

# Enhancing IoT Security through Anomaly-based Intrusion Detection Systems

MSc Research Project MSc in Data Analytics

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## Configuration Manual

# Muhammed Musthafa Keloth Poyil x23162112

#### 1 Introduction

This configuration manual outlines the prerequisites, setup, and execution details required to replicate the results of this project. The project utilises various machine learning and deep learning models for IoT intrusion detection. Key stages include data preprocessing, feature engineering, model training, evaluation, and results visualisation. This document covers the software and hardware setup, libraries used, code configuration, and steps to execute the project.

## 2 System Requirements

#### 2.1 Hardware Requirements

• Processor: Ryzen 7 or equivalent

• RAM: 8 GB

• Storage: 256 GB SSD

• GPU: AMD Radeon RX Vega 10 Graphics (or equivalent)

## 2.2 Software Requirements

• Operating System: Windows 10 or above

• Programming Language: Python 3.7 or above

- Integrated Development Environment: Jupyter Notebook (bundled with Anaconda 3)
- Deep Learning Frameworks: PyTorch (1.8), TensorFlow (2.x)

#### 2.3 Libraries Used

The following Python libraries are necessary to execute the project:

• Data Manipulation: pandas, numpy

• Visualisation: seaborn, matplotlib

• Machine Learning: scikit-learn

- Deep Learning: torch, torch\_geometric, tensorflow.keras
- Miscellaneous: warnings, scipy

```
#Import all needed libaries
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
import torch
import torch.nn as nn
import torch.nn functional as F
import to
import torch
from sklearn.svm import SVC
from sklearn.model selection import KFold import tensorflow as tf
from tensorflow.keras.models import Sequential from tensorflow.keras.layers import LSTM, GRU, SimpleRNN, Dense, Dropout
from torch geometric.nn import GCNConv, GINConv from torch geometric.nn import global_mean_pool
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from torch geometric.utils import from_scipy_sparse_matrix
from scipy.sparse import csr_matrix
from torch_geometric_data import Data
from sklearn_model_selection import cross_val_predict
from sklearn.preprocessing import LabelEncoder, StandardScaler
from sklearn.ensemble import GradientBoostingClassifier, RandomForestClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.naive bayes import GaussianNB
from sklearn.model selection import train_test_split
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_score, roc_auc_score, classification_report, confusion_matrix
warnings.filterwarnings('ignore')
```

Figure 1: List of Libraries used and Imported into Python Notebook

### 3 Data Collection

The dataset utilised is sourced from UCI ML Repository and includes samples for various IoT attacks such as Mirai and Gafgyt. These datasets are preprocessed and stored as CSV files:

#### • Files:

```
5.gafgyt.combo.csv
5.gafgyt.junk.csv
5.gafgyt.scan.csv
5.gafgyt.tcp.csv
5.gafgyt.udp.csv
5.mirai.ack.csv
5.mirai.scan.csv
5.mirai.syn.csv
5.mirai.udp.csv
5.mirai.udpplain.csv
```

#### Steps:

1. Load the datasets into pandas DataFrames.

```
# Load the CSV files from the specified location
benign = pd.read_csv(r'5.benign.csv')
gafgyt_combo = pd.read_csv(r'5.gafgyt.combo.csv')
gafgyt_junk = pd.read_csv(r'5.gafgyt.junk.csv')
gafgyt_scan = pd.read_csv(r'5.gafgyt.scan.csv')
gafgyt_tcp = pd.read_csv(r'5.gafgyt.tcp.csv')
gafgyt_udp = pd.read_csv(r'5.gafgyt.udp.csv')
mirai_ack = pd.read_csv(r'5.mirai.ack.csv')
mirai_scan = pd.read_csv(r'5.mirai.scan.csv')
mirai_syn = pd.read_csv(r'5.mirai.syn.csv')
mirai_udp = pd.read_csv(r'5.mirai.udp.csv')
mirai_udp_plain = pd.read_csv(r'5.mirai.udpplain.csv')
```

Figure 2: Reading the Dataset Files

2. Downsample datasets to address class imbalance.

```
# Downsample each dataset based on given fractions
benign_sampled = benign.sample(frac=0.25, replace=False)
gafgyt_combo_sampled = gafgyt_combo.sample(frac=0.25, replace=False)
gafgyt_junk_sampled = gafgyt_junk.sample(frac=0.5, replace=False)
gafgyt_scan_sampled = gafgyt_scan.sample(frac=0.5, replace=False)
gafgyt_tcp_sampled = gafgyt_tcp.sample(frac=0.15, replace=False)
gafgyt_udp_sampled = gafgyt_udp.sample(frac=0.15, replace=False)
mirai_ack_sampled = mirai_ack.sample(frac=0.25, replace=False)
mirai_scan_sampled = mirai_scan.sample(frac=0.15, replace=False)
mirai_syn_sampled = mirai_syn.sample(frac=0.25, replace=False)
mirai_udp_sampled = mirai_udp.sample(frac=0.1, replace=False)
mirai_udp_plain_sampled = mirai_udp_plain.sample(frac=0.27, replace=False)
```

