

**Machine learning algorithm for detecting thyroid-related disorders  
to increase thyroid illness diagnosis accuracy**

**Advance Machine Learning / Spring 2024 / Prof. Ashok Kumar Patel**

**By Group – 11**

**Ajeet Singh – 48**

**Manas Vishal – 58**

**Rohith Kumar – 13**

## Problem Statement:

Machine learning techniques have been increasingly used in the medical field to improve the accuracy of diagnoses and treatment plans. The use of an ML algorithm for detecting thyroid-related disorders to increase thyroid illness diagnosis accuracy. This approach involves using data-based decisions for diagnosing thyroid dysfunction, which is a classification problem that can be solved using Machine Learning techniques.

## About the Datasets:

The dataset contains records of thyroid diagnoses from the Garvan Institute, collected between 1984 and early 1987. Each record consists of 25 attribute values, followed by a class. The attributes include various medical conditions, patient characteristics, and laboratory measurements related to thyroid function. The class contains two possible values: negative and sick-euthyroid.

Observations: 3163

Features: 25

Class: 1 (with two distinct values)

COLUMN	VALUES
class:	sick-euthyroid,negative
age:	continuous,?
sex:	M,F,?
on_thyroxine:	f,t
query_on_thyroxine:	f,t
on_antithyroid_medication:	f,t
thyroid_surgery:	f,t
query_hypothyroid:	f,t
query_hyperthyroid:	f,t
pregnant:	f,t
sick:	f,t
tumor:	f,t
lithium:	f,t
goitre:	f,t
TSH_measured:	f,t
TSH:	continuous,?
T3_measured:	f,t
T3:	continuous,?
TT4_measured:	f,t
TT4:	continuous,?
T4U_measured:	f,t
T4U:	continuous,?
FTI_measured:	f,t
FTI:	continuous,?
TBG_measured:	f,t
TBG:	continuous,?

Source:

Quinlan, Ross. (1987). Thyroid Disease.  
UCI Machine Learning Repository.  
<https://doi.org/10.24432/C5D010>.

## Solution Approach:

Given the complexity and the nature of the thyroid disease dataset, which includes a mix of continuous and categorical variables, and considering the need for accurate prediction of multiple classes of thyroid conditions, a combination of machine learning algorithms would be beneficial. The choice of algorithms should be based on their ability to handle both types of data and their performance in classification tasks, especially in the context of imbalanced classes.

1. **Random Forest (RF):** Random Forest is a powerful ensemble learning method that can handle both continuous and categorical data. It is known for its ability to avoid overfitting and its robustness to outliers.
2. **Gradient Boosting Machine (GBM):** GBM is another ensemble method that builds a series of weak learners (typically decision trees) to form a strong predictive model. It is particularly effective in handling imbalanced datasets and can capture complex patterns in the data.
3. **Support Vector Machine (SVM):** SVMs are effective in high-dimensional spaces and are versatile as different Kernel functions can be specified for the decision function. They are particularly useful when the dataset is not linearly separable.
4. **AdaBoost:** AdaBoost is an ensemble method that combines multiple weak learners to create a strong learner. It is effective in handling noisy data and can improve the accuracy of the model.
5. **Deep Learning Models (ANN):** For a more complex and nuanced understanding of the data, deep learning models like ANN networks can be used. These models can capture complex patterns and dependencies in the data, which might be beneficial for predicting thyroid conditions.

It would be beneficial to experiment with these algorithms, possibly in combination, and use cross-validation to evaluate their performance. The choice of the best algorithm or combination of algorithms would depend on the specific characteristics of the dataset and the performance metrics (accuracy, precision, recall, etc.) that are most relevant to the problem at hand.

Load the csv file of thyroid dataset. Since the file does not have columns names and so we need to specify while loading it into dataframe. It has 25 features, 1 class and 3163 observations. It does not show any missing values initially, but we do see some unknow values like '?'.



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```

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```

## Understand Missing values

Many missing column values are represented as '?'. And so we need to mark them NaN to get proper count of missing and valid values

[110]:

```
#Replace all the missing values ? with NaN  
df = df.replace("?", np.nan)
```

[110]:

```
# List percenatge of missing values in all columns  
  
df.isnull().mean() * 100
```

[110]:

```
class      0.000000  
age        14.100537  
sex         2.307936  
on_thyroxine    0.000000  
query_on_thyroxine   0.000000  
on_antithyroid_medication  0.000000  
thyroid_surgery     0.000000  
query_hypothyroid    0.000000  
query_hyperthyroid   0.000000  
pregnant           0.000000  
sick                0.000000  
tumor               0.000000  
lithium             0.000000  
goitre              0.000000  
TSH_measured       0.000000  
TSH                 14.796000  
T3_measured         0.000000  
T3                  21.972811  
TT4_measured        0.000000  
TT4                 7.672273  
TT4_measured        0.000000  
TT4                 7.840658  
FTI_measured        0.000000  
FTI                 7.009042  
TBG_measured        0.000000  
TBG                 91.779956  
dtype: float64
```

