Machine Learning

June 8, 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

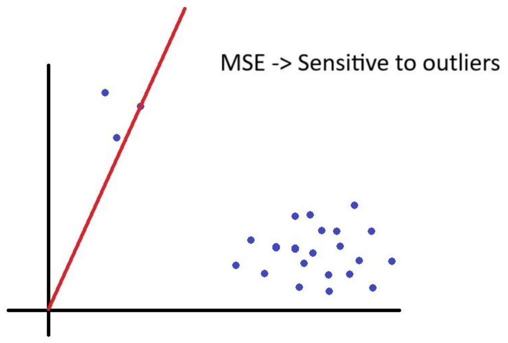
Regression losses are loss functions used in regression tasks (where the goal is to predict continuous values)

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.

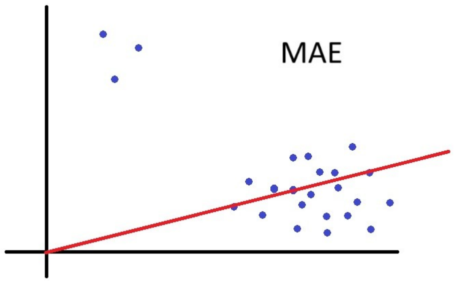


1.1.2 Mean Absolute Error

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

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.

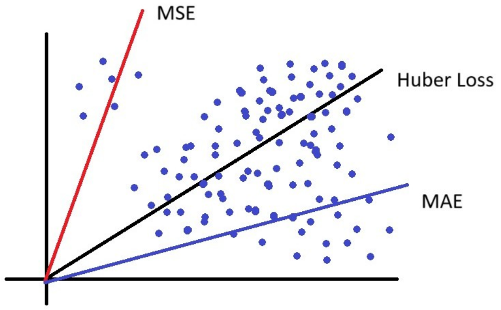


1.1.3 Huber Loss

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

$\delta - >$ 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

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

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

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

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

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

$$\text{Using gradient descent:} \quad \theta := \theta - \alpha \nabla_\theta J(\theta),$$