Figure 3: Labelling the Data with respect to Attack Type

3. Merge and encode labels into a single DataFrame.

```
# Assign attack types to each dataset
benign_sampled['type'] = 'benign'
mirai_udp_sampled['type'] = 'mirai_udp'
gafgyt_combo_sampled['type'] = 'gafgyt_combo'
gafgyt_junk_sampled['type'] = 'gafgyt_junk'
gafgyt_scan_sampled['type'] = 'gafgyt_scan'
gafgyt_tcp_sampled['type'] = 'gafgyt_tcp'
gafgyt_udp_sampled['type'] = 'gafgyt_udp'
mirai_ack_sampled['type'] = 'mirai_ack'
mirai_scan_sampled['type'] = 'mirai_scan'
mirai_syn_sampled['type'] = 'mirai_syn'
mirai_udp_plain_sampled['type'] = 'mirai_udpplain'
```

Figure 4: Labelling the Data with respect to Attack Type

Figure 5: Concatenating the Dataset

### 4 Data Visualisation

Distribution plots, bar plots, pair plots, and heatmaps are generated to analyse the dataset.



Figure 6: Plotting Histogram Plots for Four Different Features for Exploration

```
#Barplot for type and MI_dir_L5_weight
sns.barplot(x='type', y='MI_dir_L5_weight', data=df_N_BaIoT)
plt.title('Box Plot of MI_dir_L5_weight by Type')
plt.xticks(rotation=90)
plt.show()
```

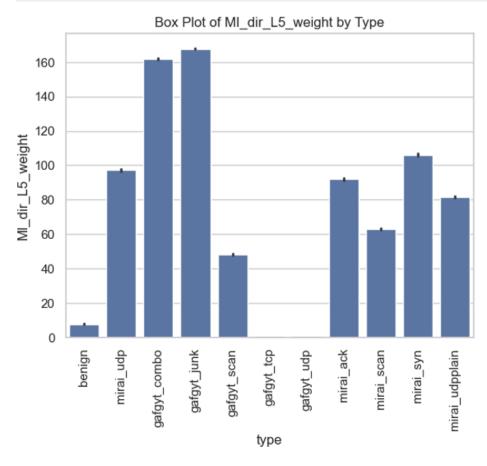


Figure 7: Boxplot for MI\_Dir\_L5\_weight

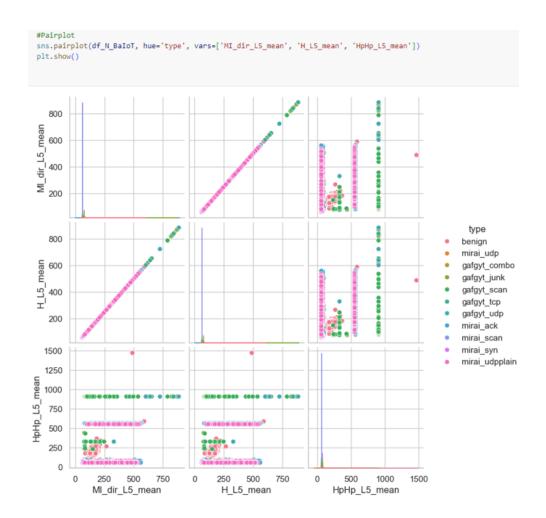


Figure 8: Pairplot for Some of the Features

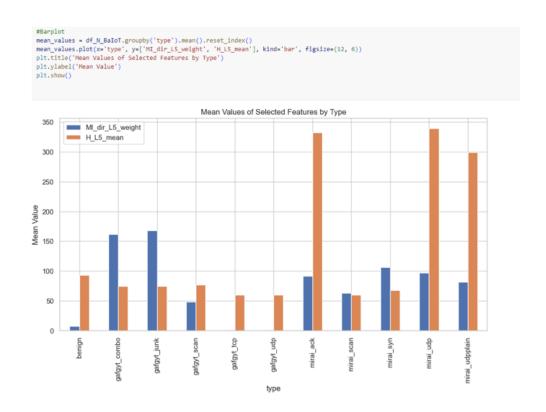


Figure 9: Barplot for MI\_dir\_L5\_weight and H\_L5\_mean w.r.t. Attack Type

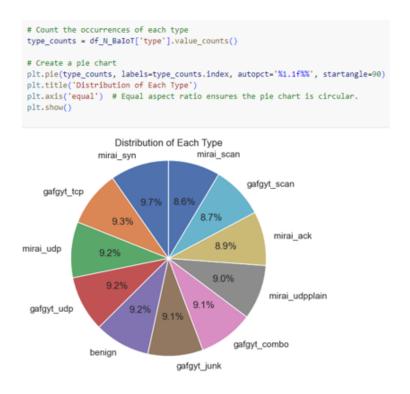


Figure 10: Pie Chart Showing the Distribution of Labels in the Dataset

## 5 Feature Engineering

Correlation matrix for all the features in the dataset are plotted for multicollinearity check. This is done by choosing subsets of 25 features at a time. Correlation matrix for the first 25 features is shown in Figure 11 below.

