForestClassifier(max_depth=3)` limits tree height to 3 levels.
- `min_samples_split` — Minimum number of samples needed to split a node.
  Example: `RandomForestClassifier(min_samples_split=5)` means a node must have at least 5 samples to be split further.
- `min_samples_leaf` — Minimum number of samples required in a leaf node.
  Example: `RandomForestClassifier(min_samples_leaf=2)` ensures each leaf has at least 2 samples.
- `max_features` — Number of features to consider when looking for the best split.
  Example: `RandomForestClassifier(max_features='sqrt')` considers only $\sqrt{\text{total features}}$ at each node.
- `bootstrap` — Whether to use bootstrap samples (sampling with replacement).
  Example: `RandomForestClassifier(bootstrap=True)` trains each tree on a random subset of the data.
- `oob_score` — Whether to use out-of-bag samples to estimate accuracy.
  Example: `RandomForestClassifier(oob_score=True)` evaluates performance using unused data from bootstrap sampling.
- `random_state` — Controls randomness for reproducibility.
  Example: `RandomForestClassifier(random_state=42)` ensures consistent results across runs.
- `ccp_alpha` — Complexity parameter for pruning. Higher value prunes more aggressively.
  Example: `RandomForestClassifier(ccp_alpha=0.01)` simplifies the tree by removing less useful splits.

7.3 Out of Bag Evaluation (OOB)

OOB (Out-of-Bag) is a validation technique used in Random Forests. When training each tree, a random subset of the data is selected using **bootstrap sampling** (sampling with replacement). The remaining data points that are not selected for training a particular tree are called **out-of-bag samples**.

These out-of-bag samples can be used as a test set to evaluate the tree's performance. The Random Forest aggregates these evaluations across all trees to estimate the model's overall accuracy — this is called the **OOB Score**.

Key Point: OOB provides an efficient, internal cross-validation mechanism without needing to hold out a dedicated test set.

7.4 Feature Importance in Random Forest

Feature importance is a score that tells us how useful or valuable each feature was in building the decision trees within a random forest model.

It helps us understand which features have the most influence on the prediction.

Why is it Useful?

- Helps in understanding the model's decision-making.
- Allows us to reduce dimensionality by removing less important features.
- Useful in feature selection for faster and better-performing models.

Example Analogy: Think of solving a puzzle. Some pieces (features) are more central to solving the image than others. Similarly, in a Random Forest, some features contribute more to accurate predictions.

How is Feature Importance Calculated?

- Every time a feature is used to split a node, the impurity (e.g., Gini or Entropy) decreases.
- This decrease in impurity is recorded and summed over all trees in the forest.
- The importance of a feature is the total reduction of the criterion (like Gini or Entropy) it brings.
- Finally, the values are normalized so that they add up to 1.

Next Steps After Identifying Important Features:

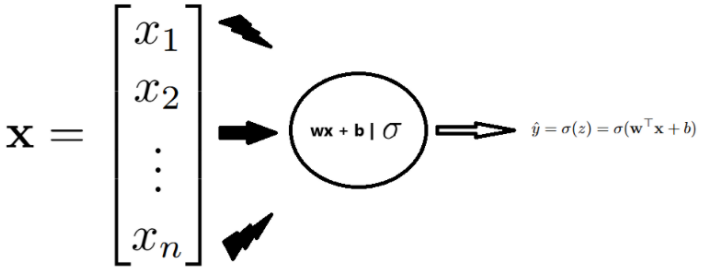
- Drop features with very low importance to reduce complexity.
- Retrain the model with only the top important features.
- Compare the new model's accuracy to check if performance improves or remains the same.
- Use the refined feature set for model interpretation or deployment.

Use in Practice: After training, you can access feature importances using the `feature_importances_` attribute of a RandomForestClassifier object.

8 Neural Network

A Neural Network is a computational model inspired by the human brain. It consists of layers of nodes (neurons) where each node applies a weighted sum and activation function

8.1 Logistic Regression



1. Initialize weights w and bias b
2. Find the optimal w and b (e.g., using gradient descent)
3. Use the model to predict:

$$\hat{y} = \sigma(w^\top x + b)$$

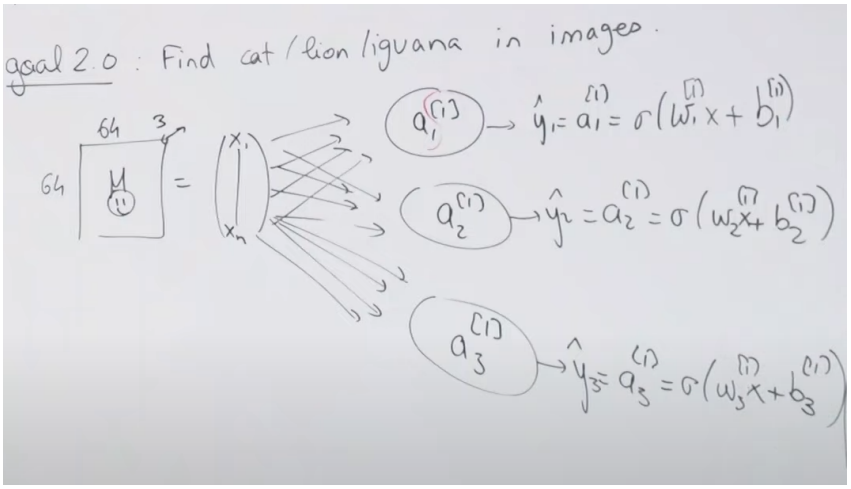
Key Concepts

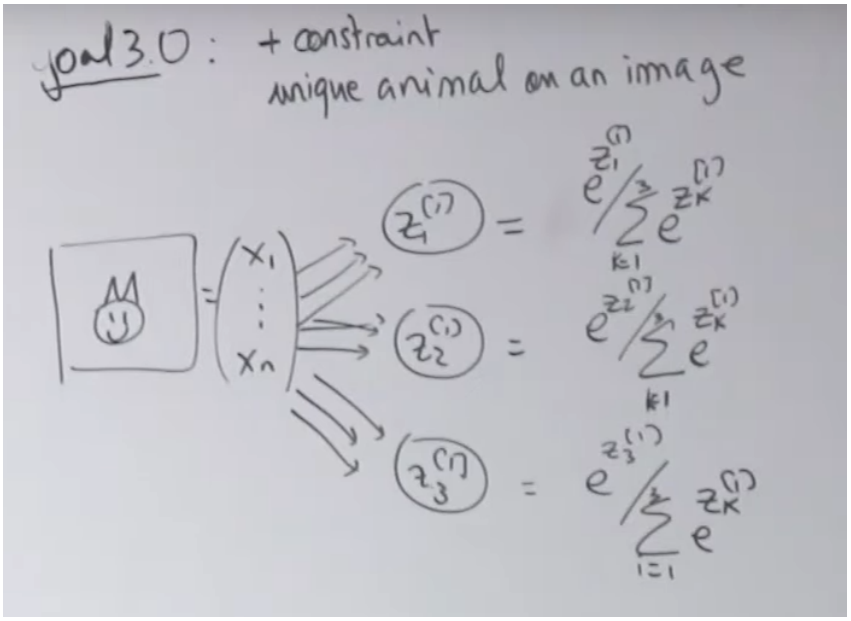
- **Neuron** = Linear transformation + Activation function