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

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 $\alpha$, number of iterations $N$
Ensure: Parameters $\theta \in R^n$
1: Initialize $\theta := \vec{0}$
2: for iter = 1 to $N$ do
3:     $h := X \cdot \theta$                                        // Hypothesis vector
4:     $error := h - y$                                             // Error vector
5:     $gradient := \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)}$
6:     $\theta := \theta + \alpha \cdot gradient$
7: end for
8: return $\theta$ =0
```

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

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

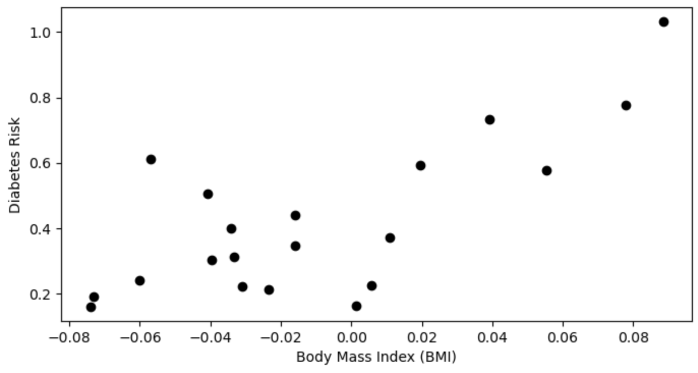
Can lead to global optimum

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

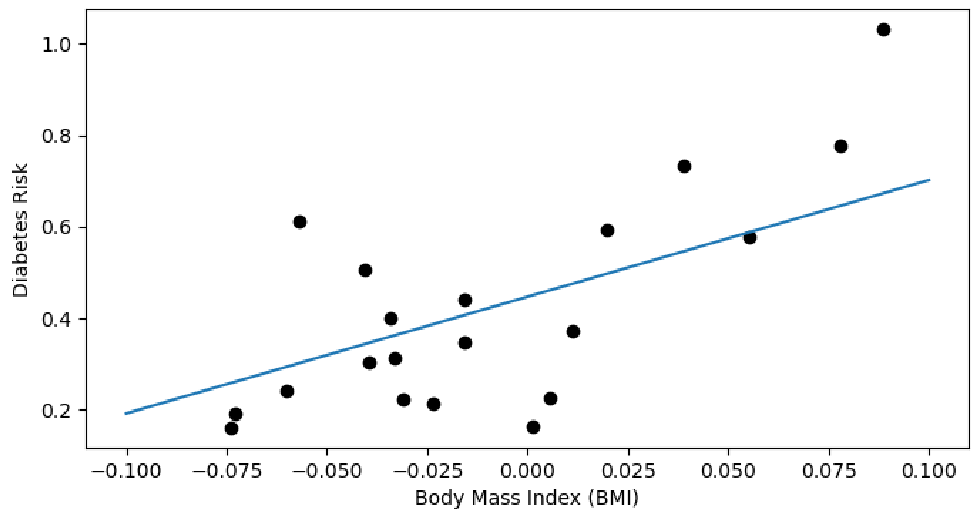
$$y = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2 + \cdots + \theta_d \cdot x_d$$

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:

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

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

$$\text{Using gradient descent:} \quad \theta := \theta - \alpha\nabla_\theta J(\theta),$$

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

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

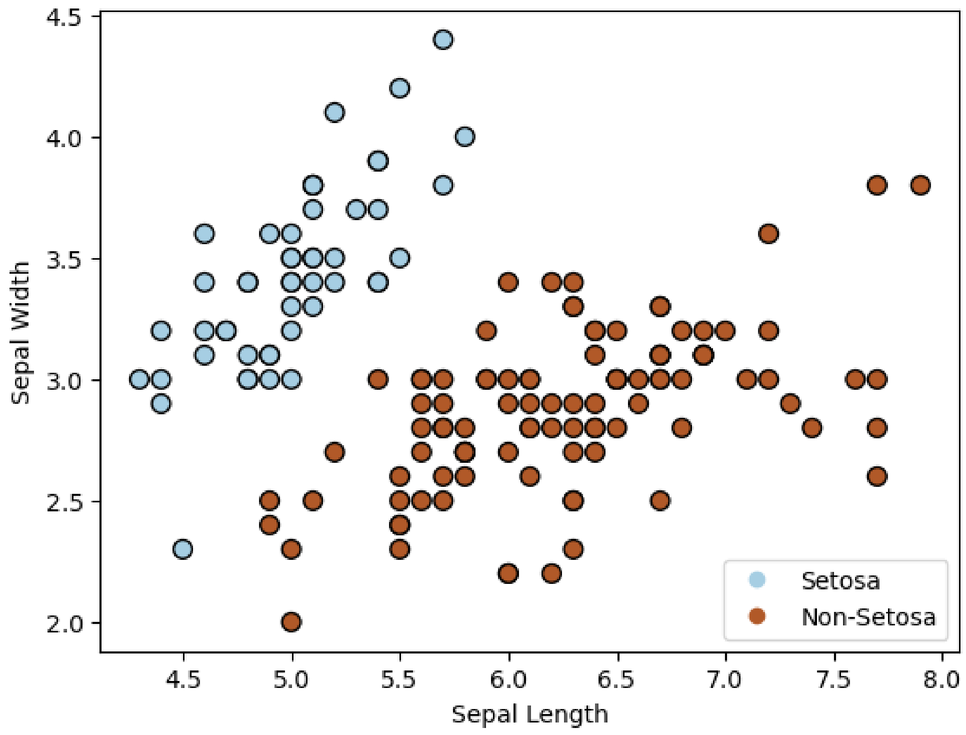
Require: Feature matrix $X \in R^{m\times n}$, target vector $y \in R^m$, learning rate α, number of iterations N

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 $\theta$ =0
```

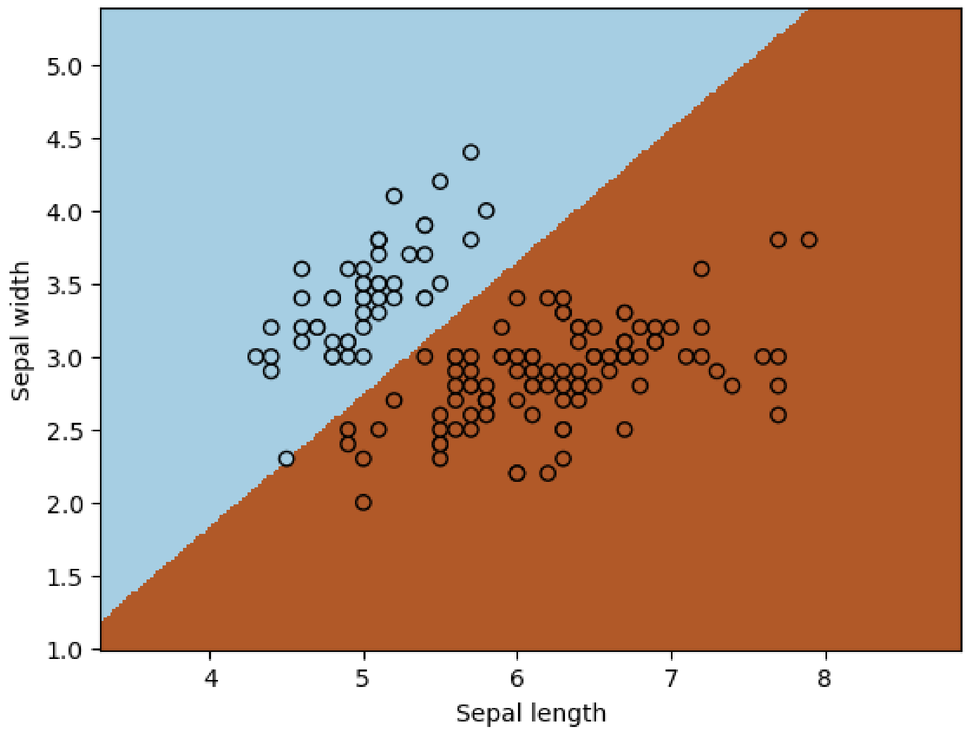
```python
import numpy as np
import pandas as pd
from sklearn import datasets
import warnings
warnings.filterwarnings('ignore')

# 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
    ↪ ')
```

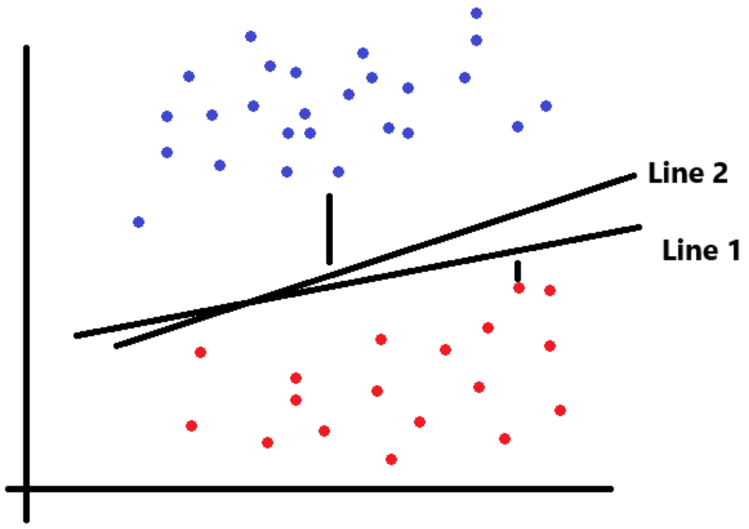


```
import numpy as np
from matplotlib import pyplot as plt

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
```

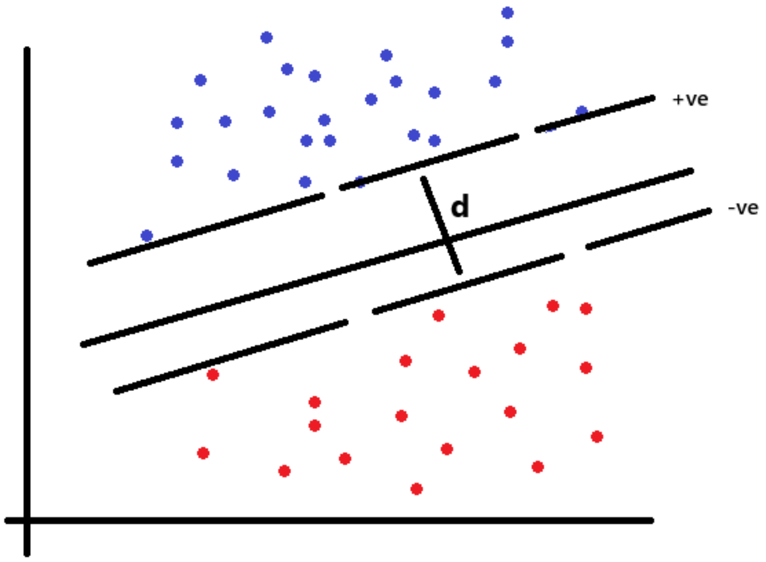


4 Support Vector Machines



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:

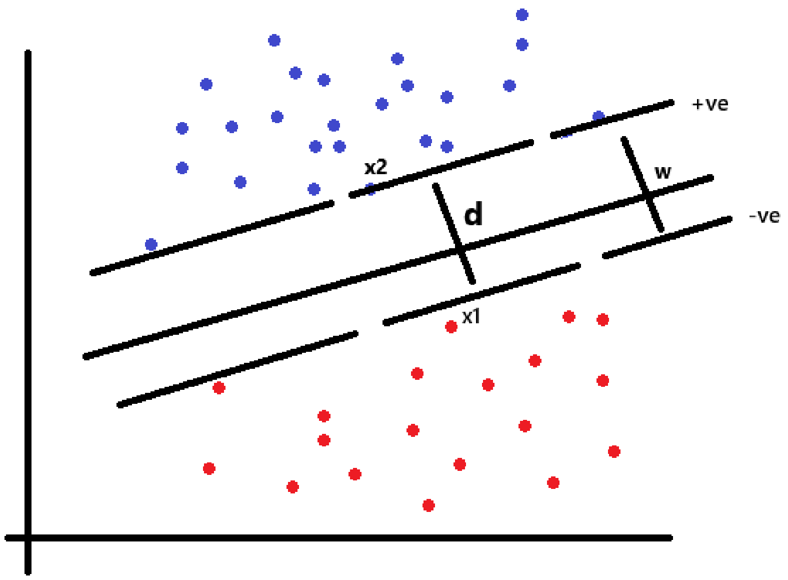
$$\hat{y} = \begin{cases} +1 & \text{if } \vec{w} \cdot \vec{x}_i + b \geq 0 \\ -1 & \text{if } \vec{w} \cdot \vec{x}_i + b < 0 \end{cases}$$

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

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

For support vectors,

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



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

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

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

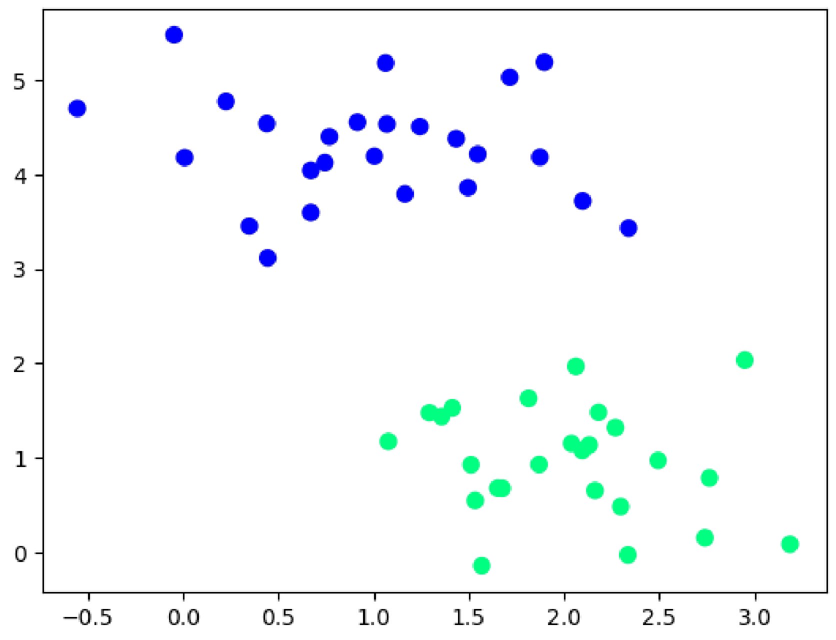
$$d = \frac{(1-b) - (-1-b)}{\|\vec{\omega}\|}$$