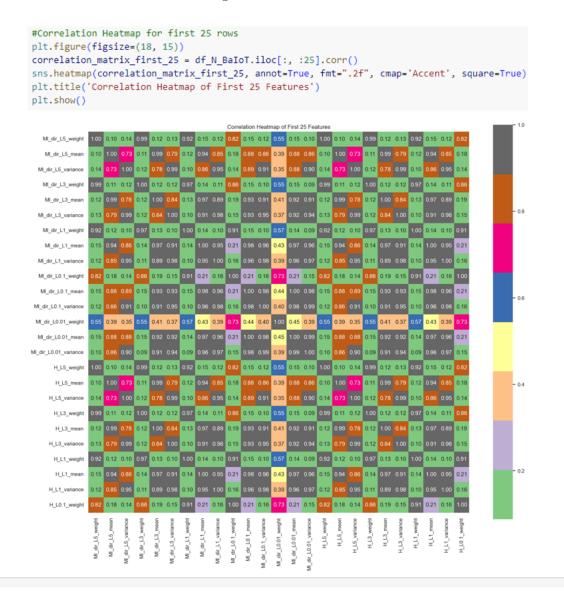


Figure 11: Correlation Matrix for First 25 Features

Next, the multicollinear features are dropped from the dataset. This is done by thresholding the Correlation Matrix by 0.8 value. Features with correlation coefficient above 0.8 are dropped. The code to implement this is shown in Figure 12.

```
# numerical columns from the dataset
numerical_columns = df_N_BaIoT.select_dtypes(include=[np.number])

# Compute the correlation matrix for numerical columns
correlation_matrix = numerical_columns.corr()

# Identify highly correlated features
least_correlated_features = correlation_matrix[correlation_matrix < 0.8]

# Print all highly correlated numerical columns
print("Least correlated numerical features (absolute correlation < 0.8):\n", least_correlated_features.columns.tolist())</pre>
```

Figure 12: Thresholding the Correlation Coefficients

As the type column representing the labels of the data is in categorical format, it needs to be converted to numerical form for modelling using Neural Network Architectures. Figure 13 below shows the implementation of LabelEncoder() from sklearn on the type column.

```
# Label Encoder
label_encoder = LabelEncoder()
df_N_BaIoT['type'] = label_encoder.fit_transform(df_N_BaIoT['type'])
```

Figure 13: Label Encoding of the Type Column

Next, the dependent and independent variables are separated for modelling. The features are separated into the X dataframe whereas the dependent variable is stored in y. Its implementation is shown in Figure 14.

```
#Sepearte dendent and independent variables
X = df_N_BaIoT[least_correlated_features.columns].values
y = df_N_BaIoT['type'].values
```

Figure 14: Separating the Dependent and Independent Columns

The dataset is then split into training and testing sets using the train\_test\_split function from sklearn's model\_selection module.

```
# Split the dataset
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)
```

Figure 15: Dividing Data into Training and Testing Sets

The data is then normalized using the StandardScaler() from sklearn. It is first fit on the training data and then used to transform it.

```
# Standardize the data
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

Figure 16: Normalizing the Data Using Standardization

PCA is then applied to get 10 components for feature reduction.

```
#PCA
pca = PCA(n_components=10)
X_train_pca = pca.fit_transform(X_train_scaled)
X_test_pca = pca.transform(X_test_scaled)
```

Figure 17: Application of PCA for Feature Reduction

```
subset_size = int(len(X_train_pca) * 0.7)
X_train_subset = X_train_pca[:subset_size]
y_train_subset = y_train[:subset_size]
```

Figure 18: Subsets of PCA Applied Data are Created for Validation Purposes

## 6 Modelling

A total of 10 models have been applied and tested on the dataset. These models, along with the libraries used, are listed below:

- 1. Gradient Boosting Machine (GBM) Sklearn
- 2. KNN Model (KNN) Sklearn
- 3. Gaussian Naïve Bayes (GNB) Sklearn
- 4. Random Forest Model (RF) Sklearn
- 5. Support Vector Machine Model (SVM) Sklearn
- 6. LSTM Model TensorFlow
- 7. RNN Model TensorFlow
- 8. GRU Model TensorFlow
- 9. Graph Convolution Network (GCN) Torch Geometric
- 10. Graph Isomorphism Network (GIN) Torch Geometric

The implementations of the different models with cross-validation are given below.

Figure 19: Implementation of the GBM Model

```
# KNN

kmn_model = KNeighborsClassifier()

#Perform 10-fold Cross-Validation on the subset
y_pred_kmn_cv = cross_val_predict(knn_model, X_train_subset, y_train_subset, cv=10)
y_pred_proba_knn_cv = cross_val_predict(knn_model, X_train_subset, y_train_subset, cv=10)
# Calculate Cross-Validation Metrics
cv_accuracy_knn = accuracy_score(y_train_subset, y_pred_knn_cv)
cv_precision_knn = precision_score(y_train_subset, y_pred_knn_cv, average='weighted')
cv_recall_knn = recall_score(y_train_subset, y_pred_knn_cv, average='weighted')
cv_ret_klnn = f_1_score(y_train_subset, y_pred_knn_cv, average='weighted')
cv_roc_auc_knn = roc_auc_score(y_train_subset, y_pred_proba_knn_cv, multi_class='ovr')

# Print Cross-Validation Metrics
print("KNN Cross-Validation Performance on Subset:")
print("Cross-Validated Accuracy:", cv_accuracy_knn)
print("Cross-Validated Accuracy:", cv_accuracy_knn)
print("Cross-Validated Faccall:", cv_precision_knn)
# Classification Report
print("Nclassification Report
print("Nclassification Report for Cross-Validated Predictions:\n", classification_report(y_train_subset, y_pred_knn_cv)
# Confusion Matrix
conf matrix_cv_knn = confusion_matrix(y_train_subset, y_pred_knn_cv)
print("Nconfusion_Matrix for Cross-Validated Predictions:\n", conf_matrix_cv_knn)
```

Figure 20: Implementation of the KNN Model

```
# Naive Bayes
gpb_model = GaussianNB()

# Perform 18-fold Cross-Validation on the subset
y_pred_gpb_cv = cross_val_predict(gpb_model, X_train_subset, y_train_subset, cv=10)
y_pred_grob_gpb_cv = cross_val_predict(gpb_model, X_train_subset, y_train_subset, cv=10)
y_pred_grob_gpb_cv = cross_val_predict(gpb_model, X_train_subset, y_train_subset, cv=10)
y_pred_grob_gpb_cv = cross_val_predict(gpb_model, X_train_subset, y_train_subset, cv=10)
# Calculate cross-validation Metrics
cv_accuracy_gpb = accuracy_score(y_train_subset, y_pred_gpb_cv)
cv_precision_gpb = precision_score(y_train_subset, y_pred_gpb_cv, average='weighted')
cv_fl_gpb = fi_score(y_train_subset, y_pred_gpb_cv, multi_class='ovr')
# Print ("cross-Validation Metrics
print("Cross-Validated Accuracy:", cv_accuracy_gpb)
print("Cross-Validated Recall:", cv_rcall_gpb)
print("Cross-Validated Recall:", cv_rcall_gpb)
print("Cross-Validated Recall:", cv_pc_auc_gpb)
# Classification Report
print("Validated Predictions:\n', classification_report(y_train_subset, y_pred_gpb_cv)
# Confusion Matrix
conf_gatrix_cv_gpb = confusion_matrix(y_train_subset, y_pred_gpb_cv)
print("Cross-Validated Predictions:\n', conf_gstrix_cv_gpb)
```

Figure 21: Implementation of the GNB Model

```
# Random Forest

# Random

# Random Forest

# Random

# Ran
```

Figure 22: Implementation of the RF Model

```
# SVM
swm_model = SVC(probability=True)

# Perform 10-fold Cross-Validation on the subset
y_pred_svm_cv = cross_val_predict(svm_model, X_train_subset, y_train_subset, cv=10)
y_pred_proba_svm_cv = cross_val_predict(svm_model, X_train_subset, y_train_subset, cv=10, method='predict_proba')

# Calculate Cross-Validation Metrics
cv_accuracy_svm = accuracy_score(y_train_subset, y_pred_svm_cv)
cv_precision_svm = precision_score(y_train_subset, y_pred_svm_cv, average='weighted')
cv_recall_svm = recall_score(y_train_subset, y_pred_svm_cv, average='weighted')
cv_recall_svm = roc_auc_score(y_train_subset, y_pred_svm_cv, average='weighted')
cv_roc_auc_svm = roc_auc_score(y_train_subset, y_pred_proba_svm_cv, multi_class='ovr')