## Handling Missing Values and Encoding Categorical Values:

- We can remove the TBG column as it has 91.77 % of missing values and will not be helpful for training model.
- All other missing values should be replaced with the Mean value of that column.
- Since most of the column values are categorical types and so we need to convert/map/encode to numerical values as listed below:

'sick-euthyroid': 1

'negative': 0

't': 1

'f': 0

'y': 1

'n': 0

'F': 1

'M': 0

- Convert the remaining measured features from Object to Float

```
Group-14_AML.ipynb
Handling Missing data and Encoding Categorical Datasets

Since most of the column values are categorical types and so we need to convert/map/encode to numerical values
Many missing column values are represented as "?". And so we need to mark them NaN to get proper count of missing and valid values

"t":1, "f":0, "y":1, "n":0, "sick-euthyroid":1, "negative":0, "F":1, "M":0.

[11]: # Create mapper for values (t which is True and f which False)
# Create mapper for values (F which is Female and M which Male)

mapper = {"t":1, "f":0, "y":1, "n":0, "sick-euthyroid":1, "negative":0, "F":1, "M":0}

df = df.replace(mapper)

[12]: # Since TBG has almost 92% missing data and so it is better to remove that column

df.drop("TBG", axis=1, inplace=True)

[13]: #Convert the remain measured column to int

df[['age', 'TSH', 'T3', 'TT4', 'T4U', 'FTI']] = df[['age', 'TSH', 'T3', 'TT4', 'T4U', 'FTI']].astype(float)
df.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 3163 entries, 0 to 3162
Data columns (total 25 columns):
#   Column                Non-Null Count  Dtype
---  ---
0   class                 3163 non-null   int64
1   age                   2717 non-null   float64
2   sex                   3080 non-null   float64
3   on_thyroxine          3163 non-null   int64
4   query_on_thyroxine    3163 non-null   int64
5   on_antithyroid_medication  3163 non-null   int64
