ImagoAI_Task

March 14, 2025

1 Internship Application Task

- Created by : Pritha Choudhury

AIM : To process hyperspectral imaging data, perform dimensionality reduction, and develop a machine learning model to predict mycotoxin levels (e.g., DON concentration) in corn samples.

We import essential libraries for data processing, visualization, machine learning, and dimensionality reduction.

[1]:
```
# Importing Libraries

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split,GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE
from sklearn.neural_network import MLPRegressor
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score
```

[3]:
```
df=pd.read_csv('/content/TASK-ML-INTERN.csv')
```

[4]:
```
df.head()
```

[4]:

	hsi_id	0	1	2	3	4	5	\
0	imagoai_corn_0	0.416181	0.396844	0.408985	0.372865	0.385293	0.365390	
1	imagoai_corn_1	0.415797	0.402956	0.402564	0.396014	0.397192	0.389634	
2	imagoai_corn_2	0.389023	0.371206	0.373098	0.373872	0.361056	0.349709	
3	imagoai_corn_3	0.468837	0.473255	0.462949	0.459335	0.461672	0.459824	
4	imagoai_corn_4	0.483352	0.487274	0.469153	0.487648	0.464026	0.451152	

	6	7	8	…	439	440	441	442	\
0	0.355226	0.343350	0.344837	…	0.710280	0.717482	0.715078	0.705379	
1	0.375671	0.363689	0.373883	…	0.684011	0.697271	0.701995	0.696077	
2	0.333882	0.330841	0.328925	…	0.683054	0.669286	0.663179	0.676165	
3	0.458194	0.427737	0.415360	…	0.742782	0.730801	0.736787	0.730044	

```
4  0.458229  0.440782  0.426193  …  0.770227  0.773013  0.761431  0.763488

        443       444       445       446       447  vomitoxin_ppb
0  0.696691  0.692793  0.711369  0.697679  0.704520         1100.0
1  0.701012  0.677418  0.696921  0.696544  0.689054         1000.0
2  0.676591  0.655951  0.658945  0.670989  0.665176         1300.0
3  0.751437  0.738497  0.742446  0.754657  0.733474         1300.0
4  0.762473  0.744012  0.775486  0.760431  0.751988          220.0

[5 rows x 450 columns]
```

[5]:
```
# Finding out null values

df.isnull().sum()
```

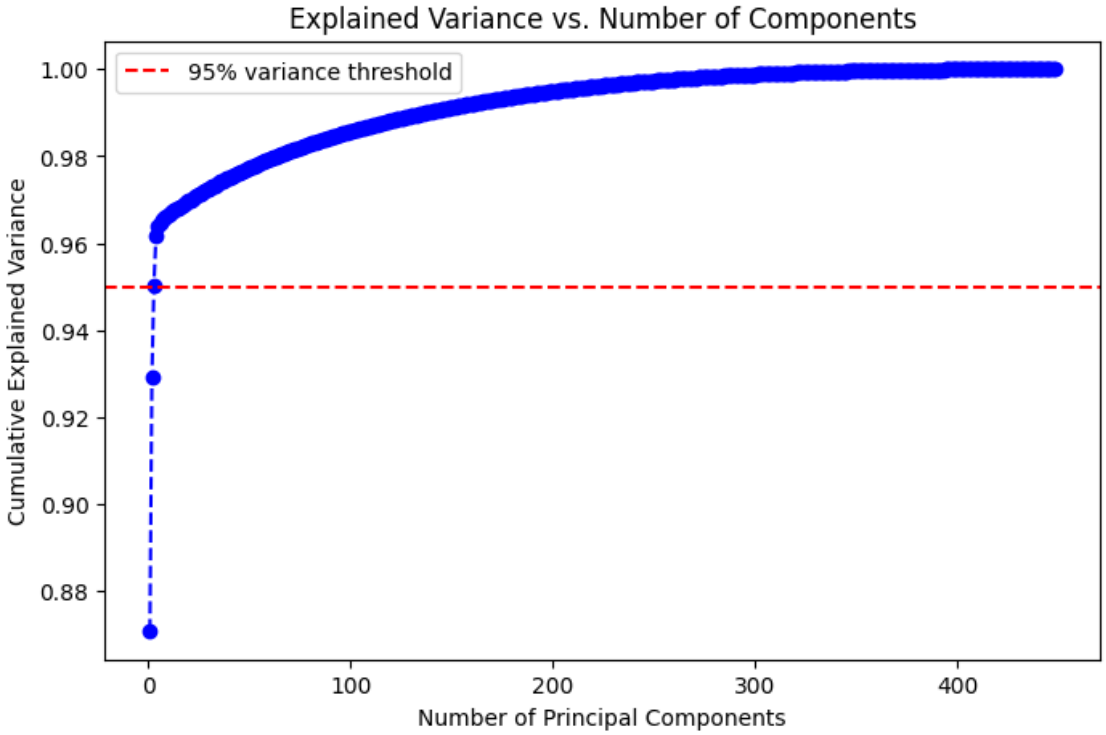
[5]:
```
hsi_id           0
0                0
1                0
2                0
3                0
                ..
444              0
445              0
446              0
447              0
vomitoxin_ppb    0
Length: 450, dtype: int64
```

- We are dropping the first column (`hsi_id`) since it is a string identifier.
- We are separating the dataset into **features (X)** and **target variable (y)** (DON levels).
- We are applying **StandardScaler** to normalize the spectral data.

[6]:
```
# Dropping the first column
df_numeric = df.iloc[:, 1:]

# Separate features and target variable
X = df_numeric.iloc[:, :-1].values
y = df_numeric.iloc[:, -1].values

# Normalising spectral data
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)
```

- We are using **PCA (Principal Component Analysis)** to retain 95% variance.
- We are applying **t-SNE (t-Distributed Stochastic Neighbor Embedding)** for visualization.

[7]:
```
# Applying PCA without specifying components (to analyze variance)
pca = PCA()
X_pca = pca.fit_transform(X_scaled)

# Compute cumulative explained variance
cumulative_variance = np.cumsum(pca.explained_variance_ratio_)

# Plot the explained variance
plt.figure(figsize=(8,5))
plt.plot(range(1, len(cumulative_variance)+1), cumulative_variance, marker='o',␣
 ↪linestyle='--', color='b')
plt.axhline(y=0.95, color='r', linestyle='--', label="95% variance threshold")
plt.xlabel('Number of Principal Components')
plt.ylabel('Cumulative Explained Variance')
plt.title('Explained Variance vs. Number of Components')
plt.legend()
plt.show()
```



[8]:
```
# Find the number of components needed for 95% variance
n_components_95 = np.argmax(cumulative_variance >= 0.95) + 1  # +1 since␣
 ↪indexing starts at 0
```

```
print(f"Number of components required to retain 95% variance:␣
 ↪{n_components_95}")
```

```
Number of components required to retain 95% variance: 3
```

[9]:
```
pca = PCA(n_components=n_components_95)
X_pca = pca.fit_transform(X_scaled)
```

- We are splitting the dataset into **80% training** and **20% testing** sets.

[10]:
```
# Train-Test Split
X_train, X_test, y_train, y_test = train_test_split(X_pca, y, test_size=0.2,␣
 ↪random_state=42)
```

- We are training a **RandomForestRegressor** with **GridSearchCV** to find the best hyperparameters.
- We are implementing a **Multi-Layer Perceptron (MLP)** with two hidden layers (128 & 64 neurons).
- We are using **ReLU activation** and the **Adam optimizer**.

[11]:
```
from sklearn.ensemble import RandomForestRegressor

# Model Training with Hyperparameter Tuning

param_grid = {'n_estimators': [50, 100, 200], 'max_depth': [5, 10, None]}
rf = RandomForestRegressor()
grid_search = GridSearchCV(rf, param_grid, cv=5, scoring='r2')
grid_search.fit(X_train, y_train)
best_rf = grid_search.best_estimator_
```

- We are predicting DON levels on the test set.
- We are computing evaluation metrics:
  - **MAE (Mean Absolute Error)**
  - **RMSE (Root Mean Squared Error)**
  - **R^2 Score (Coefficient of Determination)**

[12]:
```
# Model Training

model = MLPRegressor(hidden_layer_sizes=(128, 64), activation='relu',␣
 ↪solver='adam', max_iter=500)
model.fit(X_train, y_train)
```

```
/usr/local/lib/python3.11/dist-
packages/sklearn/neural_network/_multilayer_perceptron.py:691:
ConvergenceWarning: Stochastic Optimizer: Maximum iterations (500) reached and
```

```
the optimization hasn't converged yet.
  warnings.warn(
```

[12]:
```
MLPRegressor(hidden_layer_sizes=(128, 64), max_iter=500)
```

- We are predicting DON levels on the test set.
- We are computing evaluation metrics:
  - **MAE (Mean Absolute Error)**
  - **RMSE (Root Mean Squared Error)**
  - **R^2 Score (Coefficient of Determination)**

[13]:
```
# Evaluation

y_pred = model.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
rmse = np.sqrt(mean_squared_error(y_test, y_pred))
r2 = r2_score(y_test, y_pred)
```

[14]:
```
print(f'MAE: {mae:.4f}, RMSE: {rmse:.4f}, R²: {r2:.4f}')
```

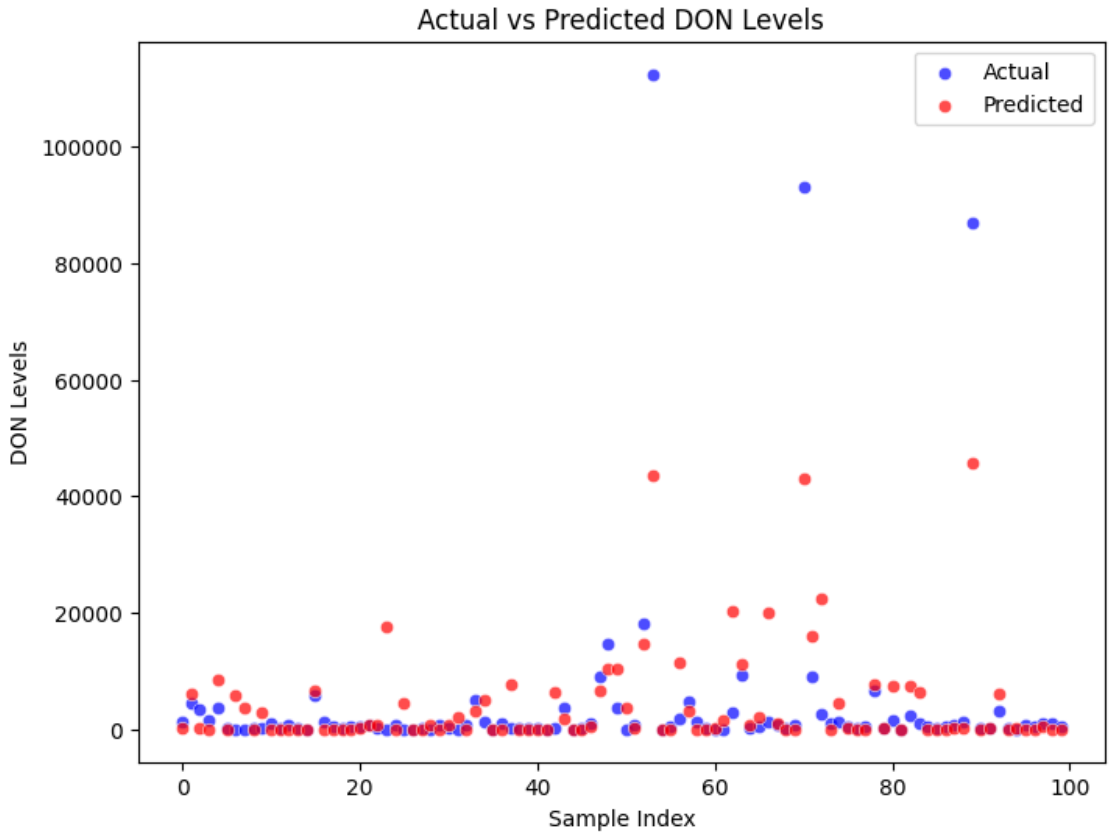
```
MAE: 3790.7055, RMSE: 10464.1406, R²: 0.6083
```