# Print Cross-Validation Metrics
print("SVM :")
print("Cross-Validated Accuracy:", cv_accuracy_svm)
print("Cross-Validated Accuracy:", cv_accuracy_svm)
print("Cross-Validated Recall:", cv_precall_svm)
print("Cross-Validated Recall:", cv_precall_svm)
print("Cross-Validated Recall:", cv_precall_svm)
print("Cross-Validated Roc AUC:", cv_fl_svm)
print("Cross-Validated Roc AUC:", cv_fl_svm)
print("Cross-Validated Roc AUC:", cv_fl_svm)
print("Cross-Validated Roc AUC:", cv_fl_svm)
# Classification Report
print("\nCassification Report:\n", classification_report(y_train_subset, y_pred_svm_cv, target_names=class_names))

# Confusion Matrix
conf_matrix_cv_svm = confusion_matrix(y_train_subset, y_pred_svm_cv)
print("\nConfusion Matrix :\n", conf_matrix_cv_svm)
```

Figure 23: Implementation of the SVM Model

```
def create_lstm_model(input_shape):
    model = Sequential()
    model.add(LSTM(64, return_sequences=False, input_shape=input_shape))
    model.add(LSTM(64, return_sequences=False, input_shape=input_shape))
    model.add(Dense(11, activation='softmax'))
    model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])
    return model
   # 10-fold Cross-Validation
   kf = KFold(n_splits=10, shuffle=True, random_state=42)
   # Lists to store metrics for each fold
   all_recall = []
   all f1 = []
   all_confusion_matrices = np.zeros((11, 11))
   # Accumulate true and predicted labels
  true_labels = []
pred_labels = []
for fold, (train_index, val_index) in enumerate(kf.split(X_train_subset, y_train_subset), 1):
      print(f"\n--- Fold {fold} ---")
      # Split the data into training and validation sets for the current fold
X_train_fold, X_val_fold = X_train_subset[train_index], X_train_subset[val_index]
y_train_fold, y_val_fold = y_train_subset[train_index], y_train_subset[val_index]
       lstm_model = create_lstm_model(input_shape=(X_train_fold.shape[1], X_train_fold.shape[2]))
       lstm\_model.fit(X\_train\_fold, y\_train\_fold, epochs=100, batch\_size=32, verbose=0)
      # Predict on validation data
y_pred_val = lstm_model.predict(X_val_fold)
y_pred_classes = np.argmax(y_pred_val, axis=1)
      # Evaluate the model for this fold
accuracy = accuracy_score(y_val_fold, y_pred_classes)
precision = precision_score(y_val_fold, y_pred_classes, average='weighted')
recall = recall_score(y_val_fold, y_pred_classes, average='weighted')
f1 = fi_score(y_val_fold, y_pred_classes, average='weighted')
       conf_matrix = confusion_matrix(y_val_fold, y_pred_classes, labels=np.arange(11))
all_confusion_matrices += conf_matrix # Accumulate confusion matrices across folds
       # Collect true and predicted labels for the overall classification report
       true_labels.extend(y_val_fold)
       pred_labels.extend(y_pred_classes)
       all_accuracy.append(accuracy)
all_precision.append(precision)
all_recall.append(recall)
       all_f1.append(f1)
# average metrics across all folds
average_accuracy = np.mean(all_accuracy)
average_precision = np.mean(all_precision)
average_recall = np.mean(all_recall)
average_f1 = np.mean(all_f1)
     # Generate overall classification report and confusion matrix
overall_classification_report = classification_report(true_labels, pred_labels,target_names=class_names)
average_confusion_matrix = all_confusion_matrices / 10 # Average confusion matrix across folds
    # Print the average metrics, classification report, and confusion matrix print("\n--- Average Metrics across all folds ---") print(f"Average Accuracy: {average_accuracy: .4f;"} print(f"Average Precision: {average_precision: .4f;") print(f"Average Recall: (average_recall: .4f;") print(f"Average Fi Score: {average_f1:.4f}")
     # Print overall classification report
print("\n--- Overall Classification Report ---")
print(overall_classification_report)
print("\nConfusion Matrix for Cross-Validated Predictions:\n", average_confusion_matrix)
```

Figure 24: Implementation and Evaluation of the LSTM Model

13

```
# RNN model function

def create_rnn_model(input_shape):

model = Sequential()

model.add(SimpleRNN(64, return_sequences=false, input_shape=input_shape))

model.add(Dense(11, activation='softmax'))

model.comple(potimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])

return model
                         # 10-fold Cross-Validation
kf = KFold(n_splits=10, shuffle=True, random_state=42)
                        # Lists to store metrics for each fold
all_accuracy = []
all_precision = []
all_reall = []
all_fi = []
all_cofusion_matrices = np.zeros((11, 11))
                         # Accumulate true and predicted labels
true_labels = []
pred_labels = []
                              for fold, (train_index, val_index) in enumerate(kf.split(X_train_subset, y_train_subset), 1):
    print(f"\n--- Fold (fold) ---")
                                      # Split the data into training and validation sets

