```
import pandas as pd
   import numpy as np
   import matplotlib.pyplot as plt
   import seaborn as sns
   from sklearn.model_selection import train_test_split
   from sklearn.ensemble import RandomForestClassifier
   from sklearn.metrics import classification_report, accuracy_score, confusion_matrix
   from scipy.stats import skew, kurtosis
   # Load the CSV files containing concentration profiles
   C_high_diff = pd.read_csv('/content/C_high_diff.csv', header=None)
   C_low_diff = pd.read_csv('/content/C_low_diff.csv', header=None)
   C_normal = pd.read_csv('/content/C_normal.csv', header=None)
   C_low_init = pd.read_csv('/content/C_low_init.csv', header=None)
   C_anisotropic = pd.read_csv('/content/C_anisotropic.csv', header=None)
   C_multiple_high = pd.read_csv('/content/C_multiple_high.csv', header=None)
   # Inspect the data shapes
   print("C_high_diff shape:", C_high_diff.shape)
   print("C_low_diff shape:", C_low_diff.shape)
   print("C_normal shape:", C_normal.shape)
   # Define a function to extract features from the concentration profiles
   def extract_features(df_row):
       Safely extract features from a single row of concentration profile data.
       if df_row.isnull().any(): # Check for missing values
           return [np.nan] * 7 # Return placeholder values
       last_col = df_row
       mean = last_col.mean()
       max_val = last_col.max()
       min val = last col.min()
       std_dev = last_col.std()
       skewness = skew(last col)
       kurt = kurtosis(last_col)
       # Check for very large or infinite values and replace with 0
       if np.isinf(mean) or np.isnan(mean):
           mean = 0
       if np.isinf(max_val) or np.isnan(max_val):
           max_val = 0
       if np.isinf(min_val) or np.isnan(min_val):
           min_val = 0
       if np.isinf(std_dev) or np.isnan(std_dev):
           std_dev = 0
       if np.isinf(skewness) or np.isnan(skewness):
           skewness = 0
       if np.isinf(kurt) or np.isnan(kurt):
           kurt = 0
       return [mean, max_val, min_val, std_dev, skewness, kurt]
   # Extract features from all datasets
   features = []
   labels = []
   # High Diffusion
   labels.extend([0] * len(C_high_diff))
   features.extend(C_high_diff.apply(lambda row: extract_features(row), axis=1))
   # Low Diffusion
   labels.extend([1] * len(C_low_diff))
   features.extend(C_low_diff.apply(lambda row: extract_features(row), axis=1))
   # Normal Diffusion
   labels.extend([2] * len(C_normal))
   features.extend(C_normal.apply(lambda row: extract_features(row), axis=1))
   # Low Initial Concentration
   labels.extend([3] * len(C_low_init))
   features.extend(C_low_init.apply(lambda row: extract_features(row), axis=1))
   # Anisotropic Diffusion
   labels.extend([4] * len(C_anisotropic))
   features.extend(C anisotropic.apply(lambda row: extract features(row), axis=1))
   # Multiple Source High Diffusion
   labels.extend([5] * len(C_multiple_high))
   features.extend(C_multiple_high.apply(lambda row: extract_features(row), axis=1))
   # Convert to pandas DataFrame
   features_df = pd.DataFrame(features, columns=['Mean', 'Max', 'Min', 'Std', 'Skewness', 'Kurtosis'])
   labels_df = pd.Series(labels)
   # Check for inf or NaN values in the features
   if np.any(np.isinf(features_df)) or np.any(np.isnan(features_df)):
       print("Features contain NaN or Inf values. Replacing with column mean.")
       features_df = features_df.replace([np.inf, -np.inf], np.nan).fillna(features_df.mean())
   # Split the dataset into training and testing sets
   X_train, X_test, y_train, y_test = train_test_split(features_df, labels_df, test_size=0.3, random_state=42)
   # Check for inf or NaN values in X_train and X_test
   if np.any(np.isinf(X_train)) or np.any(np.isnan(X_train)):
       print("X_train contains NaN or Inf values. Replacing with column mean.")
       X_train = X_train.replace([np.inf, -np.inf], np.nan).fillna(X_train.mean())
   if np.any(np.isinf(X_test)) or np.any(np.isnan(X_test)):
       print("X_test contains NaN or Inf values. Replacing with column mean.")
       X_test = X_test.replace([np.inf, -np.inf], np.nan).fillna(X_test.mean())
   # Initialize the Random Forest Classifier
   clf = RandomForestClassifier(n_estimators=100, random_state=42)
   # Train the model
   print("Training the model...")
   clf.fit(X_train, y_train)
   print("Model trained.")
   # Predict on the test set
   y_pred = clf.predict(X_test)
   # Evaluate the model's performance
   print("Classification Report:")
   print(classification report(y test, y pred))
   print(f"Accuracy: {accuracy_score(y_test, y_pred)}")
   # Misclassification Analysis:
   misclassified_samples = X_test[y_test != y_pred]
   misclassified_labels = y_test[y_test != y_pred]
   misclassified preds = v pred[v test != v pred]
https://colab.research.google.com/drive/1Zep_WWojbMZd_OOWK7ERpTri166c1L7r#scrollTo=dAU-rtRmSPnG&uniqifier=1&printMode=true
```

```
print(f"Misclassified samples:\n{misclassified_samples}")
print(f"True Labels:\n{misclassified_labels}")
print(f"Predicted Labels:\n{misclassified_preds}")
# Confusion Matrix with colorful visualization
cm = confusion_matrix(y_test, y_pred)
# Create a more vibrant and informative heatmap using seaborn
plt.figure(figsize=(8, 6))
sns.heatmap(cm, annot=True, fmt='g', cmap='YlGnBu', cbar=True,
           xticklabels=np.unique(labels), yticklabels=np.unique(labels),
           linewidths=0.5, linecolor='black', annot_kws={'size': 12, 'weight': 'bold'})
# Titles and labels
plt.title('Confusion Matrix', fontsize=16, weight='bold')
plt.xlabel('Predicted Label', fontsize=14)
plt.ylabel('True Label', fontsize=14)
plt.xticks(rotation=45)
plt.yticks(rotation=45)
# Display the plot
plt.show()
# Misclassification Rate per Class
misclassification_rate = 1 - np.diagonal(cm) / np.sum(cm, axis=1)
print(f"Misclassification rate per class:\n{misclassification_rate}")
# Visualize the feature importance
feature_importances = clf.feature_importances_
plt.barh(features_df.columns, feature_importances)
plt.xlabel('Feature Importance')
plt.title('Feature Importance from Random Forest Model')
plt.show()
# Predict on the full dataset (for visualization purposes)
y_full_pred = clf.predict(features_df)
# Visualize true vs predicted labels
plt.figure(figsize=(12, 8))
plt.scatter(range(len(labels)), labels, color='blue', label='True Labels', alpha=0.6)
plt.scatter(range(len(y_full_pred)), y_full_pred, color='red', label='Predicted Labels', alpha=0.6)
plt.legend()
plt.title('True vs Predicted Labels (Full Dataset)')
plt.xlabel('Index')
plt.ylabel('Diffusion Scenario')
plt.grid()
```