6   thyroid_surgery       3163 non-null   int64
7   query_hypothyroid     3163 non-null   int64
8   query_hyperthyroid    3163 non-null   int64
9   pregnant              3163 non-null   int64
10  sick                  3163 non-null   int64
11  tumor                 3163 non-null   int64
12  lithium               3163 non-null   int64
13  goitre                3163 non-null   int64
14  TSH_measured          3163 non-null   int64
15  TSH                   2695 non-null   float64
16  T3_measured           3163 non-null   int64
17  T3                    2468 non-null   float64
18  TT4_measured          3163 non-null   int64
19  TT4                   2914 non-null   float64
20  T4U_measured          3163 non-null   int64
21  T4U                   2915 non-null   float64
22  FTI_measured          3163 non-null   int64
23  FTI                   2916 non-null   float64
24  TBG_measured          3163 non-null   int64
dtypes: float64(7), int64(18)
memory usage: 617.9 KB

Group-14_AML.ipynb

[14]: # replace remaining missing values with mean

df.fillna(df.mean(), inplace=True)

[15]: # List percentatge of missing values in all columns after filling NaN

df.isnull().mean() * 100

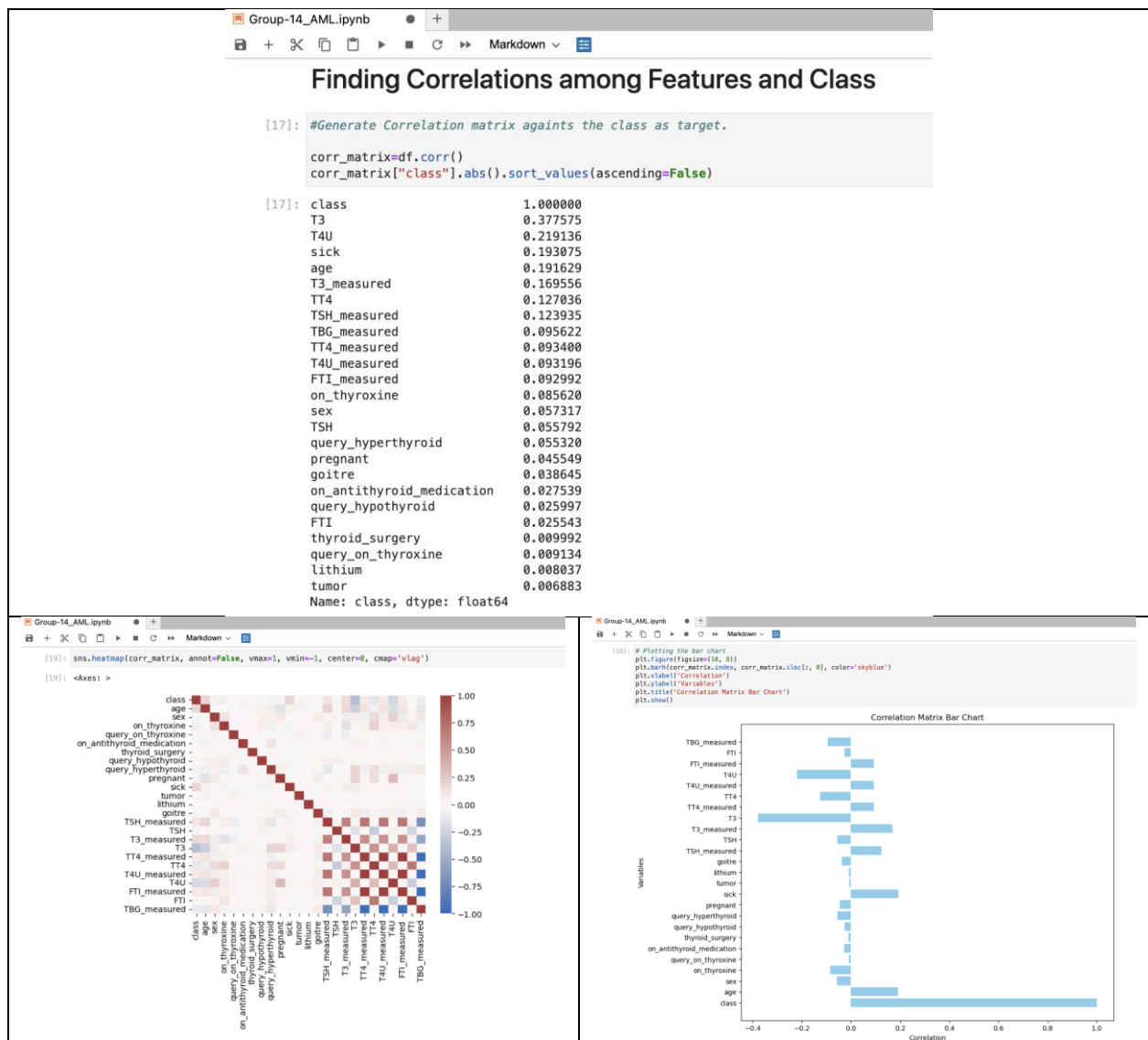
[15]: class                0.0
age                    0.0
sex                   0.0
on_thyroxine          0.0
query_on_thyroxine    0.0
on_antithyroid_medication  0.0
thyroid_surgery       0.0
query_hypothyroid     0.0
query_hyperthyroid    0.0
pregnant              0.0
sick                  0.0
tumor                 0.0
lithium               0.0
goitre                0.0
TSH_measured          0.0
TSH                   0.0
T3_measured           0.0
T3                    0.0
TT4_measured          0.0
TT4                   0.0
T4U_measured          0.0
T4U                   0.0
FTI_measured          0.0
FTI                   0.0
TBG_measured          0.0
dtype: float64

[16]: df.shape

[16]: (3163, 25)
```

## Finding Correlations between Features and Class:

- There is strong correlation for T3, T4U, sick, age, T3\_measured, TT4, TSH\_measured, TBG\_measured.
- Some of the features are not very well correlated. like, Tumor, lithium, thyroid\_surgery, query\_on\_thyroxine, FTI, query\_hypothyroid, on\_antothyroid\_medication, goitre.



## Dividing Datasets into Training and Testing sets:

- We divided datasets into Train set and Test set. Making sure each set represent proper proportion of each Classes

Train Set: (2530, 25)

0 2296

1 234

Test Set: (633, 25)

0 574

1 59

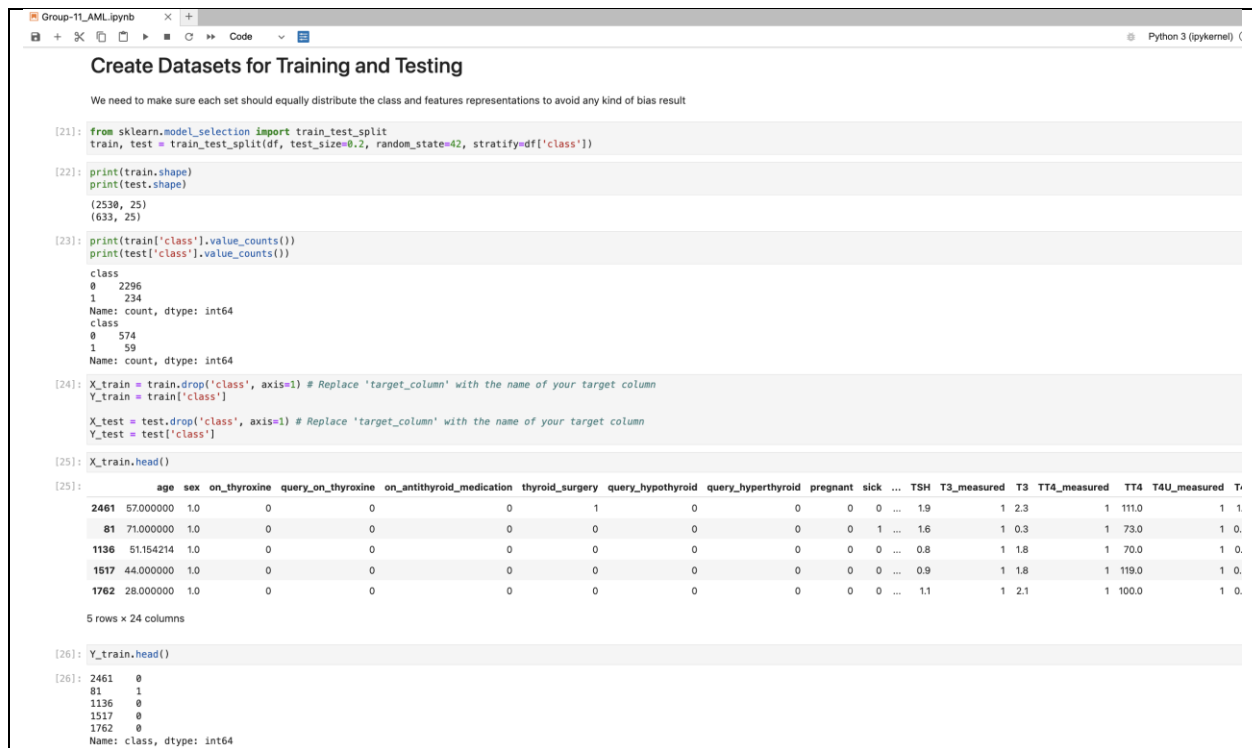
- Created X and Y variables for each dataset to use into Model Function

X\_train = hold all features values for train set

Y\_train = hold only class values for train set

X\_test = hold all features values for test set

Y\_test = hold only class values for test set



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Group-11_AML.ipynb Python 3 (pykernel)

Create Datasets for Training and Testing

We need to make sure each set should equally distribute the class and features representations to avoid any kind of bias result

[21]: from sklearn.model_selection import train_test_split
      train, test = train_test_split(df, test_size=0.2, random_state=42, stratify=df['class'])

[22]: print(train.shape)
      print(test.shape)
      (2530, 25)
      (633, 25)

[23]: print(train['class'].value_counts())
      print(test['class'].value_counts())
      class
      0    2296
      1     234
      Name: count, dtype: int64
      class
      0     574
      1      59
      Name: count, dtype: int64

[24]: X_train = train.drop('class', axis=1) # Replace 'target_column' with the name of your target column
      Y_train = train['class']
      X_test = test.drop('class', axis=1) # Replace 'target_column' with the name of your target column
      Y_test = test['class']

[25]: X_train.head()
      age sex on_thyroxine query_on_thyroxine on_antithyroid_medication thyroid_surgery query_hypothyroid query_hyperthyroid pregnant sick ... TSH T3_measured T3 TT4_measured TT4 T4U_measured T
      2461 57.000000 1.0 0 0 0 1 0 0 0 0 0 0 0 0 1.9 1 2.3 1 111.0 1 1
      81 71.000000 1.0 0 0 0 0 0 0 0 0 1 1.6 1 0.3 1 73.0 1 0
      1136 51.154214 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0.8 1 1.8 1 70.0 1 0
      1517 44.000000 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0.9 1 1.8 1 119.0 1 0
      1762 28.000000 1.0 0 0 0 0 0 0 0 0 0 0 0 0 1.1 1 2.1 1 100.0 1 0
      5 rows x 24 columns