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

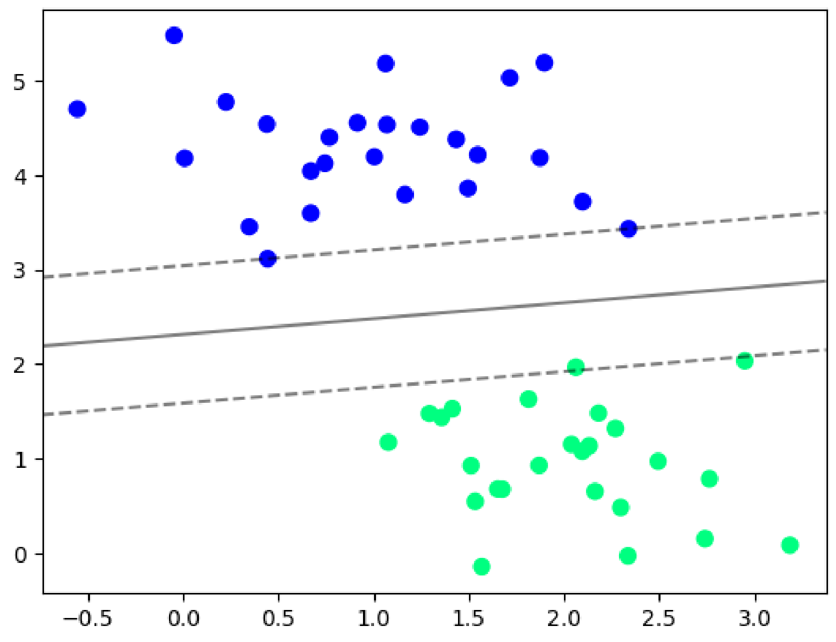
$$\arg \max_{(\vec{\omega}^*, b^*)} \frac{2}{\|\vec{\omega}\|} \quad \text{subject to} \quad y_i(\vec{\omega} \cdot \vec{x}_i + b) \geq 1$$