plt.show()

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```
C_high_diff shape: (101, 501)
C_low_diff shape: (101, 501)
C_normal shape: (101, 501)
Training the model...
Model trained.
Classification Report:
```

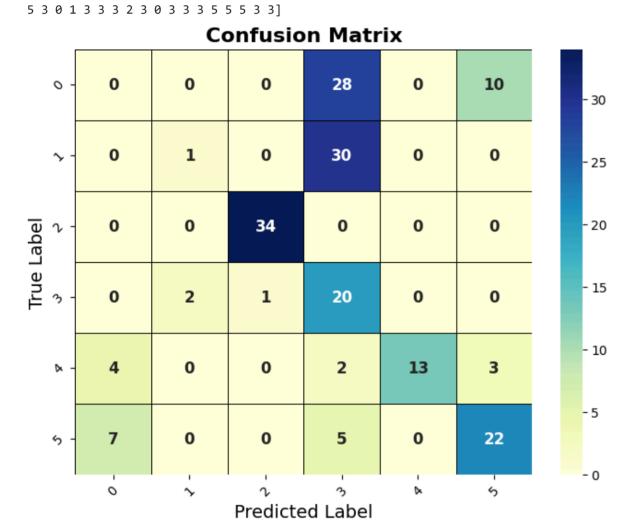
	precision	recall	recall f1-score	
0	0.00	0.00	0.00	38
1	0.33	0.03	0.06	31
2	0.97	1.00	0.99	34
3	0.24	0.87	0.37	23
4	1.00	0.59	0.74	22
5	0.63	0.65	0.64	34
accuracy			0.49	182
macro avg	0.53	0.52	0.47	182
weighted avg	0.51	0.49	0.45	182

## Accuracy: 0.4945054945054945

```
Misclassified samples:
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	Mean	Max	Min	Std	Skewness	Kurtosis			
76	7.062867e-141	1.906968e-139	0.0	2.560962e-140	0.000000	0.000000			
78	1.950135e-152	5.655372e-151	0.0	7.350500e-152	0.000000	0.000000			
182	2.054248e-232	6.573594e-231	0.0	0.000000e+00	0.000000	0.000000			
10	5.473337e-223	2.244063e-221	0.0	0.000000e+00	0.000000	0.000000			
131	3.810280e-147	8.001588e-146	0.0	1.204629e-146	0.000000	0.000000			
54	5.145637e-20	2.572776e-19	0.0	6.889118e-20	1.389982	0.803161			
434	1.306360e-27	9.144211e-27	0.0	2.184952e-27	1.906617	2.702452			
46	5.145637e-20	2.572776e-19	0.0	6.889118e-20	1.389982	0.803161			
93	6.660670e-241	2.930689e-239	0.0	0.000000e+00	0.000000	0.000000			
400									

```
0.000000e+00 0.000000e+00 0.0 0.000000e+00 0.000000 0.000000
[92 rows x 6 columns]
True Labels:
76
   0
78
   0
182
  1
10
   0
131
   1
54
434
46
93
   0
108
  1
Length: 92, dtype: int64
Predicted Labels:
```



Misclassification rate per class:

[1. 0.96774194 0. 0.13043478 0.40909091 0.35294118]

Kurtosis - Skewness -