X_train_fold, X_val_fold = X_train_subset[train_index], X_train_subset[val_index]
y_train_fold, y_val_fold - y_train_subset[train_index], y_train_subset[val_index]
                                        # Define and compile the RNN model
rnn_model = create_rnn_model(input_shape=(X_train_fold.shape[1], X_train_fold.shape[2]))
                                       # Train the model for 100 epochs rnn_model.fit(X_train_fold, y_train_fold, epochs=100, batch_size=32, verbose=0)
                                       # Predict on validation data
y_pred_val = rnn_model.predict(X_val_fold)
y_pred_classes = np.argmax(y_pred_val, axis=1)
                                      # Evaluate the model for this fold
accuracy = accuracy_score(y_val_fold, y_pred_classes)
precision = precision_score(y_val_fold, y_pred_classes, average='weighted')
recall = recall_score(y_val_fold, y_pred_classes, average='weighted')
f1 = f1_score(y_val_fold, y_pred_classes, average='weighted')
                                       # Generate confusion matrix for this fold and accumulate conf_matrix = confusion_matrix(y_val_fold, y_pred_classes, labels=np.arange(11)) all_confusion_matrices += conf_matrix
                                        # Collect true and predicted labels for the overall classification report true_labels.extend(y_val_fold) pred_labels.extend(y_pred_classes)
                                      # Store metrics
all_accuracy.append(accuracy)
all_precision.append(precisio
all_recall.append(recall)
all_f1.append(f1)
                              # Calculate average metrics across all folds
average_accuracy_rnn = np.mean(all_accuracy)
average_precision_rnn = np.mean(all_precision)
average_recil_rnn = np.mean(all_precision)
average_fci_rnn = np.mean(all_fci)
# Generate overall classification report and confusion matrix overall_classification_report_rnn = classification_report(true_labels, pred_labels,target_names=class_names) average_confusion_matrix_rnn = all_confusion_matrices / 10
# Print the average metrics, classification report, and confusion matrix print("\n-- Average Metrics across all folds ---") print(f"Average Accuracy: (average_accuracy_rnn:.4f)") print(f"Average Precision: (average_precision_rnn:.4f)") print(f"Average Recall: (average_recall_rnn:.4f)") print(f"Average Fi Score: (average_f1_rnn:.4f)")
# Print overall classification report
print("\n--- Overall classification Report ---")
print(overall_classification_report_rnn)
print("\ncofrusion Matrix for Cross-Validated Predictions:\n", average_confusion_matrix_rnn)
```

Figure 25: Implementation and Evaluation of the RNN Model

```
# GBU model | def create_gru_model(input_shape):
model_sequential()
model_sequential()
model_sequential()
model_add(punse(ii, activation='softmas'))
model.complie(potisizer-adam', loss-'sparse_categorical_crossentropy', metrics-('accuracy'))
model.complie(potisizer-adam', loss-'sparse_categorical_crossentropy', metrics-('accuracy'))
return model
# 10-fold cross-validation
# it its to store metrics for each fold
all_accuracy = []
all_precision = []
all_cri = []
for fold, (train_index, val_index) in enumerate(kf.split(X_train_subset, y_train_subset), 1):
print(f'nn--rold(fold)---")
# Split the data into training and validation sets for the current fold
X_train_fold, y_val_fold = y_train_subset[train_index], y_train_subset[val_index]
y_train_fold, y_val_fold = y_train_subset[train_index], y_train_subset[val_index]
# Define and compile the GBU model
gru_model = create_gru_model(input_shape+(X_train_fold.shape[a]), X_train_fold.shape[a]))
# Train the model for 100 epochs
gru_model.fit(X_train_fold, y_train_fold, epochs-i00, batch_size-i2, verbose-e)
# Predict on validation data
y_pred_classes = np_argmax(y_pred_val_atis)
# Evaluate the model for this fold
accuracy = accuracy_score(y_val_fold, y_pred_classes)
precision = precision_score(y_val_fold, y_pred_classes)
precision = precision_score(y_val_fold, y_pred_classes, average='weighted')
# Generate confusion matrix for this fold and accumalate
conf_matrix = confusion_matrix(s_val_fold, y_pred_classes, labels=np_arange(ii))
all_confusion_matrices += conf_matrix
# Collect true and predicted labels
true_labels.extend(y_yal_fold)
pred_labels.extend(y_nal_fold)
pred_labels.extend(y_nal_fold)
pred_labels.extend(y_nal_fold)
pred_labels.extend(y_nal_fold)
pred_labels.extend(y_nal_fold)
# Calculate average metrics across all folds
# Print the average me
```

Figure 26: Implementation and Evaluation of the GRU Model

```
# Define a threshold
threshold = 0.5

edges = np.argwhere(np.abs(correlation_matrix) > threshold)
edges = edges[edges[:, 0] != edges[:, 1]]
edge_index = torch.tensor(edges.T, dtype=torch.long)
```

Figure 27: Generating Graph Data from the PCA Components

```
# Initialize the model
          class GCN(torch.nn.Module):
                       def __init__(self, num_features, num_classes):
                                super(GCN, self).__init__()
self.conv1 = GCNConv(num_features, 16)
                                    self.conv2 = GCNConv(16, num_classes)
                       def forward(self, data):
                                  x, edge_index = data.x, data.edge_index
                                   x = self.conv1(x, edge_index)
                                  x = F.relu(x)
                                   x = self.conv2(x, edge_index)
                            return F.log_softmax(x, dim=1)
         # Prepare your data tensors
x_tensor = torch.tensor(X_train_pca, dtype=torch.float)
y_tensor = torch.tensor(y_train, dtype=torch.long)
        **Cross-validation setup

kf = KFold(n_splits=5, shuffle=True, random_state=42) # 5-fold cross-validation
accuracies1, precisions1, recalls1, f1_scores1, roc_aucs1 = [], [], [], [],
all_preds = [] # To store all predictions for confusion matrix
all_true_labels = [] # To store all true labels for confusion matrix
# Cross-validation loop
for train_idx, val_idx in kf.split(x_tensor):
    # Split the data into training and validation
    x_train_cv, x_val_cv = x_tensor[train_idx], x_tensor[val_idx]
    y_train_cv, y_val_cv = y_tensor[train_idx], y_tensor[val_idx]
          # Create data objects for training and validation
train_data = Data(x=x_train_cv, edge_index=edge_index)
val_data = Data(x=x_val_cv, edge_index=edge_index)
          # Initialize the model and optimizer
          = anazazize tne model and optinizer
model = GCN(num features=X_train_pca.shape[1], num_classes=len(set(y_train)))
optinizer = torch.optin.Adam(model.parameters(), lr=0.01)
criterion = torch.nn.NLLLloss()
         # Training the model
model.train()
for epoch in range(200):
    optimizer.zero_grad()
    output = model(train_data)
    loss = criterion(output, y_train_cv)
    loss.backward()
    optimizer.step()
          # Validation the model
          # Get probabilities for ROC AUC
val_probs = F.softmax(val_output, dim=1)
val_preds = val_output.argmax(dim=1).numpy()
         # Evaluate the model
accuracy = accuracy_score(y_val_cv, val_preds)
precision = precision_score(y_val_cv, val_preds, average='weighted')
recall = recall_score(y_val_cv, val_preds, average='weighted')
f1 = f1_score(y_val_cv, val_preds, average='weighted')
          # Calculate ROC AUC
roc_auc = roc_auc_score(y_val_cv, val_probs.numpy(), multi_class='ovr', average='weighted')
         # Append results for cross-validation accuracies1.append(accuracy) precisions1.append(precision) recalls1.append(recall) fl_scores1.append(fl) roc_aucs1.append(foc_auc)
          # Store predictions and true labels for confusion matrix all preds.extend(val_preds) all_true_labels.extend(y_val_cv.numpy())
  # Calculate the average performance across all folds print(f*Average Accuracy: (pp.mean(accuracles):.4f)") print(f*Average Precision: (pp.mean(pecialos):.4f)") print(f*Average Recall: (pp.mean(*ecalls):.4f)") print(f*Average Fis Gene: (pp.mean(fis_Gones):.4f)") print(f*Average ROC-AUC: (pp.mean(foc_aucs):.4f)") print(f*Average ROC-AUC: (pp.mean(foc_aucs):.4f)")
  # Classification report and confusion matrix for all folds
print("\nClassification Report:\n", classification_report(all_true_labels, all_preds))
  # Confusion Matrix
cm = confusion_matrix(all_true_labels, all_preds)
print(cm)
```

Figure 28: Implementation and Evaluation of the GCN Model

16

```
# GIN model class
           class GIN(torch.nn.Module):
                def __init__(self, num_features, num_classes):
    super(GIN, self).__init__()
    self.conv1 = GINConv(torch.nn.Sequential()
                               torch.nn.Linear(num_features, 16),
                               torch.nn.ReLU(),
torch.nn.Linear(16, 16)
                        self.conv2 = GINConv(torch.nn.Sequential(
                                torch.nn.Linear(16, 16),
torch.nn.ReLU(),
                                torch.nn.Linear(16, num_classes)
                 def forward(self, data):
                        x, edge_index = data.x, data.edge_index
                         x = self.conv1(x, edge_index)
                         x = self.conv2(x, edge\_index)
                        return F.log_softmax(x, dim=1)
          # Prepare your data tensors
          x_tensor = torch.tensor(X_train_pca, dtype=torch.float)
y_tensor = torch.tensor(y_train, dtype=torch.long)
           # Cross-validation setup
          kf = KFold(n_splits=5, shuffle=True, random_state=42) # 5-fold cross-validation
accuracies, precisions, recalls, fi_scores, roc_aucs = [], [], [], []
all_preds = []
          all_true_labels = []
# Cross-validation loop
# Cross-validation loop
for train_idx, val_idx in kf.split(x_tensor):
# Split the data into training and validation
x_train_cv, x_val_cv = x_tensor[train_idx], x_tensor[val_idx]
y_train_cv, y_val_cv = y_tensor[train_idx], y_tensor[val_idx]
      # Create data objects for training and validation train_data = Data(x=x_train_cv, edge_index=edge_index) val_data = Data(x=x_val_cv, edge_index=edge_index)
      # Initialize the model and optimizer
model = GIN(num_features=X_train_pca.shape[1], num_classes=len(set(y_train)))
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
criterion = torch.nn.NLLLoss()
      # Training the model
      # Training the mode
model.train()
for epoch in range(200):
    optimizer.zero_grad()
    output = model(train_data)
    loss = criterion(output, y_train_cv)
      # Validation the model
            val output - model(val data)
      # Get probabilities for ROC AUC
val_probs = F.softmax(val_output, dim=1)
val_preds = val_output.argmax(dim=1).numpy()
      # tvaluate the model
accuracy = accuracy_score(y_val_cv, val_preds)
precision = precision_score(y_val_cv, val_preds, average='weighted')
recall = recall_score(y_val_cv, val_preds, average='weighted')
f1 = f1_score(y_val_cv, val_preds, average='weighted')
      # Calculate ROC AUC
       roc_auc = roc_auc_score(y_val_cv, val_probs.numpy(), multi_class='ovr', average='weighted')
       # Append results for cross-validation
      accuracies.append(accuracy)
precisions.append(precision)
recalls.append(recall)
f1_scores.append(f1)
            # Store predictions and true labels for confusion matrix
            all preds.extend(val preds)
            all_true_labels.extend(y_val_cv.numpy())
     # Calculate the average performance across all folds
    print(f"Average Accuracy: (np.mean(accuracies):.4f)")
print(f"Average Precision: (np.mean(precisions):.4f)")
print(f"Average Precision: (np.mean(precisions):.4f)")
print(f"Average Fi Score: (np.mean(fi_scores):.4f)")
print(f"Average ROC-AUC: (np.mean(roc_aucs):.4f)")
     # Classification report and confusion matrix for all folds
     print("\nClassification Report:\n", classification_report(all_true_labels, all_preds))
     # Confusion Matrix
    cm = confusion_matrix(all_true_labels, all_preds)
     print(cm)
```

Figure 29: Implementation and Evaluation of the GIN Model

```
model_results = []

# Appand model metrics
model_results.append('Model': 'GCM', 'Accuracy': np.mean(accuracies), 'Precision': np.mean(precisions1), 'Bacall': np.mean(recalls1), 'Fi Score': np.mean(fl_scores1))
model_results.append('Model': 'GCM', 'Accuracy': np.mean(accuracies), 'Mrecision': np.mean(precisions1), 'Becall': np.mean(recalls1), 'Fi Score': np.mean(fl_scores1))
model_results.append('Model': 'GLM', 'Accuracy': np.mean(accuracies), 'Mrecision': np.mean(precision), 'Becall': np.mean(recall), 'Fi Score': np.mean(fl))
model_results.append('Model': 'KLM', 'Accuracy': np.mean(accuracies), 'Mrecision': np.mean(np.mp, 'Recall': np.meall', np.meall'
```

Figure 30: Combining the Model Results

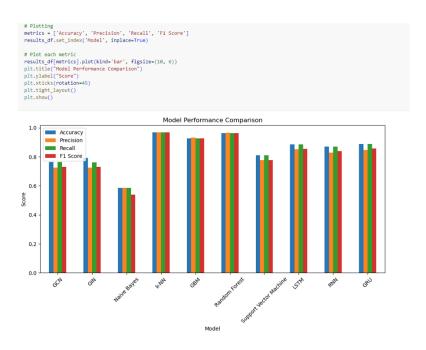


Figure 31: Plotting the Results Graphically

Similar to the above implementation, the models are used without cross-validation. The implementation of the models is exactly the same.

## 7 Execution Steps

#### 1. Setup Environment:

- Install required libraries using pip install or Anaconda.
- Launch Jupyter Notebook.

#### 2. Run Code:

- Execute the provided .ipynb file in sequence.
- Configure file paths for datasets.

#### 3. View Results:

• Outputs and visualisations will be generated within the notebook.

## 8 References

- Guide (no date). https://www.tensorflow.org/guide.
- PyG Documentation pytorch\_geometric documentation (no date). https://pytorch-geometric.readthedocs.io/en/latest/.
- scikit-learn: machine learning in Python scikit-learn 0.16.1 documentation (no date). https://scikit-learn.org/.
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