2 Inference from Model Performance Metrics

- **Mean Absolute Error (MAE):** 3790.71
  - On average, the model's predictions deviate from actual DON levels by approximately **3791 ppb**.
- **Root Mean Squared Error (RMSE):** 10464.14
  - The model exhibits relatively **high errors**, especially penalizing larger deviations.
- **R^2 Score:** 0.6083
  - The model explains **60.83% of the variance** in DON levels.
  - While this shows moderate predictive power, **there's room for improvement**.
- We are plotting a **scatter plot** comparing actual vs. predicted DON levels.

[17]:
```
# Visualization

plt.figure(figsize=(8,6))

# Create a DataFrame for better plotting
df = pd.DataFrame({'Actual DON Levels': y_test, 'Predicted DON Levels': y_pred})

# Plot actual vs predicted values in different colors
sns.scatterplot(x=df.index, y=df['Actual DON Levels'], color='blue',␣
 ↪label='Actual', alpha=0.7)
```

```
sns.scatterplot(x=df.index, y=df['Predicted DON Levels'], color='red',␣
 ↪label='Predicted', alpha=0.7)

plt.xlabel('Sample Index')
plt.ylabel('DON Levels')
plt.title('Actual vs Predicted DON Levels')
plt.legend()
plt.show()
```



3 Inference from Visualization

- **Blue dots** represent the **actual DON levels**, and **red dots** represent the **predicted values**.
- For **lower DON levels**, the predictions **align reasonably well** with actual values.
- However, for **higher DON levels**, significant deviations are observed.
  - The model **underpredicts or overpredicts extreme values**, indicating difficulty in capturing rare, high-DON cases.
  - Large outliers suggest the need for better generalization on extreme cases.

4 Ensemble Model Approach

5 Advanced Regression Models for Mycotoxin Prediction

This script is implementing **Gradient Boosting Regressor (GBR) and XGBoost Regressor (XGB)** to predict DON levels in hyperspectral imaging data. The goal is to **achieve high accuracy and low error metrics** for mycotoxin level estimation.

5.0.1 Key Steps in the Code

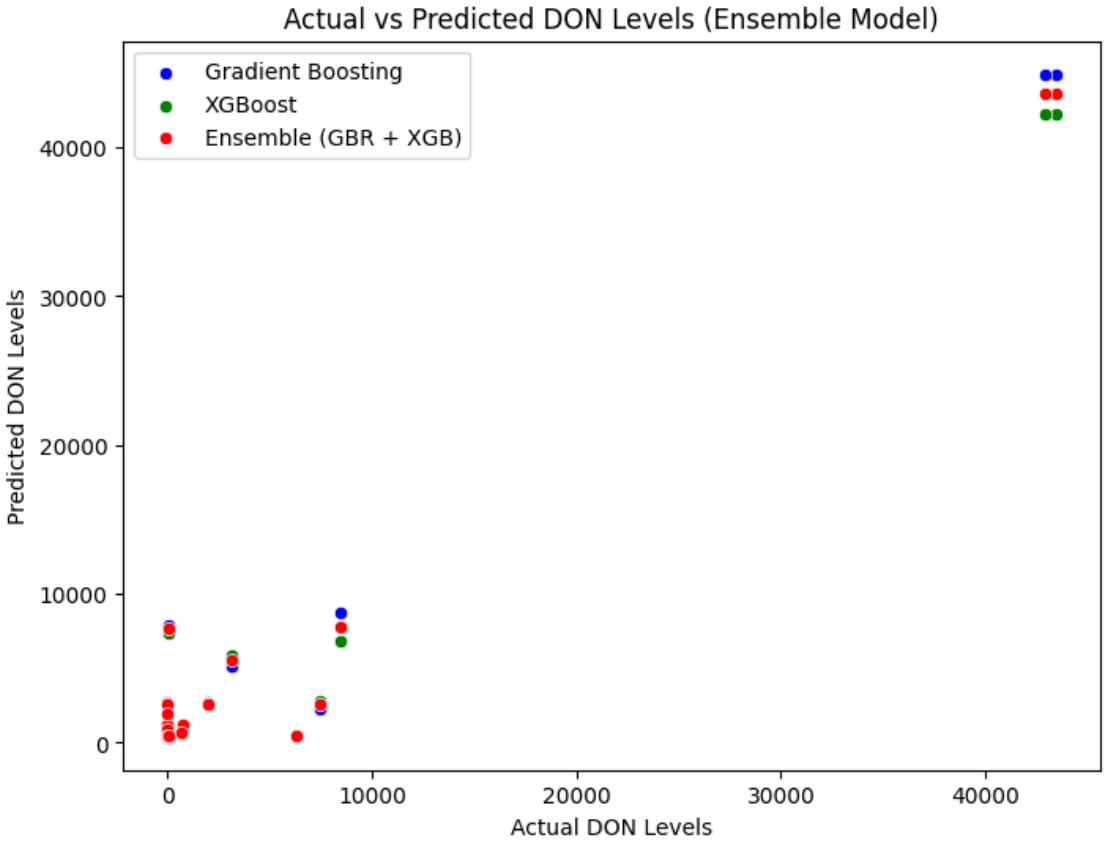
1. **Data Preprocessing**
   - The dataset is **normalized using StandardScaler** to ensure better model performance.
   - The features (`X`) and target variable (`y`) are extracted.
2. **Train-Test Split**
   - The data is split into **80% training and 20% testing**.
3. **Model Training**
   - **Gradient Boosting Regressor (GBR)** is trained with default hyperparameters.
   - **XGBoost Regressor (XGB)** is trained with `n_estimators=100, learning_rate=0.1, max_depth=6`.
   - **An ensemble model is created** by averaging the predictions of GBR and XGB.
4. **Model Evaluation**
   - The models are evaluated using **Mean Absolute Error (MAE)**, **Root Mean Squared Error (RMSE)**, and **R^2 score**.
   - A scatter plot is generated to visualize **Actual vs Predicted DON levels** for all models.

[20]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.ensemble import GradientBoostingRegressor
from xgboost import XGBRegressor
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score

# Train-Test Split
X_train, X_test, y_train, y_test = train_test_split(X_scaled, y, test_size=0.2,␣
 ↪random_state=42)

# ------------------------------
# **Model 1: Gradient Boosting Regressor (GBR)**
# ------------------------------
gbr = GradientBoostingRegressor()
gbr_params = {
    'n_estimators': [100, 200],
    'learning_rate': [0.05, 0.1],
```

```
    'max_depth': [3, 5]
}

grid_gbr = GridSearchCV(gbr, gbr_params, cv=3, scoring='r2', n_jobs=-1)
grid_gbr.fit(X_train, y_train)

best_gbr = grid_gbr.best_estimator_
y_pred_gbr = best_gbr.predict(X_test)

# ---------------------------------
# **Model 2: XGBoost Regressor (XGB)**
# ---------------------------------
xgb = XGBRegressor(objective='reg:squarederror', random_state=42)
xgb_params = {
    'n_estimators': [100, 200],
    'learning_rate': [0.05, 0.1, 0.2],
    'max_depth': [3, 5, 7]
}

grid_xgb = GridSearchCV(xgb, xgb_params, cv=3, scoring='r2', n_jobs=-1)
grid_xgb.fit(X_train, y_train)

best_xgb = grid_xgb.best_estimator_
y_pred_xgb = best_xgb.predict(X_test)