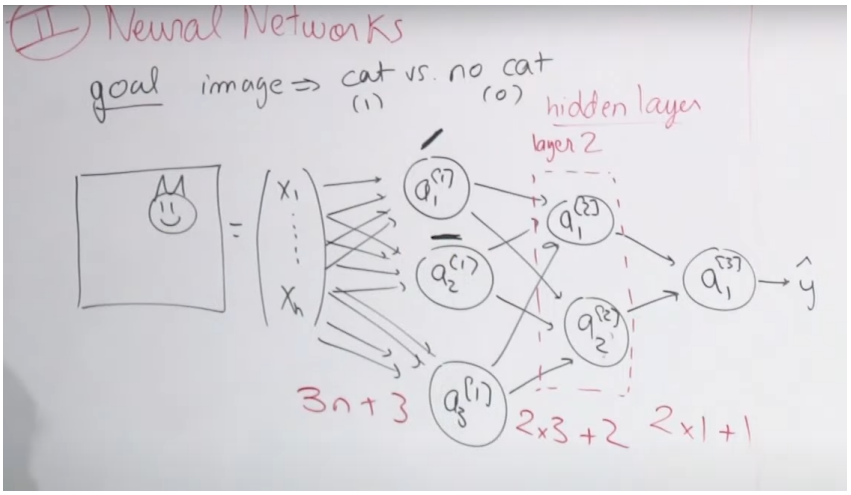
$$\text{Neuron output: } \hat{y} = \sigma(w^\top x + b)$$

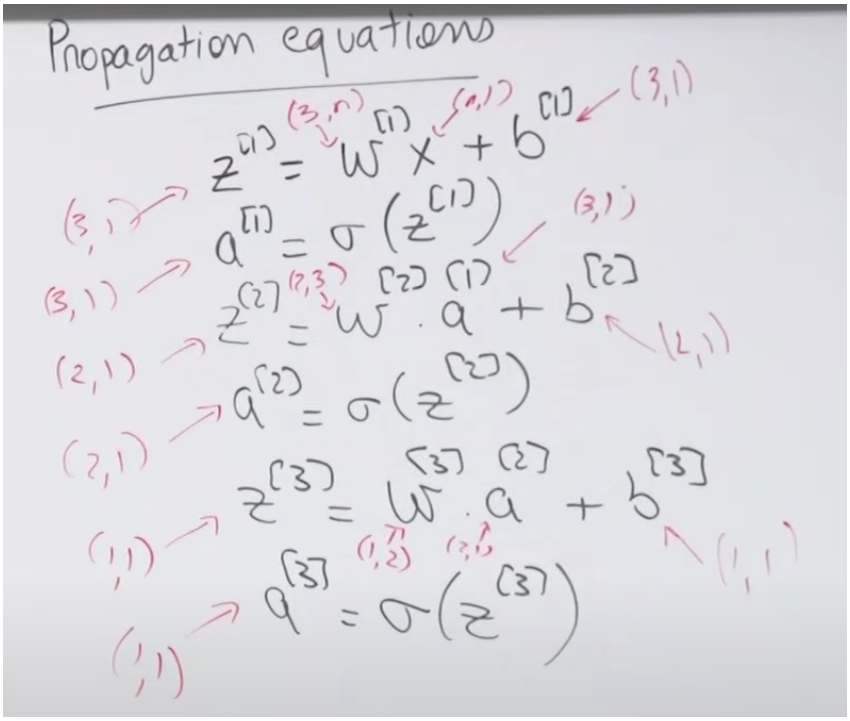
- **Model** = Architecture + Parameters

Architecture: structure of layers and connectionsParameters: weights w and biases b


goal 2.0 : Find cat / lion / iguana in images.
64
3
64
$a_1^{[1]} \rightarrow \hat{y}_1 = a_1^{[1]} = \sigma(w_1^{[1]} x + b_1^{[1]})$
$a_2^{[1]} \rightarrow \hat{y}_2 = a_2^{[1]} = \sigma(w_2^{[1]} x + b_2^{[1]})$
$a_3^{[1]} \rightarrow \hat{y}_3 = a_3^{[1]} = \sigma(w_3^{[1]} x + b_3^{[1]})$


goal 3.0 : + constraint
unique animal on an image
$z_1^{[1]} = e^{z_1^{[1]}} / \sum_{k=1}^{3} e^{z_k^{[1]}}$
$z_2^{[1]} = e^{z_2^{[1]}} / \sum_{k=1}^{3} e^{z_k^{[1]}}$
$z_3^{[1]} = e^{z_3^{[1]}} / \sum_{i=1}^{3} e^{z_k^{[1]}}$


II Neural Networks
goal image ⇒ cat vs. no cat
(1) (0)
hidden layer
layer 2
$a_1^{[1]}$
$a_2^{[1]}$
$a_3^{[1]}$
$a_1^{[2]}$
$a_2^{[2]}$
$a_1^{[3]} \rightarrow \hat{y}$
3n+3
2x3+2
2x1+1



8.2 Gradient Descent Variants

Batch Gradient Descent: Uses the entire training dataset to compute the gradient of the loss function.

- Stable convergence
- Slow for large datasets
- Update: $\theta := \theta - \eta \nabla J(\theta)$

Batch Gradient Descent: Use all data at once
model.fit(`X_train, y_train, batch_size = len(X_train)`, epochs=100)

Mini-Batch Gradient Descent: Divides the training set into small batches and updates parameters using each mini-batch.

- Faster and more memory-efficient
- Introduces noise that can help escape local minima
- Update: $\theta := \theta - \eta \nabla J_{\text{mini-batch}}(\theta)$

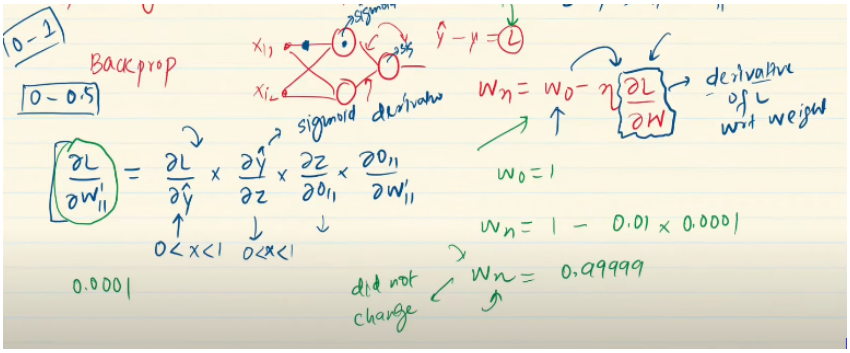
Mini-Batch Gradient Descent:

Mini-Batch Gradient Descent: Use small batch (e.g., 32)
model.fit(`X_train, y_train, batch_size = 32`, epochs=100)

8.3 Vanishing Gradient Problem

Vanishing Gradient Problem is encountered when training artificial neural networks with gradient based learning methods and backpropagation. In such methods, during each iteration of training each of the neural network's weights receives an update proportional to the partial derivative of the error function with respect to the current weight. The problem is that in some cases, the gradient will be vanishingly small, effectively preventing the weight from changing its value. In the worst case, this may completely stop the neural network from further training
0.1 x 0.1 x 0.1 x .... = 0.00000..1
Occurs in deep neural networks
Particulary with sigmoid / tanh. These functions map a large range of input values to a small output range. The gradients

of these activation functions become very small and if multiplied by each other across many layers, cause them to shrink exponentially.



How to recognize ?

- Loss focus ⇒ no changes
- Weights graph ⇒ if constant

How to handle Vanishing Gradient Problem ?

- Reduce model complexity
- Use different activation function
- Proper weight initialization
- Batch normalization
- Residual Network

8.4 Improving the Performance

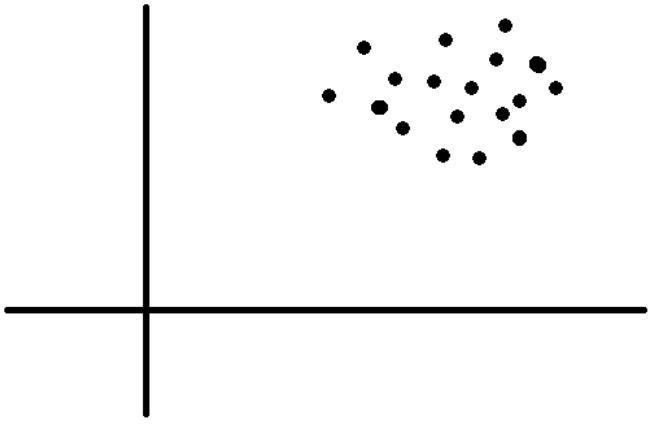
8.4.1 Standardization

Formula:

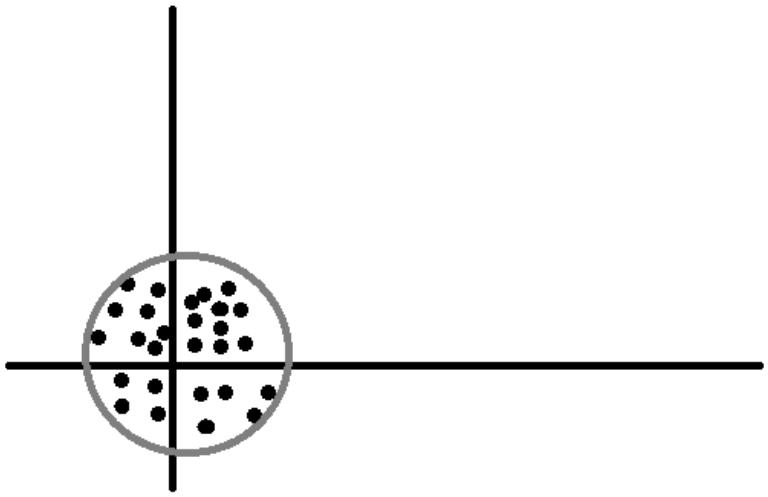
$$z = \frac{x - \mu}{\sigma}$$

where x is the data point, μ is the mean, and σ is the standard deviation.

When to Use: Use standardization when features have different scales and the data follows (or approximately follows) a Gaussian distribution. It is commonly used in algorithms like SVM, logistic regression, and k-means.



After Standardization



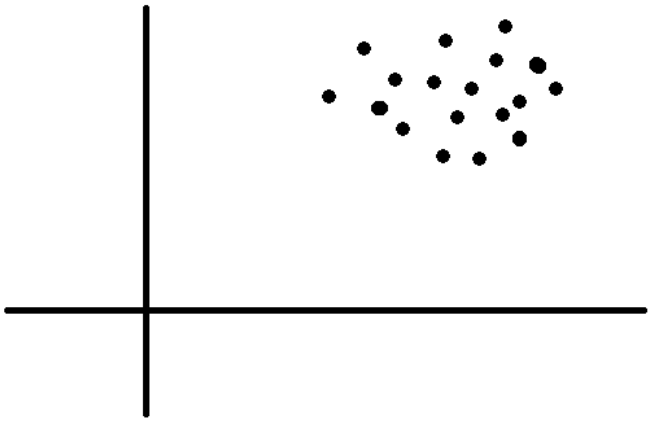
8.4.2 Normalization

Formula:

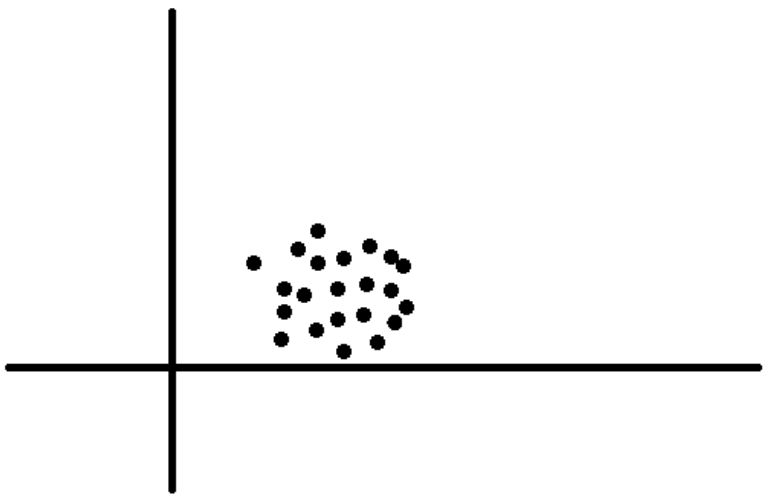
$$x_{\text{norm}} = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$

where x is the data point, x_{min} and x_{max} are the minimum and maximum values of the feature.

When to Use: Use normalization when the data does not follow a Gaussian distribution and needs to be scaled to a specific range, typically $[0, 1]$. It is useful for distance-based algorithms like k-NN and neural networks.



After Normalization



8.4.3 Difference

Standardization

- Transforms data to have **zero mean and unit variance**.
- Use when the data is (approximately) **normally distributed**.
- Suitable for **linear models, SVM, logistic regression**, and PCA.

Normalization

- Scales data to a fixed range, usually $[0, 1]$.
- Use when the distribution is **not Gaussian**.
- Preferred for **distance-based algorithms** like k-NN, K-Means, or Neural Networks.

8.5 Dropout

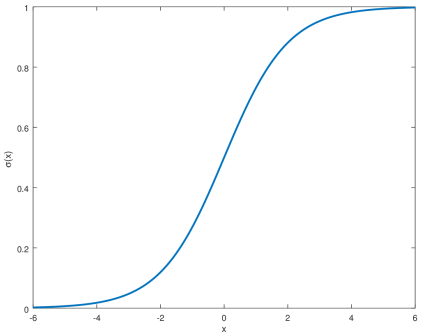
Dropout is a regularization technique used in neural networks to reduce overfitting. It works by randomly deactivating a fraction of neurons during training, which prevents the model from relying too heavily on specific neurons and encourages redundancy and robustness in learning.

- Randomly sets a fraction of input units to zero at each update during training.
- Helps improve generalization by reducing reliance on any specific neurons.
- Typically used in fully connected (dense) layers.
- Inactive during inference (testing).

```
model.add(tf.keras.layers.Dropout(0.5))
```

8.6 Activation Functions

8.6.1 Sigmoid



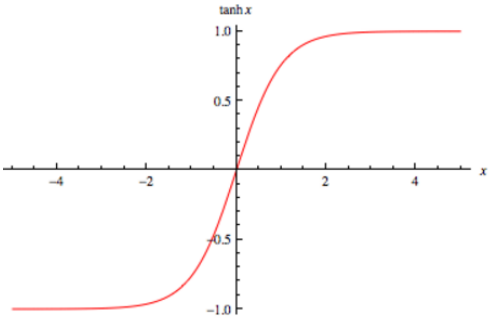
Advantages

- $[0, 1] \Rightarrow$ Probability $\Rightarrow$ Output Layer $\Rightarrow$ Binary Classification
- Non-Linear $\Rightarrow$ It can capture non linear data pattern
- Differentiable

Disadvantages

- Saturating Function $\Rightarrow$ Vanishing Gradient Problem
- Non zero centered $\Rightarrow$ Training gets slow

8.6.2 Tanh



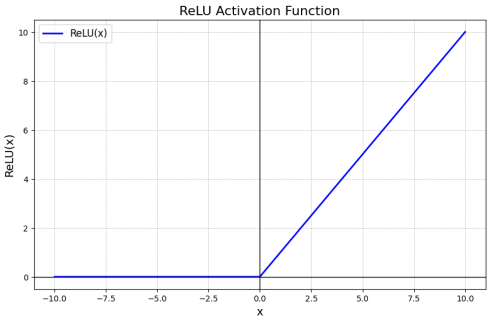
Advantages

- Non-Linear $\Rightarrow$ It can capture non linear data pattern
- Zero centered $\Rightarrow$ Training faster
- Differentiable

Disadvantages

- Saturating Function $\Rightarrow$ Vanishing Gradient Problem
- Computationally expensive

8.6.3 ReLU



Advantages

- Non-Linear $\Rightarrow$ It can capture non linear data pattern
- Not Saturated in the positive region
- Computationally inexpensive
- Converge faster

Disadvantages

- Not purely differentiable
- Not zero centered $\Rightarrow$ Use Batch Normalization

8.6.4 Dying ReLU

Dying ReLU refers to a situation where a large number of neurons output zero for all inputs and stop learning during training.

Causes:

- If the weighted input to the ReLU is negative, the output becomes zero.
- During backpropagation, gradients also become zero, so weights stop updating.
- Large negative bias initialization or high learning rate can push neurons into this inactive state permanently.

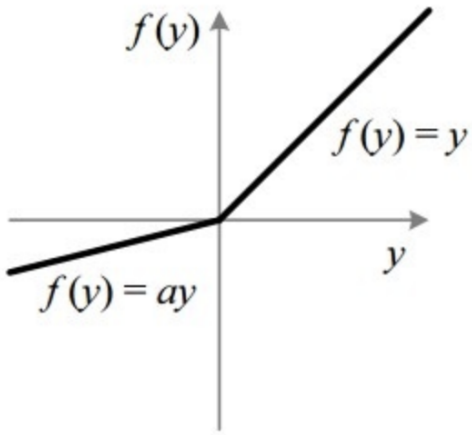
Solution:

- Use variants like Leaky ReLU, Parametric ReLU (PReLU), or ELU.
- Proper weight initialization (e.g., He initialization).
- Lower learning rate to avoid large negative updates.

8.6.5 Leaky ReLU

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha x & \text{if } x \leq 0 \end{cases}$$

where α is a small constant (e.g., 0.01).



Advantages

- Non saturated
- Easily computed
- No dying relu
- Close to zero centre

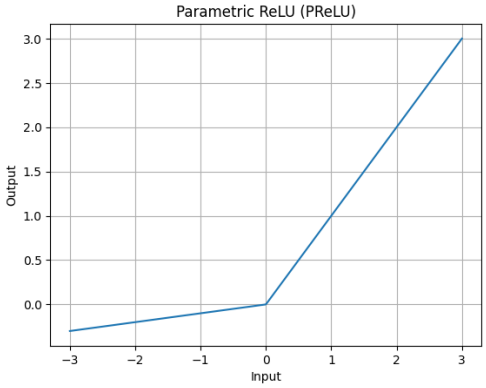
Disadvantages

- The value of α (slope for negative inputs) is fixed and manually set. If not chosen properly, it may not completely solve the Dying ReLU problem.
- It introduces a small gradient for negative values, which might still lead to slow learning for those neurons.

8.6.6 Parametric ReLU (PReLU)

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha x & \text{if } x \leq 0 \end{cases} \quad \text{where } \alpha \text{ is a learnable parameter.}$$

where α is a small constant (e.g., 0.01).



Advantages:

- Learns the optimal slope for negative inputs during training.
- Can adapt better to different types of data compared to fixed-slope functions like Leaky ReLU.
- Helps mitigate the Dying ReLU problem more effectively.

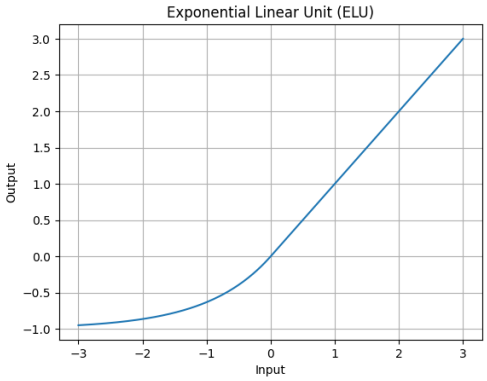
Disadvantages:

- Introduces additional parameters, increasing model complexity.
- Risk of overfitting if not properly regularized.

8.6.7 Exponential Linear Unit (ELU)

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha(e^x - 1) & \text{if } x \leq 0 \end{cases} \quad \text{where } \alpha > 0 \text{ is a hyperparameter (commonly } \alpha = 1).$$

where α is a small constant (e.g., 0.01).



Advantages:

- Smooth and differentiable at all points, including at 0.
- Avoids dying ReLU problem with non-zero gradients for negative inputs.
- Helps bring the mean activation closer to zero, which speeds up learning.

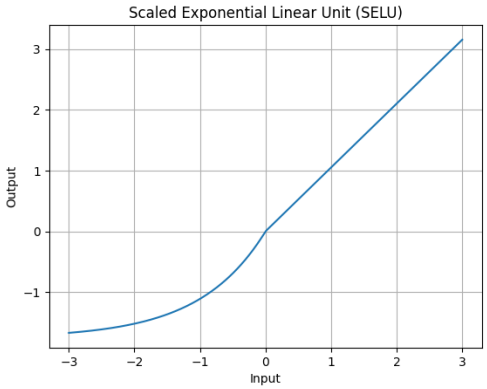
Disadvantages:

- Computationally more expensive due to the exponential function.
- May cause exploding gradients if α is not properly chosen.

8.6.8 Scaled Exponential Linear Unit (SELU)

$$f(x) = \lambda \begin{cases} x & \text{if } x > 0 \\ \alpha(e^x - 1) & \text{if } x \leq 0 \end{cases}$$

where $\lambda \approx 1.0507$ and $\alpha \approx 1.6733$ are fixed constants.



Advantages:

- Self-normalizing: maintains zero mean and unit variance across layers.
- Speeds up training and improves convergence in deep networks.
- Reduces need for explicit normalization techniques like Batch Normalization.

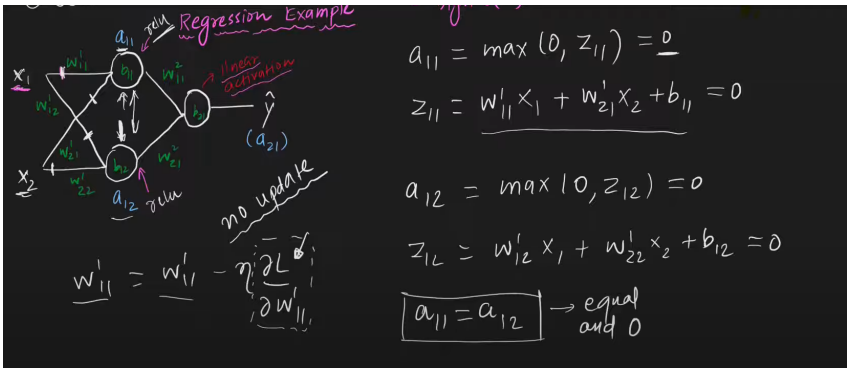
Disadvantages:

- Requires careful initialization (e.g., LeCun normal) and use of specific architectures (e.g., no dropout).
- Only works well with specific types of networks (e.g., fully connected feedforward networks).

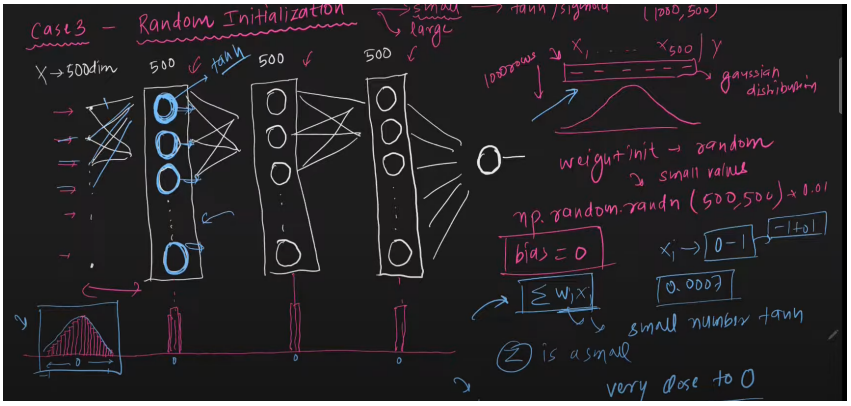
8.7 Weight Initialization

8.7.1 What not to do ?

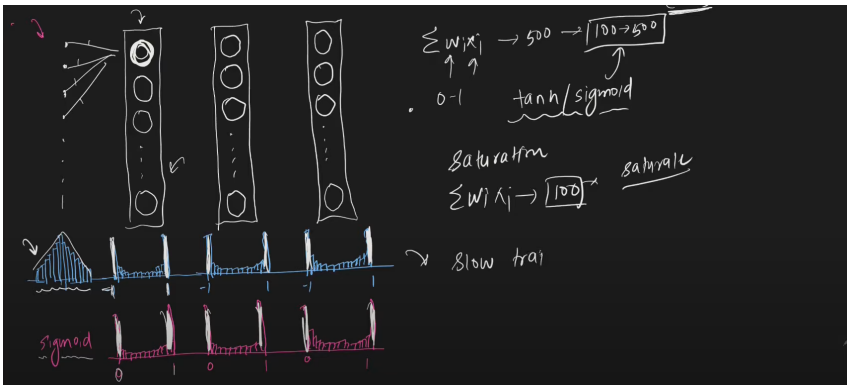
- Zero Initialization



- Non 0 Constant Value ⇒ Model acts like a linear model
- Randomly initialized: Small values



- Randomly initialized: Large values



8.8 Weight Initialization Technique

- **Xavier / Glorot Initialization** (used with `tanh`, `sigmoid`):
  - Normal distribution:
$$\mathcal{N}\left(0, \sqrt{\frac{1}{\text{fan\_in}}}\right)$$
  - Uniform distribution:
$$\mathcal{U}\left[-\text{limit}, \text{limit}\right], \quad \text{where limit} = \sqrt{\frac{6}{\text{fan\_in} + \text{fan\_out}}}$$
- **He Initialization** (used with `ReLU`):
  - Normal distribution:
$$\mathcal{N}\left(0, \sqrt{\frac{2}{\text{fan\_in}}}\right)$$
  - Uniform distribution:
$$\mathcal{U}\left[-\text{limit}, \text{limit}\right], \quad \text{where limit} = \sqrt{\frac{6}{\text{fan\_in}}}$$

8.9 Batch Normalization

Batch-Normalization (BN) is an algorithmic method which makes the training of Deep Neural Networks (DNN) faster and more stable.

It consists of normalizing activation vectors from hidden layers using the mean and variance of the current batch. This normalization step is applied right before (or right after) the nonlinear function.

8.9.1 Internal Covariate Shift

Internal Covariate Shift refers to the change in the distribution of layer inputs during training, as the parameters of the previous layers change. This shift can slow down training and make it harder for the network to converge.

Batch Normalization mitigates this problem by normalizing the inputs of each layer to have a consistent mean and variance across mini-batches. By stabilizing the input distribution, Batch Normalization allows for faster training, enables higher learning rates, and can act as a form of regularization.

8.10 Optimizers

Optimizers play a crucial role in training neural networks by updating the model's weights to minimize the loss function. They determine how the model learns from data by adjusting the weights based on the computed gradients during backpropagation.

- **EWMA (Exponentially Weighted Moving Average)**
  Formula:
  $$v_t = \beta v_{t-1} + (1-\beta)x_t$$
  Use: Not an optimizer by itself, but a key component in optimizers like Momentum and Adam. It helps smooth values like gradients.
  Advantage: Smoothens noisy data and reacts gradually to recent changes.
  Disadvantage: Introduces bias at the beginning which may require correction.

- **SGD with Momentum**
  Formula:
  $$v_t = \beta v_{t-1} + (1-\beta)\nabla L(\theta_t), \quad \theta_{t+1} = \theta_t - \eta v_t$$
  Advantage: Accelerates convergence by dampening oscillations, especially in ravines.
  Disadvantage: Requires tuning of momentum coefficient β and learning rate η.

- **Nesterov Accelerated Gradient (NAG)**
  Formula:
  $$v_t = \beta v_{t-1} + \eta \nabla L(\theta_t - \beta v_{t-1}), \quad \theta_{t+1} = \theta_t - v_t$$
  Advantage: Looks ahead before updating weights, leading to more informed and often faster convergence.
  Disadvantage: Slightly more computational overhead due to the look-ahead step.

- **AdaGrad (Adaptive Gradient)**
  Formula:
  $$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \nabla L(\theta_t)$$
  where G_t is the sum of squares of past gradients.
  Advantage: Adapts learning rates per parameter, beneficial for sparse data.
  Disadvantage: Learning rate decays too aggressively, may stop learning early.

- **RMSprop**
  Formula:
  $$E[g^2]_t = \beta E[g^2]_{t-1} + (1-\beta)(\nabla L(\theta_t))^2, \quad \theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} \nabla L(\theta_t)$$
  Advantage: Solves AdaGrad's decaying learning rate issue, suitable for non-stationary objectives.
  Disadvantage: Sensitive to hyperparameters, requires tuning β and η.

- **Adam (Adaptive Moment Estimation)**
  Formula:
  $$m_t = \beta_1 m_{t-1} + (1-\beta_1)\nabla L(\theta_t), \quad v_t = \beta_2 v_{t-1} + (1-\beta_2)(\nabla L(\theta_t))^2$$
  $$\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1-\beta_2^t}$$
  $$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$$
  Advantage: Combines Momentum and RMSprop, widely used, performs well in many tasks.
  Disadvantage: Can sometimes lead to non-converging or overly adaptive behavior, especially with noisy gradients.

9 Recurrent Neural Networks (RNNs)

Recurrent Neural Networks (RNNs) are a class of artificial neural networks designed to recognize patterns in sequences of data, such as time series, natural language, or audio. Unlike traditional feedforward neural networks, RNNs have connections that form directed cycles, allowing information to persist. This means RNNs can use their internal state (memory) to process sequences of inputs.

Mathematically, for an input sequence $x = (x_1, x_2, \ldots, x_T)$, the hidden state h_t at time step t is computed as:

$$h_t = \tanh(W_{hx}x_t + W_{hh}h_{t-1} + b_h)$$

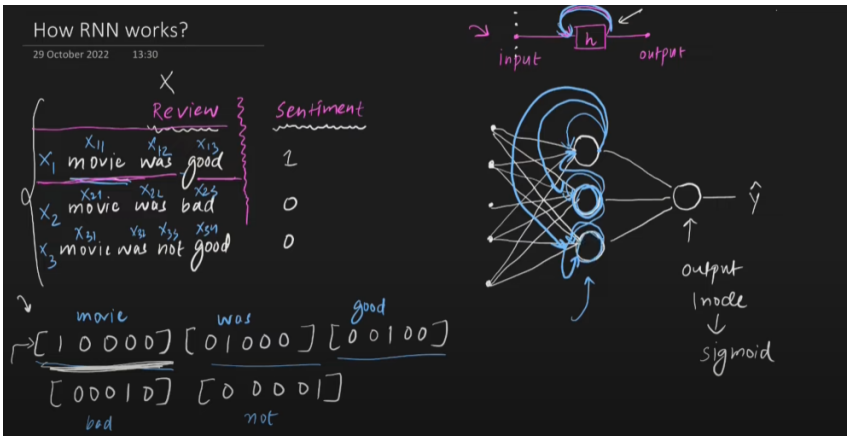
$$y_t = W_{hy}h_t + b_y$$

where W_{hx}, W_{hh}, and W_{hy} are weight matrices, and b_h, b_y are bias vectors.

9.1 Comparison with Artificial Neural Networks (ANNs)

- **Temporal Dependencies:** RNNs are better suited than ANNs for tasks involving sequential data, as they maintain a memory of previous inputs via hidden states.
- **Parameter Sharing:** In RNNs, weights are shared across time steps, making them more efficient when dealing with sequences of arbitrary length.
- **Context Awareness:** RNNs can learn contextual relationships over time, which is not possible with standard ANNs that treat each input independently.
- **Applications:** RNNs are widely used in natural language processing, speech recognition, and time-series forecasting, whereas ANNs are more suited for static input-output mappings like image classification or tabular data tasks.

9.2 How RNN works?



Recurrent Neural Networks (RNNs) process sequential data by maintaining a hidden state that captures information from previous time steps. The given image illustrates sentiment analysis using RNN on text reviews.

- Each review (e.g., "movie was good") is broken into words and converted into one-hot encoded vectors.
- These vectors are fed into the RNN one at a time across time steps $t = 1, 2, 3, \ldots$.
- At each step, the hidden state h_t is updated using the current input x_t and the previous hidden state h_{t-1}.
- The final hidden state is passed through a sigmoid-activated output node to predict the sentiment (positive = 1, negative = 0).

$$h_t = \tanh(W_{hx}x_t + W_{hh}h_{t-1} + b_h), \quad \hat{y} = \sigma(W_{hy}h_T + b_y)$$

This allows the RNN to capture word dependencies and context across the sentence for better classification.

Basic RNN in TensorFlow

```
import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import SimpleRNN, Dense, Embedding

# Sample input parameters
vocab_size = 1000  # Vocabulary size
embedding_dim = 64
rnn_units = 32
sequence_length = 10

# Build the model
model = Sequential([
    Embedding(input_dim=vocab_size, output_dim=embedding_dim, input_length=
        ↪ sequence_length),
    SimpleRNN(rnn_units),
    Dense(1, activation='sigmoid')
])

# Compile the model
model.compile(optimizer='adam', loss='binary_crossentropy', metrics=['accuracy'])

# Print model summary
model.summary()
```

9.3 Types of RNN Architectures (Based on Input-Output Patterns)

RNNs can be categorized based on how sequences are handled at the input and output levels. The main types are:

- **One-to-One:** Standard neural network (e.g., image classification). Single input and single output.
- **One-to-Many:** One input leads to a sequence of outputs. Example: Image captioning (image in, sentence out).
- **Many-to-One:** A sequence of inputs results in a single output.
  Example: Sentiment analysis of a sentence.
  The RNN processes the entire input sequence and outputs a single value (like a sentiment score) at the end.
- **Many-to-Many (synchronized):** Each input time step corresponds to an output time step.
  Example: POS tagging or time-series prediction.
- **Many-to-Many (unsynchronized):** The number of input and output time steps are different.
  Example: Machine translation.

Many-to-One RNN is especially useful for classification tasks where the full context of a sequence determines a single outcome.

9.4 Problem with RNN

Recurrent Neural Networks (RNNs) are powerful for sequence modeling, but they suffer from certain limitations:

Long-Term Dependency

RNNs often struggle to retain information from earlier time steps when processing long sequences. This is due to the vanishing gradient problem, where gradients become too small to influence learning during backpropagation through time.

Example: Consider the sentence:
"The movie that I watched last night with my friends was incredibly good."
To predict the sentiment ('good' → positive), the network needs to remember the earlier context. Vanilla RNNs may forget crucial words if the sentence is too long.

Unstable Training

During training, RNNs may experience exploding or vanishing gradients, especially with deep sequences. This makes optimization difficult, resulting in poor convergence or unstable learning dynamics.

Example: When training on long paragraphs or time series, the loss might fluctuate wildly or become stuck because early layers receive either extremely small or extremely large gradients.

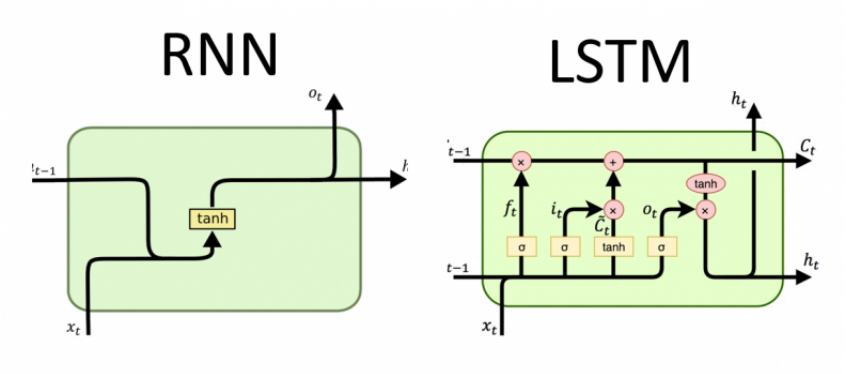
Solutions: These issues are commonly addressed using architectures like LSTM (Long Short-Term Memory) or GRU (Gated Recurrent Unit), which use gating mechanisms to better manage information flow over time.

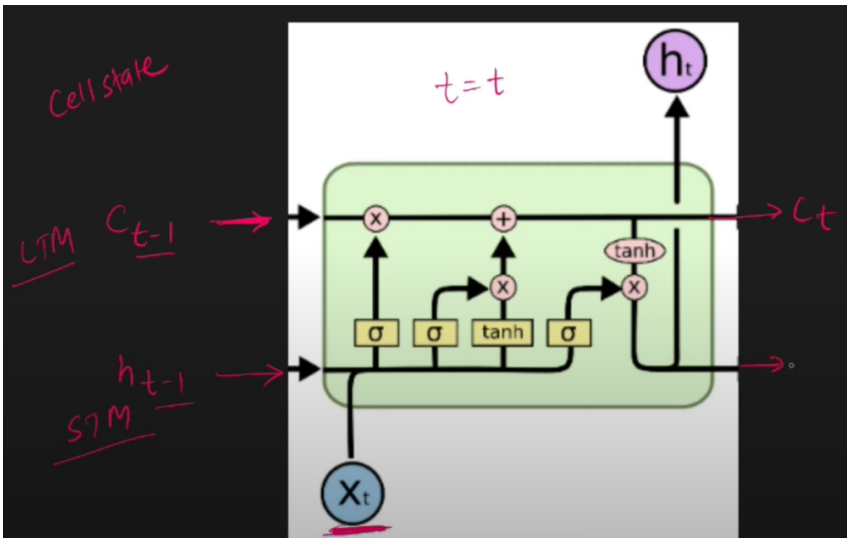
10 Long Short-Term Memory (LSTM)

10.1 Core Idea

The core idea of **LSTM (Long Short-Term Memory)** is to introduce a mechanism that can preserve and manage both short-term and long-term dependencies in sequential data, thereby overcoming the limitations of traditional RNNs, particularly the vanishing gradient problem.

- Traditional RNNs struggle with remembering long-range dependencies because all past information is compressed into a single hidden state, which tends to lose important context over time.
- LSTM addresses this by introducing two separate memory components:
  - **Short-term memory** (h_t): captures the immediate, recent context.
  - **Long-term memory** (c_t): carries important long-range information through the entire sequence.
- These memory components are controlled by **gates**:
  - **Forget Gate**: Decides what information to remove from the long-term memory.
  - **Input Gate**: Decides what new information should be added to the long-term memory.
  - **Output Gate**: Determines what should be output from the current state.
- At every time step, the LSTM cell uses these gates to intelligently control what to remember, what to forget, and what to output.





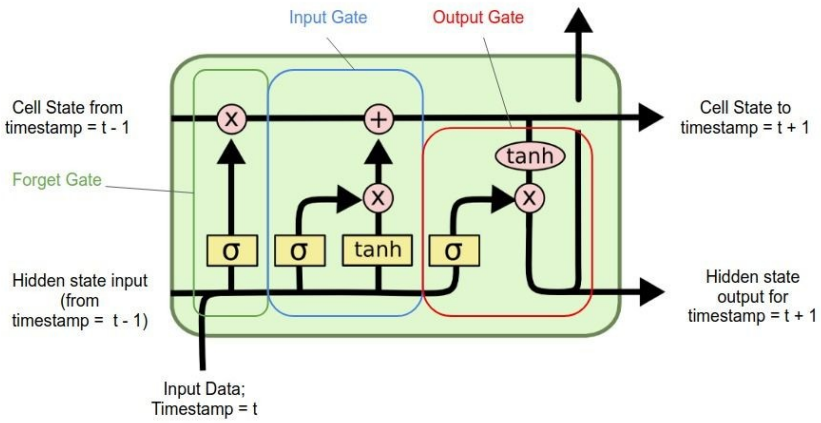
At each time step, the LSTM cell takes the following **three inputs**:

- C_{t-1}: Long-term memory from the previous time step.
- h_{t-1}: Short-term memory (hidden state) from the previous time step.
- x_t: Input at the current time step.

The LSTM cell produces the following **two outputs**:

- C_t: Updated long-term memory (cell state) for the next time step.
- h_t: Updated short-term memory (hidden state) for the next time step.

10.2 LSTM Architecture



10.2.1 Forget Gate

Based on the current input and short term context, forget gate decides which one to remove from long term memory.

10.2.2 Input Gate

Based on the current input, the input gate decides what new should be added to LSTM

10.2.3 Output Gate

Based on the current input, it decides what should be given as output from LSTM. It also creates short-term memory.
For a more in-depth explanation, refer to the following video:
https://www.youtube.com/watch?v=Akv3poqqwI4&list=PLKnIA16_RmvYuZauWaPlRTC54KxSNLtNn&index=62&t=2s

Basic LSTM in TensorFlow

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from tensorflow.keras.layers import LSTM, Dense, Embedding

# Sample input parameters
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sequence_length = 10

# Build the model
model = Sequential([
    Embedding(input_dim=vocab_size, output_dim=embedding_dim, input_length=
        ↪ sequence_length),
    LSTM(lstm_units),
    Dense(1, activation='sigmoid')
])

# Compile the model
model.compile(optimizer='adam', loss='binary_crossentropy', metrics=['accuracy'])

# Print model summary
model.summary()
```

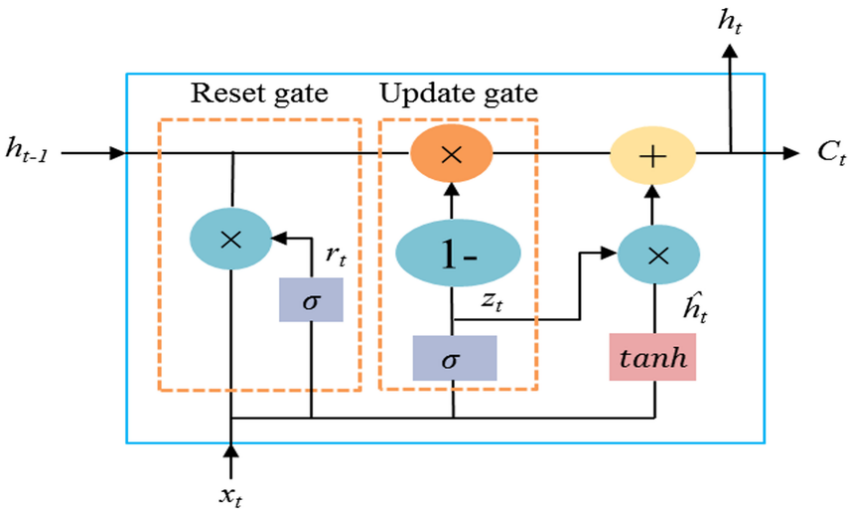
11 Gated Recurrent Neural Network (GRU)

Flaws with LSTM:

- It was complex ⇒ it had large number of parameters ⇒ took more training time

Solution:

- GRU ⇒ Simple architecture ⇒ Less training time



The GRU (Gated Recurrent Unit) is a simplified version of the LSTM, designed to solve the vanishing gradient problem while using fewer gates and parameters.

- The GRU has two main gates:
  1. **Reset Gate** (r_t): Controls how much of the previous hidden state (h_{t-1}) to forget.
  2. **Update Gate** (z_t): Decides how much of the previous hidden state to retain and how much of the new candidate state ($\hat{h}_t$) to use.

- The **candidate hidden state** $\hat{h}_t$ is calculated using the reset gate and current input:

$$\hat{h}_t = \tanh(W_h[r_t * h_{t-1}, x_t])$$

- The **final hidden state** h_t is computed as:

$$h_t = z_t * h_{t-1} + (1 - z_t) * \hat{h}_t$$

- σ is the sigmoid activation function, and tanh is the hyperbolic tangent activation function.

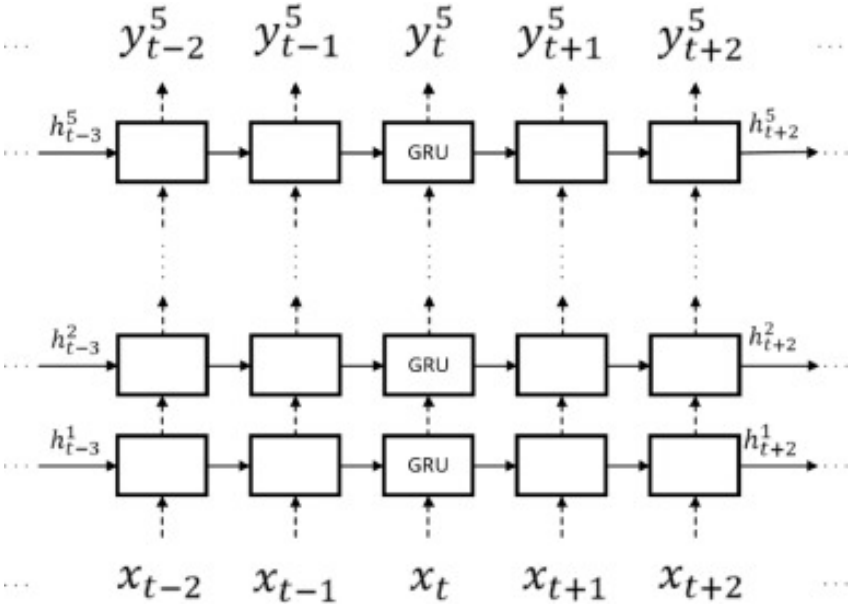
12 Deep RNN

A **Deep RNN** is an extension of a standard RNN architecture where multiple recurrent layers are stacked on top of each other. In this setup, each layer captures features at different levels of abstraction.

Architecture Overview

As shown in the figure below, the input sequence $x_{t-2}, x_{t-1}, x_t, x_{t+1}, x_{t+2}$ is passed through multiple recurrent layers (GRUs in this case). Each layer processes the sequence and passes its hidden states to the next layer above it:

- The bottom layer receives the raw input sequence.
- Intermediate layers process hidden states from the layer below.
- The final layer generates outputs at each time step (e.g., y_t^5).



Difference from Basic RNN, LSTM, and GRU

- **Basic RNN:** Processes sequences with a single recurrent layer. It struggles with long-term dependencies due to vanishing gradients.
- **LSTM:** Introduces memory cells and gating mechanisms to preserve long-term dependencies more effectively.
- **GRU:** A simplified version of LSTM that uses fewer gates and is computationally more efficient.
- **Deep RNN:** Regardless of whether it uses RNN, LSTM, or GRU cells, a Deep RNN stacks multiple layers of them to capture hierarchical temporal features.

Advantages of Deep RNNs

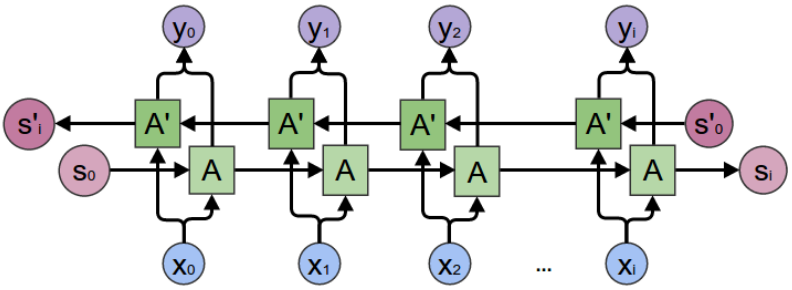
- Learn complex representations from sequential data.
- Lower layers capture short-term patterns; upper layers learn more abstract and long-range dependencies.
- Especially useful in applications like speech recognition, machine translation, and time-series forecasting.

13 Bidirectional RNN — BiLSTM

Use LSTM ⇒ When only past information matters.
Use BiLSTM ⇒ Both past and future content is needed

Eg: for NER, consider the following examples;
"I love Amazon river"
"I love Amazon website"

Bidirectional RNN uses two RNNs, forward RNN and backward RNN. Forward RNN reads the sentence from beginning, backward RNN reads the sentence from the end and then we concatenate both the output



14 When to Use Different RNN Architectures

- **Basic RNN:**
  - Use when sequences are short and dependencies are local.
  - Suitable for simple tasks like character-level prediction or small time series problems.
  - Not ideal for long sequences due to vanishing gradient issues.
- **LSTM (Long Short-Term Memory):**
  - Use when long-term dependencies are important.
  - Great for language modeling, machine translation, and time series forecasting with long history.
  - Preferable when model interpretability (e.g., gating) is beneficial.
- **GRU (Gated Recurrent Unit):**
  - Use when you need faster training with comparable performance to LSTM.
  - Suitable for large datasets or low-resource environments.
  - Good default when experimenting with sequence models.
- **Deep RNN (Stacked RNN/LSTM/GRU):**
  - Use when you want to capture hierarchical or more abstract temporal patterns.
  - Ideal for complex tasks like speech recognition, music generation, or handwriting synthesis.
  - Typically used with dropout or batch normalization to prevent overfitting.
- **Bidirectional RNN (or BiLSTM, BiGRU):**
  - Use when the entire input sequence is available at once.
  - Ideal for tasks where both past and future context improves performance (e.g., Named Entity Recognition, POS tagging, sentiment analysis).
  - Not suitable for real-time prediction or streaming data.