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)
```



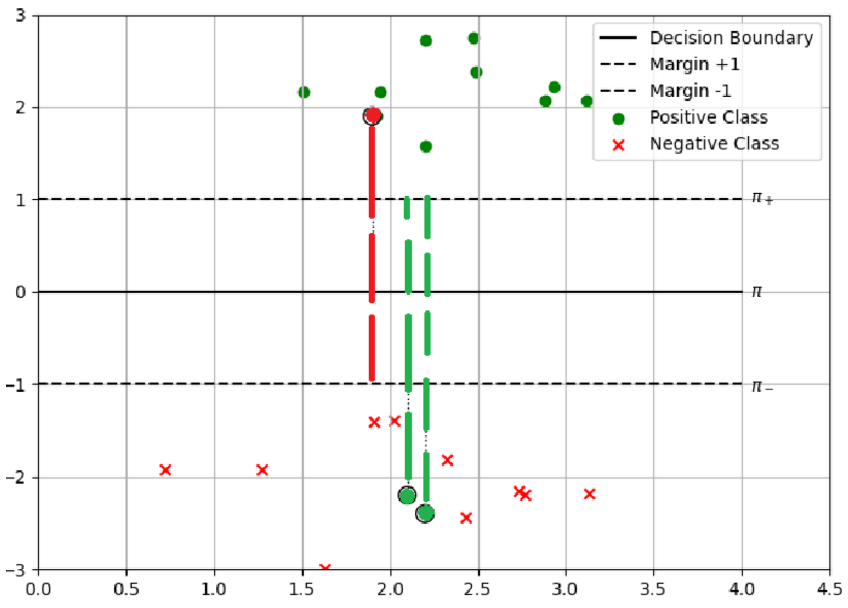
4.2 Non Linear Separable Data

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.

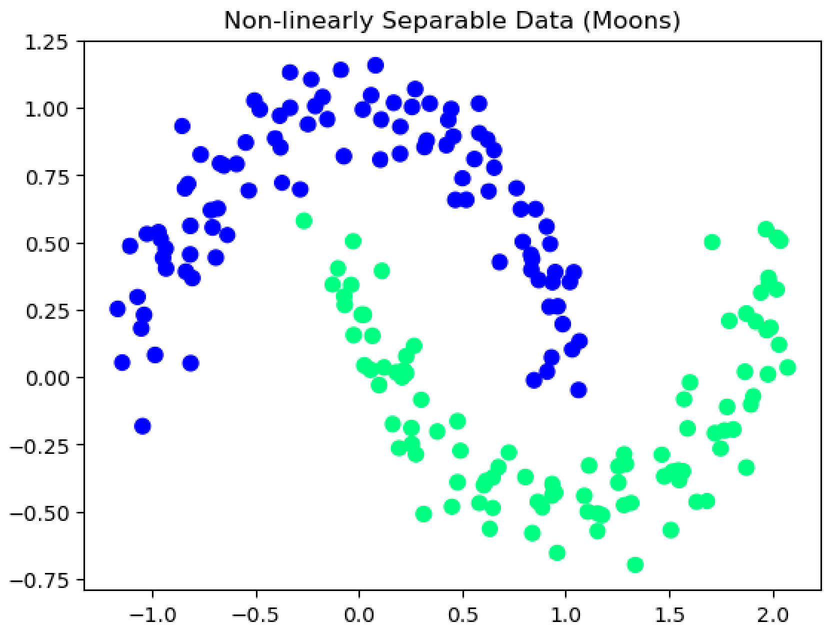
4.3 Kernel

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.

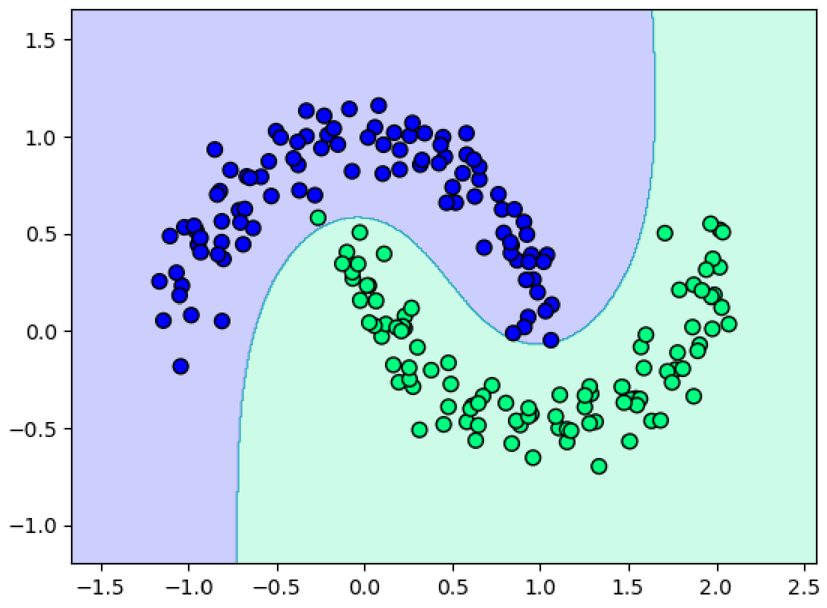
Types of Kernels:

- **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()
```



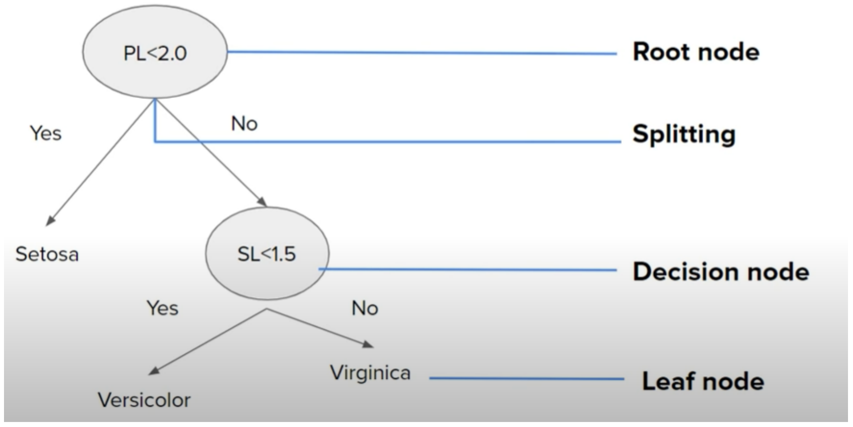
```python
from sklearn.svm import SVC    # Support Vector Classifier
model = SVC(kernel='rbf', C = 1)
model.fit(X,y)
```