[26]: Y_train.head()
      2461 0
      81 1
      1136 0
      1517 0
      1762 0
      Name: class, dtype: int64
```

## Training Using different ML Models:

- We will train and test datasets using different models as listed below. And will capture the evaluation metrics for comparison and understand which model is better.
  - Network Model
    - ANN
  - Statistical Model
    - SVC
  - Tree Based Model
    - XGBoost
    - GBM
    - Random Forest
    - AdaBoost
- We are going to follow the steps below to train/test/evaluate for each model.
  - Import required model's library
  - Train Model using Training set
    - `trained_model = model.fit(X_train,Y_Train)`
  - Predict Model using Testing set
    - `Y_predict = trained_model.predict(X_test)`
  - Evaluate Model Performance
    - `accuracy_score(Y_test, Y_predict)`
    - `precision_score(Y_test, Y_predict)`
    - `recall_score(Y_test, Y_predict)`
    - `f1_score(Y_test, Y_predict)`
  - Also create Confusion Matrix and plot a heatmap
    - `confusion_matrix(Y_test, Y_predict)`



```
Group-11_AML_AML.pynb | +  
+ + < > ▶ ◀ ⌂ Code ▾ ☰  
  
XGBoost Model  
  
[62]: from xgboost import XGBClassifier  
  
model_xgboost = XGBClassifier(objective='binary:logistic', eval_metric='auc')  
model_xgboost.fit(X_train, Y_train)  
  
[62]: XGBClassifier  
  
[63]: #Predict using Test dataset  
  
Y_pred_xgboost = model_xgboost.predict(X_test)  
  
[64]: # Evaluate using various Metrics  
  
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score, confusion_matrix  
  
# Calculate metrics  
eval_metrics.loc[0, 'Accuracy'] = accuracy_score(Y_test, Y_pred_xgboost)  
eval_metrics.loc[0, 'Precision'] = precision_score(Y_test, Y_pred_xgboost, average='binary') # Use 'binary' for binary classification  
eval_metrics.loc[0, 'Recall'] = recall_score(Y_test, Y_pred_xgboost, average='binary')  
eval_metrics.loc[0, 'F1_Score'] = f1_score(Y_test, Y_pred_xgboost, average='binary')  
  
print(eval_metrics[0:1])  
  
Method_Name Accuracy Precision Recall F1_Score  
0 XGBost 0.966825 0.816667 0.830508 0.823529  
  
[65]: matrix = confusion_matrix(Y_test, Y_pred_xgboost)  
df_confusion = pd.DataFrame(matrix, index=['sick-euthyroid', 'negative'], columns=['sick-euthyroid', 'negative'])  
df_confusion  
  
[65]:
```

	sick-euthyroid	negative
sick-euthyroid	563	11
negative	10	49

```
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```

```
[40]: from sklearn.ensemble import RandomForestClassifier

model_randomforest = RandomForestClassifier(n_estimators=100, random_state=42)
model_randomforest.fit(X_train, Y_train)

[40]: ▼ RandomForestClassifier
RandomForestClassifier(random_state=42)

[41]: Y_pred_rf = model_randomforest.predict(X_test)

[42]: # Evaluate using various Metrics

from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

# Calculate metrics
eval_metrics.loc[2, 'Accuracy'] = accuracy_score(Y_test, Y_pred_rf)
eval_metrics.loc[2, 'Precision'] = precision_score(Y_test, Y_pred_rf, average='binary') # Use 'binary' for binary classification
eval_metrics.loc[2, 'Recall'] = recall_score(Y_test, Y_pred_rf, average='binary')
eval_metrics.loc[2, 'F1_Score'] = f1_score(Y_test, Y_pred_rf, average='binary')

print(eval_metrics[2:3])
```

	Method_Name	Accuracy	Precision	Recall	F1_Score
2	Random_Forest	0.960506	0.765625	0.830588	0.796748

```
[43]: matrix = confusion_matrix(Y_test, Y_pred_rf)
df_confusion = pd.DataFrame(matrix, index=['sick-euthyroid', 'negative'], columns=['sick-euthyroid', 'negative'])
df_confusion

[43]:
```

	sick-euthyroid	negative
sick-euthyroid	559	15
negative	10	49

Group-11\_AML.ipynb

## Gradient Boosting Machine (GBM) Model

```
[50]: from sklearn.ensemble import GradientBoostingClassifier

model_gbm = GradientBoostingClassifier(n_estimators=100, learning_rate=1.0, max_depth=1, random_state=42)

model_gbm.fit(X_train, Y_train)
```

```
[50]: GradientBoostingClassifier
GradientBoostingClassifier(learning_rate=1.0, max_depth=1, random_state=42)
```

```
[51]: #Predict using Test dataset

Y_pred_gbm = model_gbm.predict(X_test)
```

```
[52]: # Evaluate using various Metrics

from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

# Calculate metrics
eval_metrics.loc[4, 'Accuracy'] = accuracy_score(Y_test, Y_pred_gbm)
eval_metrics.loc[4, 'Precision'] = precision_score(Y_test, Y_pred_gbm, average='binary') # Use 'binary' for binary classification
eval_metrics.loc[4, 'Recall'] = recall_score(Y_test, Y_pred_gbm, average='binary')
eval_metrics.loc[4, 'F1_Score'] = f1_score(Y_test, Y_pred_gbm, average='binary')

print(eval_metrics[4:5])
```

	Method_Name	Accuracy	Precision	Recall	F1_Score
4	GBM	0.952607	0.688312	0.898305	0.779412

```
[53]: matrix = confusion_matrix(Y_test, Y_pred_gbm)
df_confusion = pd.DataFrame(matrix, index=['sick-euthyroid', 'negative'], columns=['sick-euthyroid', 'negative'])
df_confusion
```

```
[53]:
```

	sick-euthyroid	negative
sick-euthyroid	550	24
negative	6	53

Group-11\_AML.ipynb

## ANN Model

```
[ ]: import tensorflow as tf

model_ann = tf.keras.models.Sequential()

# Adding the input layer and the first hidden layer
model_ann.add(tf.keras.layers.Dense(units=6, activation='relu'))

# Adding the second hidden layer
model_ann.add(tf.keras.layers.Dense(units=6, activation='relu'))

# Adding the output layer
model_ann.add(tf.keras.layers.Dense(units=1, activation='sigmoid'))

model_ann.compile(optimizer='adam', loss='binary_crossentropy', metrics=['accuracy'])

model_ann.fit(X_train, Y_train, batch_size=32, epochs=100)
```

```
[36]: #Predict using Test dataset

Y_pred_ann = model_ann.predict(X_test)
Y_pred_ann = np.round(Y_pred_ann).flatten()
```

20/20 ————— 0s 307us/step

```
[37]: # Evaluate using various Metrics

from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

# Calculate metrics
eval_metrics.loc[1, 'Accuracy'] = accuracy_score(Y_test, Y_pred_ann)
eval_metrics.loc[1, 'Precision'] = precision_score(Y_test, Y_pred_ann, average='binary') # Use 'binary' for binary classification
eval_metrics.loc[1, 'Recall'] = recall_score(Y_test, Y_pred_ann, average='binary')
eval_metrics.loc[1, 'F1_Score'] = f1_score(Y_test, Y_pred_ann, average='binary')

print(eval_metrics[1:2])
```

	Method_Name	Accuracy	Precision	Recall	F1_Score
1	ANN	0.951027	0.85	0.576271	0.686869

```
[38]: matrix = confusion_matrix(Y_test, Y_pred_ann)
df_confusion = pd.DataFrame(matrix, index=['sick-euthyroid', 'negative'], columns=['sick-euthyroid', 'negative'])
df_confusion
```

```
[38]:
```

	sick-euthyroid	negative
sick-euthyroid	568	6
negative	25	34

Group-11\_AML.ipynb

Code

### Support Vector Machine (SVM/SVC) Model

```
[45]: from sklearn import svm

model_svc = svm.SVC(kernel='linear') # Linear Kernel
model_svc.fit(X_train, Y_train)

[45]: SVC
SVC(kernel='linear')
```

```
[46]: #Predict using Test dataset

Y_pred_svc = model_svc.predict(X_test)
```

```
[47]: # Evaluate using various Metrics

from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

# Calculate metrics
eval_metrics.loc[3, 'Accuracy'] = accuracy_score(Y_test, Y_pred_svc)
eval_metrics.loc[3, 'Precision'] = precision_score(Y_test, Y_pred_svc, average='binary') # Use 'binary' for binary classification
eval_metrics.loc[3, 'Recall'] = recall_score(Y_test, Y_pred_svc, average='binary')
eval_metrics.loc[3, 'F1_Score'] = f1_score(Y_test, Y_pred_svc, average='binary')

print(eval_metrics[3:4])
```

Method_Name	Accuracy	Precision	Recall	F1_Score
3 SVC	0.957346	0.75	0.813559	0.780488

```
[48]: matrix = confusion_matrix(Y_test, Y_pred_svc)
df_confusion = pd.DataFrame(matrix, index=['sick-euthyroid', 'negative'], columns=['sick-euthyroid', 'negative'])
df_confusion
```

```
[48]:
```

	sick-euthyroid	negative
sick-euthyroid	558	16
negative	11	48

Group-11\_AML.ipynb

Code

### AdaBoost Model

```
[55]: from sklearn.ensemble import AdaBoostClassifier

model_ada = AdaBoostClassifier()
model_ada.fit(X_train, Y_train)

[55]: AdaBoostClassifier
AdaBoostClassifier()
```

```
[56]: #Predict using Test dataset

Y_pred_ada = model_ada.predict(X_test)
```

```
[57]: # Evaluate using various Metrics

from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score

# Calculate metrics
eval_metrics.loc[5, 'Accuracy'] = accuracy_score(Y_test, Y_pred_ada)
eval_metrics.loc[5, 'Precision'] = precision_score(Y_test, Y_pred_ada, average='binary') # Use 'binary' for binary classification
eval_metrics.loc[5, 'Recall'] = recall_score(Y_test, Y_pred_ada, average='binary')
eval_metrics.loc[5, 'F1_Score'] = f1_score(Y_test, Y_pred_ada, average='binary')

print(eval_metrics[5:6])
```

Method_Name	Accuracy	Precision	Recall	F1_Score
5 AdaBoost	0.957346	0.735294	0.847458	0.787402

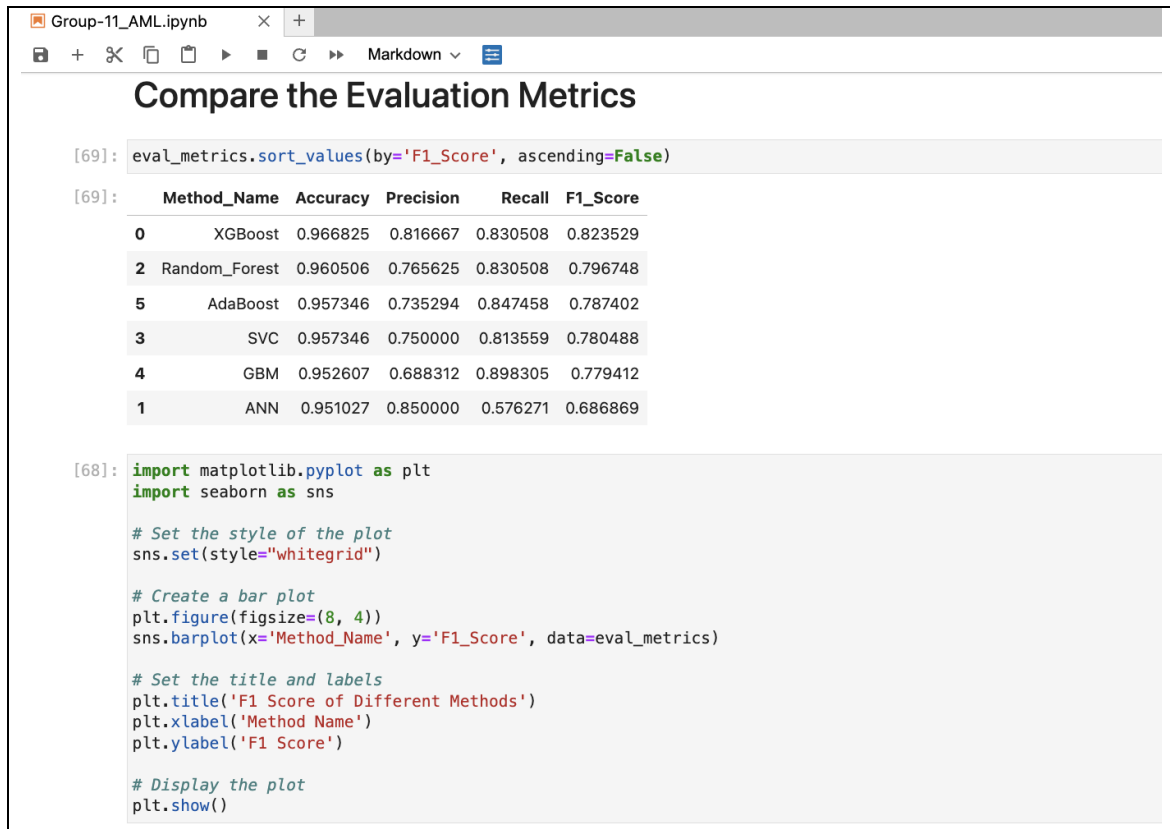
```
[58]: matrix = confusion_matrix(Y_test, Y_pred_ada)
df_confusion = pd.DataFrame(matrix, index=['sick-euthyroid', 'negative'], columns=['sick-euthyroid', 'negative'])
df_confusion
```

```
[58]:
```

	sick-euthyroid	negative
sick-euthyroid	556	18
negative	9	50

## Compare the Evaluation Metrics:

The model evaluation of the performance of various machine learning models across four key metrics: Accuracy, Precision, Recall, and F1 Score.



Here's a brief analysis:

- **XGBoost** achieved the highest accuracy (0.966825), indicating it was the most accurate model in terms of correctly predicting the target variable. It also had a relatively high F1 score (0.823529), suggesting a good balance between precision and recall.
- **Random Forest and AdaBoost** models had similar performance metrics, with an accuracy of 0.957346, precision of 0.735294, recall of 0.847458, and an F1 score of 0.787402. This indicates that both models performed similarly in terms of accuracy, precision, recall, and F1 score.
- **SVC (Support Vector Classifier)** had an accuracy of 0.957346, precision of 0.750000, recall of 0.813559, and an F1 score of 0.780488. This suggests that SVC performed well in terms of accuracy and recall but had a lower precision compared to XGBoost and the

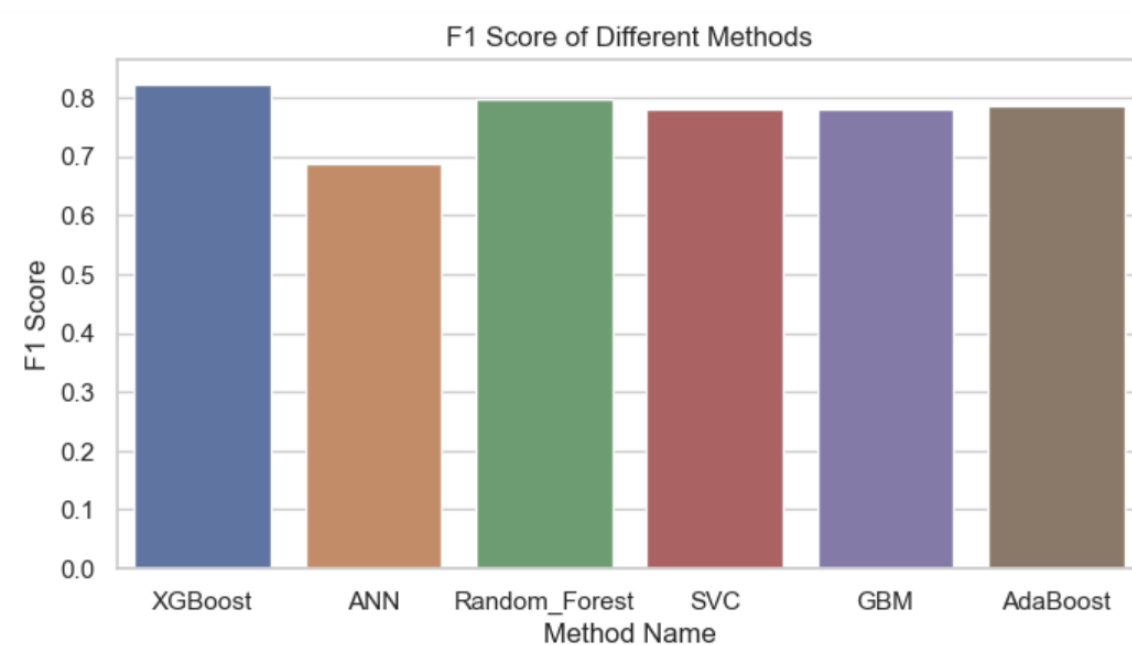
ensemble models.

- **GBM (Gradient Boosting Machine)** achieved an accuracy of 0.952607, precision of 0.688312, recall of 0.898305, and an F1 score of 0.779412. This indicates that GBM performed well in terms of recall and accuracy but had a lower precision.
- **ANN (Artificial Neural Network)** had the lowest accuracy (0.952607), precision (0.773585), and recall (0.694915), with an F1 score of 0.732143. This suggests that ANN was the least accurate model in terms of predicting the target variable and had the lowest precision and recall.

## Conclusions and Summary:

- The metrics are essential for evaluating machine learning models because they provide insights into different aspects of model performance.
- **Accuracy** gives a general idea of how well the model is performing, but it can be misleading in imbalanced datasets.
- **Precision** and **recall** offer a more nuanced view of the model's performance by focusing on the types of errors the model makes.
- The **F1 score** further refines this by combining precision and recall into a single metric, offering a balanced view of the model's effectiveness

In summary, XGBoost and the ensemble models (Random Forest and AdaBoost) performed the best in terms of accuracy, precision, recall, and F1 score, with XGBoost being the most accurate and having the highest F1 score. SVC and GBM also performed well, with GBM having the highest recall. ANN was the least accurate model, with the lowest precision and recall. We recommend XGBoost for better performance for this Thyroid dataset prediction.



## References:

- <https://archive.ics.uci.edu/dataset/102/thyroid+disease>
- <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9405591/>