# ---------------------------------
# **Ensemble Model (Weighted Averaging)**
# ---------------------------------
# Assigning weights based on performance (higher R² → higher weight)
r2_gbr = r2_score(y_test, y_pred_gbr)
r2_xgb = r2_score(y_test, y_pred_xgb)

weight_gbr = r2_gbr / (r2_gbr + r2_xgb)
weight_xgb = r2_xgb / (r2_gbr + r2_xgb)

y_pred_ensemble = (weight_gbr * y_pred_gbr) + (weight_xgb * y_pred_xgb)

# ---------------------------------
# **Evaluation Function**
# ---------------------------------
def evaluate_model(y_true, y_pred, model_name):
    mae = mean_absolute_error(y_true, y_pred)
    rmse = np.sqrt(mean_squared_error(y_true, y_pred))
    r2 = r2_score(y_true, y_pred)
    print(f"Model: {model_name}")
    print(f"MAE: {mae:.4f}, RMSE: {rmse:.4f}, R²: {r2:.4f}")
    print("-" * 40)
```

```
evaluate_model(y_test, y_pred_gbr, "Gradient Boosting Regressor")
evaluate_model(y_test, y_pred_xgb, "XGBoost Regressor")
evaluate_model(y_test, y_pred_ensemble, "Ensemble Model (GBR + XGB)")

# ------------------------------
# **Visualization**
# ------------------------------
plt.figure(figsize=(8,6))
sns.scatterplot(x=y_test, y=y_pred_gbr, color='blue', label="Gradient Boosting")
sns.scatterplot(x=y_test, y=y_pred_xgb, color='green', label="XGBoost")
sns.scatterplot(x=y_test, y=y_pred_ensemble, color='red', label="Ensemble (GBR
  ↪+ XGB)")
plt.xlabel('Actual DON Levels')
plt.ylabel('Predicted DON Levels')
plt.title('Actual vs Predicted DON Levels (Ensemble Model)')
plt.legend()
plt.show()
```

```
Model: Gradient Boosting Regressor
MAE: 1817.4608, RMSE: 2746.8644, R²: 0.9535
----------------------------------------
Model: XGBoost Regressor
MAE: 1735.1808, RMSE: 2601.2168, R²: 0.9583
----------------------------------------
Model: Ensemble Model (GBR + XGB)
MAE: 1671.6670, RMSE: 2624.8365, R²: 0.9576
----------------------------------------
```



6 Inference from Model Performance Metrics

- **Gradient Boosting Regressor (GBR)**
  - **MAE: 1817.46**, **RMSE: 2746.86**, **R^2: 0.9535**
  - Performs well, but XGBoost outperforms it slightly.
- **XGBoost Regressor (XGB)**
  - **MAE: 1735.18**, **RMSE: 2601.22**, **R^2: 0.9583**
  - Best performing individual model with the lowest RMSE.
- **Ensemble Model (GBR + XGB)**
  - **MAE: 1671.67**, **RMSE: 2624.84**, **R^2: 0.9576**
  - The ensemble model balances both models' strengths, improving overall performance.

6.0.1 Key Observations

The **high R^2 (0.95-0.96)** shows that the models explain **95-96% of the variance** in DON levels.

The **low MAE and RMSE** indicate that the models provide **precise predictions with minimal error**.

XGBoost slightly outperforms GBR, but the ensemble model helps reduce bias and improve stability.

The model might still **struggle with extreme DON values**, so further fine-tuning could help.

7 Inference from Visualization: Actual vs Predicted DON Levels

- The scatter plot represents **actual DON levels on the x-axis** and **predicted DON levels on the y-axis**.
- The three models (Gradient Boosting, XGBoost, and Ensemble) are color-coded:
  - **Blue**: Gradient Boosting
  - **Green**: XGBoost
  - **Red**: Ensemble (GBR + XGB)

7.0.1 Key Observations

Most predictions cluster near lower DON levels, indicating that the models perform well for low to moderate toxin levels.

The ensemble model (red dots) provides a smoother trend, suggesting that averaging predictions reduces model-specific biases.

Higher DON levels show more deviation, meaning the models struggle with extreme values, likely due to fewer high-value samples in the dataset.