5 Decision Trees

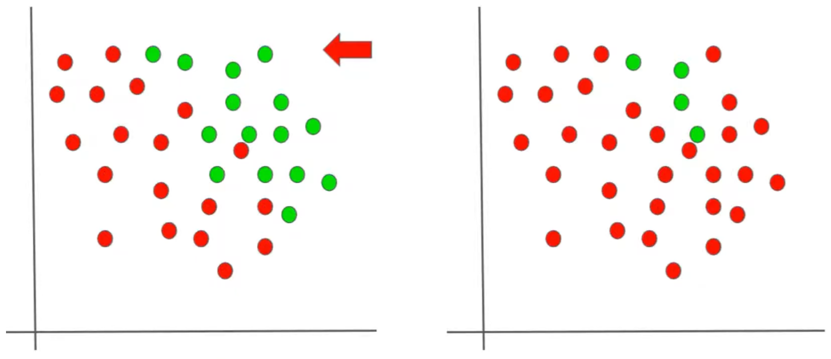
A **Decision Tree** is a supervised machine learning algorithm used for both *classification* and *regression* tasks. It models decisions and their possible consequences using a tree-like structure.

- 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 $\Rightarrow$ **Less Entropy**


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

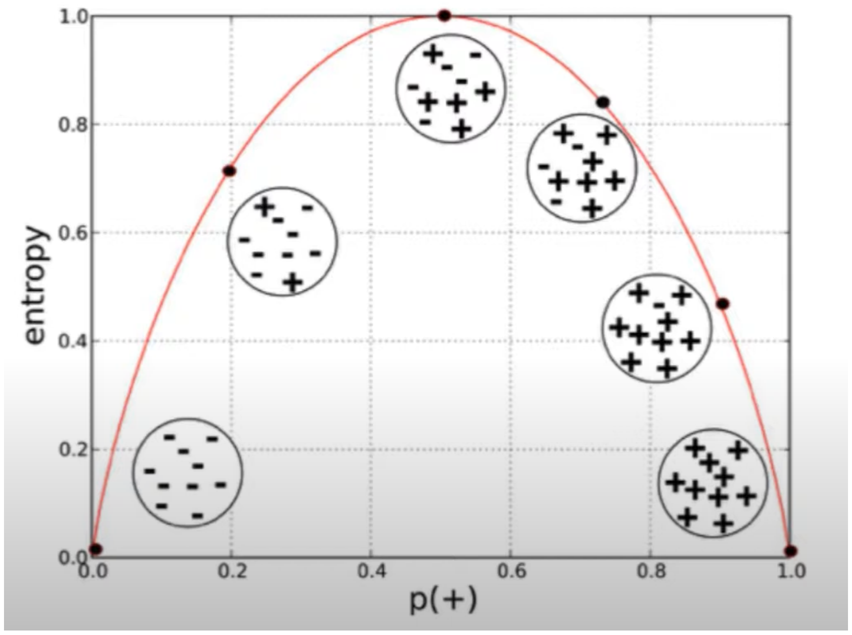
Let:

- 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

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

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

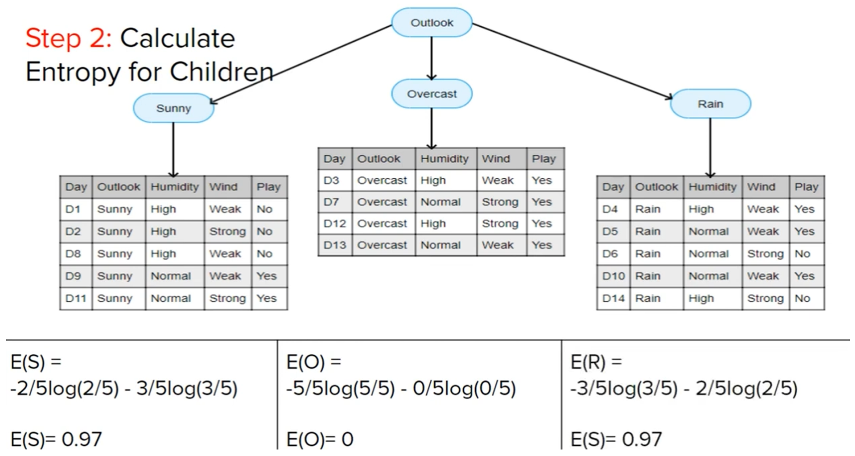
Entropy of Parent Dataset:

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

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

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

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

E(S) =
-2/5log(2/5) - 3/5log(3/5)

E(S)= 0.97

E(O) =
-5/5log(5/5) - 0/5log(0/5)

E(O)= 0

E(R) =
-3/5log(3/5) - 2/5log(2/5)

E(S)= 0.97

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

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

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

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

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.

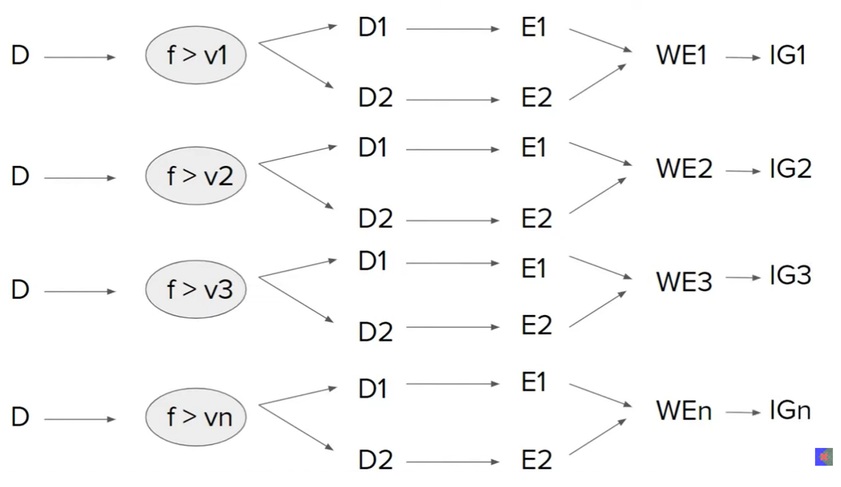
Solution: Perform **hyperparameter tuning** to choose between Gini and Entropy based on the performance of your specific dataset.

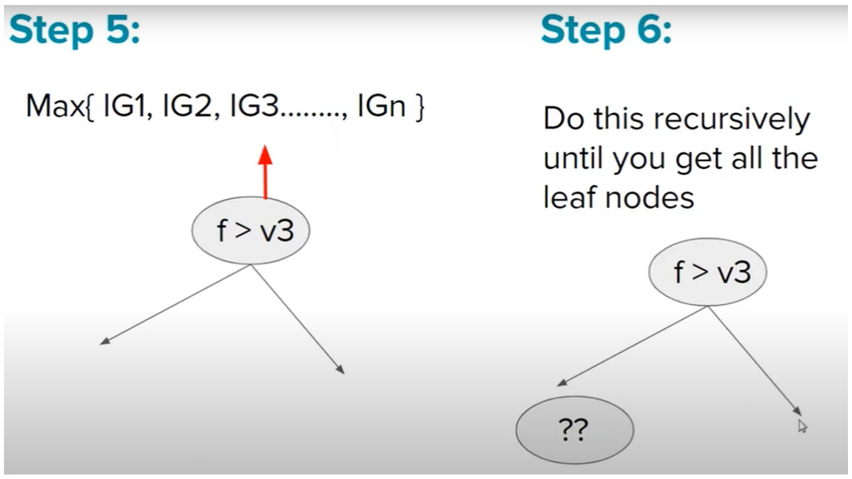
5.4 Handling Numerical values in Decision Trees

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




Step 5:
Max{ IG1, IG2, IG3........, IGn }
f > v3
Step 6:
Do this recursively until you get all the leaf nodes
f > v3
??

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.

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.

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.