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[34]: import pandas as pd
      from sklearn.model_selection import train_test_split
      from sklearn.ensemble import RandomForestClassifier
      from sklearn.metrics import accuracy_score, classification_report
      import numpy as np
      import joblib
[16]: # Step 1: Load the updated CSV file with balanced water quality data
      file_path = 'balanced_water_quality_with_nanoparticles.csv' # Replace with the_
       ⇔correct path
      data = pd.read_csv(file_path)
[17]: # Step 2: Data Overview
      print("Data Overview:")
      print(data.head())
     Data Overview:
              pH Lead (mg/L) Mercury (mg/L)
                                               Bacteria (cfu/mL) Arsenic (mg/L) \
                     0.004525
     0 9.065749
                                     0.000441
                                                       162.574511
                                                                         0.010283
     1 6.733394
                     0.001154
                                     0.001659
                                                       69.677048
                                                                         0.001700
     2 7.782632
                     0.003603
                                     0.000154
                                                       84.726990
                                                                         0.003943
     3 7.586133
                     0.002265
                                     0.000172
                                                        3.167012
                                                                         0.001132
     4 7.975943
                     0.013698
                                     0.000356
                                                       169.508169
                                                                         0.002695
        Contaminant Level Nanomaterial Required Water Safe to Drink
     0
                 0.799450 Silver Nanoparticles
                                                                  No
                 0.910240 Silver Nanoparticles
                                                                 No
     1
                                 Graphene Oxide
                 0.584275
                                                                 Yes
     3
                 0.207570
                                 Graphene Oxide
                                                                 Yes
                 0.075436 Silver Nanoparticles
                                                                 No
[18]: # Step 3: Data Preprocessing
      # Convert the 'Nanomaterial Required' and 'Water Safe to Drink' columns to \Box
       ⇔categorical variables
      data['Nanomaterial Required'] = data['Nanomaterial Required'].
       ⇒astype('category').cat.codes
```

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data['Water Safe to Drink'] = data['Water Safe to Drink'].map({'Yes': 1, 'No': u
       →0})
      # Define the features (input variables) and the target (output variable)
      features = ['pH', 'Lead (mg/L)', 'Mercury (mg/L)', 'Bacteria (cfu/mL)', |
      target = 'Nanomaterial Required'
      X = data[features]
      y = data[target]
[19]: # Step 4: Split the data into training and testing sets
      X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,_
       →random_state=42)
[20]: # Step 5: Train a RandomForest Classifier
      model = RandomForestClassifier(n estimators=100, random state=42)
      model.fit(X_train, y_train)
[20]: RandomForestClassifier(random_state=42)
[21]: # Step 6: Make predictions on the test set
      y_pred = model.predict(X_test)
[30]: # Step 7: Evaluate the model's performance
      accuracy = accuracy_score(y_test, y_pred)
      print(f"Nanomaterial Prediction Model Accuracy: {accuracy * 100:.2f}%")
      # Ensure the predicted and true labels cover all classes
      unique_classes_in_test = np.unique(y_test)
      unique_classes_in_pred = np.unique(y_pred)
      print(f"Unique classes in test data: {unique_classes_in_test}")
      print(f"Unique classes in predictions: {unique_classes_in_pred}")
      # Classification Report for nanomaterial prediction
      # Dynamically adjusting target names based on unique predicted classes
      target_names = ['Graphene Oxide', 'Silver Nanoparticles', 'Zinc Oxide_
      ⇔Nanoparticles']
      report = classification_report(y_test, y_pred, labels=unique_classes_in_pred,_u
       atarget_names=[target_names[i] for i in unique_classes_in_pred])
      print("Nanomaterial Classification Report:\n", report)
     Nanomaterial Prediction Model Accuracy: 100.00%
     Unique classes in test data: [0 1]
     Unique classes in predictions: [0 1]
     Nanomaterial Classification Report:
```

```
precision
                                    recall f1-score
                                                        support
                           1.00
                                     1.00
                                                           581
      Graphene Oxide
                                                1.00
Silver Nanoparticles
                           1.00
                                      1.00
                                                1.00
                                                           419
                                                1.00
                                                          1000
            accuracy
           macro avg
                           1.00
                                      1.00
                                                1.00
                                                          1000
                                                1.00
        weighted avg
                           1.00
                                      1.00
                                                          1000
```

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[32]: # Step 8: Predict whether the water is safe to drink (binary classification)
      # Define a new target for water safety prediction
     target_safety = 'Water Safe to Drink'
     y_safety = data[target_safety]
      # Split the data for water safety prediction
     X_train_safety, X_test_safety, y_train_safety, y_test_safety =_
      strain_test_split(X, y_safety, test_size=0.2, random_state=42)
     # Train a RandomForest Classifier for water safety prediction
     model_safety = RandomForestClassifier(n_estimators=100, random_state=42)
     model_safety.fit(X_train_safety, y_train_safety)
     # Make predictions for water safety
     y_pred_safety = model_safety.predict(X_test_safety)
     # Evaluate the water safety model
     accuracy_safety = accuracy_score(y_test_safety, y_pred_safety)
     print(f"Water Safety Model Accuracy: {accuracy_safety * 100:.2f}%")
      # Classification Report for water safety
      # Ensure the correct number of target names for the binary classification
     report_safety = classification_report(y_test_safety, y_pred_safety,_u
      print("Water Safety Classification Report:\n", report_safety)
```

Water Safety Model Accuracy: 100.00% Water Safety Classification Report:

	precision	recall	f1-score	support
Not Safe	1.00	1.00	1.00	442
Safe	1.00	1.00	1.00	558
accuracy			1.00	1000
macro avg	1.00	1.00	1.00	1000
weighted avg	1.00	1.00	1.00	1000

```
[37]: # Save the trained models as .pkl files
joblib.dump(model, 'model_nanomaterial.pkl')
joblib.dump(model_safety, 'model_safety.pkl')

print("Models have been saved as 'model_nanomaterial.pkl' and 'model_safety.

→pkl'")
```

Models have been saved as 'model_nanomaterial.pkl' and 'model_safety.pkl'

[]: