EMLM_Exercise2_lkmail

February 7, 2024

Lauri Maila Student number 2209361 February, 6, 2024

1 Exercise 2 | TKO_7092 Evaluation of Machine Learning Methods 2024

1.0.1 Prediction of the metal ion content from multi-parameter data

Use K-Nearest Neighbor Regression with euclidean distance to predict total metal concentration (c_total), concentration of Cadmium (Cd) and concentration of Lead (Pb), using number of neighbors k = 1, 3, 5, 7.

Instructions:

```
- You may use Nearest Neighbor Regression from https://scikit-learn.org/stable/modules/neighbo
- The data should be standarized using z-score (using sklearn.preprocessing.StandardScaler is 
- Implement Leave-One-Out cross-validation and calculate the C-index for each output (c_total,
- Implement Leave-Replicas-Out cross-validation and calculate the C-index for each output (c_t
- Explain your code by adding detailed comments.
- Only provide code that is relevant to the exercise.
- Please submit your solution as a Jupyter Notebook (.ipynb) and as a PDF file. Ensure to incl
- Submit to moodle your solution on ** Wednesday 7 of February ** at the latest.
```

Please follow the instructions and note that you are expected to submit your individual solution. Identical or overly similar submissions will result in the exercise being marked as failed.

1.1 Import libraries

[ ]:
```python
# In this cell import all libraries you need. For example:
import numpy as np
import pandas as pd
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import LeaveOneOut, LeaveOneGroupOut
from sklearn.neighbors import KNeighborsRegressor
import matplotlib.pyplot as plt
```

1.2 Read and visualize the dataset

[ ]:
```
# In this cell read the file Water_data.csv
waterdata_df = pd.read_csv('water_data.csv')
dim = waterdata_df.shape
print("Number of rows:", dim[0])
print("Number of columns:", dim[1])
waterdata_df.head()
```

```
Number of rows: 268
Number of columns: 6
```

[ ]:

	Mod1	Mod2	Mod3	c_total	Cd	Pb
0	9945	119	72335	0	0.0	0.0
1	9596	119	110542	0	0.0	0.0
2	10812	120	98594	0	0.0	0.0
3	10786	117	82977	0	0.0	0.0
4	10566	108	136416	14	0.0	14.0

1.3 Standardization of the dataset

[ ]:
```
```

[ ]:
```
```

[ ]:
```
# In this cell, standardize the dataset features by removing the mean and␣
↪scaling to unit variance.
# In other words, use z-score to scale the dataset features (Mod1, Mod2, Mod3)
# Print the 5 first samples (i.e. rows) of the scaled dataset

# I'll use sklearn StandardScaler to scale the features Mod1, Mod2 and Mod3
scaler = StandardScaler()

# Fit and transform the chosen features
scaled_features = scaler.fit_transform(waterdata_df[['Mod1', 'Mod2', 'Mod3']])

# Create a fd with the scaled features
scaled_features_df = pd.DataFrame(scaled_features, columns=['Mod1', 'Mod2',␣
↪'Mod3'])

# Print the first 5 samples of the scaled dataset
scaled_features_df.head()
```

[ ]:

	Mod1	Mod2	Mod3
0	-0.972283	-0.670482	-0.358179
1	-0.975878	-0.670482	0.259488
2	-0.963351	-0.670394	0.066333
3	-0.963619	-0.670657	-0.186137

```
4 -0.965885 -0.671447  0.677776
```

1.4 C-index code

```
[ ]: # I'm using the same C-index implementation given in the first exercise
"""
C-index function:
- INPUTS:
'y' an array of the true output values
'yp' an array of predicted output values
- OUTPUT:
The c-index value
"""
def cindex(y, yp):
    n = 0
    h_num = 0
    for i in range(0, len(y)):
        t = y[i]
        p = yp[i]
        for j in range(i+1, len(y)):
            nt = y[j]
            np = yp[j]
            if (t != nt):
                n = n + 1
                if (p < np and t < nt) or (p > np and t > nt):
                    h_num += 1
                elif (p == np):
                    h_num += 0.5
    return h_num/n
```

```
[ ]: # Test the cindex function with following values
true_labels = np.array([-1, 1, 1, -1, 1])
predictions = np.array([0.60, 0.80, 0.75, 0.75, 0.70])
cindx = cindex(true_labels, predictions)
print(cindx) # This shoudl give 0.75, works fine
```

```
0.75
```

1.5 Leave-One-Out cross-validation

In the following cell, write and execute your code for Leave-One-Out cross-validation using K-Nearest Neighbor Regression with k values of 1, 3, 5, and 7. Print the corresponding Leave-One-Out C-index for c_total, Cd and Pb for each k value.

```
[ ]: # We'll use the scaled features for X data
X = scaled_features_df[['Mod1', 'Mod2', 'Mod3']]
y = waterdata_df[['c_total', 'Cd', 'Pb']]
```

```python
# K-values to test
k_values = [1, 3, 5, 7]

# Dict for the results for plotting at the end
results_dict = []

# Iterate for each target variable c_total, Cd and Pb
for target_col in y.columns:
    print(f"Target variable: {target_col}")
    # Iterate for each k-value for the kNN
    for k in k_values:
        # Using LeaveOneOut() to get LOOCV indices
        loocv = LeaveOneOut()

        # Lists to store the predictions and actual values for C-index␣
↪calculation
        predictions = []
        true_values = []

        # Split the data using LOOCV
        for train_index, test_index in loocv.split(X):

            X_train, X_test = X.iloc[train_index], X.iloc[test_index]
            # Separate for each variable
            y_train, y_test = y[target_col].iloc[train_index], y[target_col].
↪iloc[test_index]

            # Initialize the kNN model
            knn = KNeighborsRegressor(n_neighbors=k)
            knn.fit(X_train, y_train)

            # Predict on the single test data using previously trained model
            y_pred = knn.predict(X_test)
            predictions.append(y_pred.tolist())
            true_values.append(y_test.values.tolist())

        # Calculate the C-index for the current k-value/variable and store it
        loocv_cindex = cindex(np.array(true_values), np.array(predictions))
        results_dict.append({'type': 'loocv', 'variable': target_col, 'k': k,␣
↪'cindex': loocv_cindex})

        print(f"K = {k}: Leave-One-Out C-index: {loocv_cindex:.3f}")
```

```
Target variable: c_total

K = 1: Leave-One-Out C-index: 0.908
K = 3: Leave-One-Out C-index: 0.920
K = 5: Leave-One-Out C-index: 0.896
```

```
K = 7: Leave-One-Out C-index: 0.884
Target variable: Cd
K = 1: Leave-One-Out C-index: 0.914
K = 3: Leave-One-Out C-index: 0.912
K = 5: Leave-One-Out C-index: 0.866
K = 7: Leave-One-Out C-index: 0.832
Target variable: Pb
K = 1: Leave-One-Out C-index: 0.880
K = 3: Leave-One-Out C-index: 0.885
K = 5: Leave-One-Out C-index: 0.861
K = 7: Leave-One-Out C-index: 0.841
```

1.6 Leave-Replicas-Out cross-validation

In the following cell, write and execute your code for Leave-Replicas-Out cross-validation using K-Nearest Neighbor Regression with k values of 1, 3, 5, and 7. Print the corresponding Leave-Replicas-Out C-index for c_total, Cd and Pb for each k value.

[ ]:
```
# Create the replica groups for Leave-Replicas-Out CV
def create_replica_groups(data):
    # Get unique rows and their counts
    _, idx, counts = np.unique(data, return_index=True, return_counts=True,␣
 ↪axis=0)
    groups = np.repeat(np.arange(len(counts)), counts)
    return groups

# Group labels based on replicas for each target variable
groups = {}
for target_col in y.columns:
    # Create replica groups for each variable
    groups[target_col] = create_replica_groups(y[target_col].to_numpy())

# K-values to test
k_values = [1, 3, 5, 7]

# Iterate for each target variable c_total, Cd and Pb
for target_col in y.columns:
    print(f"Target variable: {target_col}")
    # Iterate for each k-value for the kNN
    for k in k_values:
        # Using LeaveOneGroupOut() to get CV indices based on replica groups
        lro = LeaveOneGroupOut()

        # Lists to store the predictions and actual values for C-index␣
 ↪calculation
        predictions = []
        true_values = []
```

```
        # Split the data using Leave-Replicas-Out CV
        for train_index, test_index in lro.split(X, groups=groups[target_col]):␣
↪# Use groups for correct variable
            X_train, X_test = X.iloc[train_index], X.iloc[test_index]
            y_train, y_test = y[target_col].iloc[train_index], y[target_col].
↪iloc[test_index]

            # Initialize the kNN model
            knn = KNeighborsRegressor(n_neighbors=k)
            knn.fit(X_train, y_train)

            # Predict on the left out group data using previously trained model
            y_pred = knn.predict(X_test)
            predictions.extend(y_pred.tolist())
            true_values.extend(y_test.values.tolist())

        # Calculate the C-index for the current k-value/variable and store it
        lro_cindex = cindex(np.array(true_values), np.array(predictions))
        res = {'type': 'lro', 'variable': target_col, 'k': k, 'cindex':␣
↪lro_cindex}
        results_dict.append(res)

        print(f"K = {k}: Leave-Replicas-Out C-index: {lro_cindex:.3f}")
```

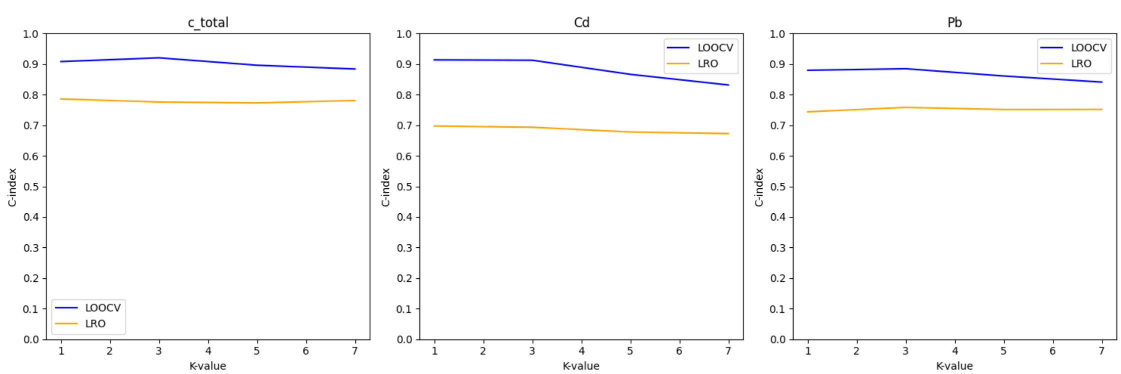
```
Target variable: c_total
K = 1: Leave-Replicas-Out C-index: 0.786
K = 3: Leave-Replicas-Out C-index: 0.776
K = 5: Leave-Replicas-Out C-index: 0.773
K = 7: Leave-Replicas-Out C-index: 0.781
Target variable: Cd
K = 1: Leave-Replicas-Out C-index: 0.697
K = 3: Leave-Replicas-Out C-index: 0.693
K = 5: Leave-Replicas-Out C-index: 0.678
K = 7: Leave-Replicas-Out C-index: 0.673
Target variable: Pb
K = 1: Leave-Replicas-Out C-index: 0.744
K = 3: Leave-Replicas-Out C-index: 0.758
K = 5: Leave-Replicas-Out C-index: 0.751
K = 7: Leave-Replicas-Out C-index: 0.752
```

1.7 Plot Leave-One-Out and Leave-Replicas-Out Results

Note: You may plot the results as they were presented in the video lecture (refer to MOOC2-Module 2 .pptx slides).

[ ]:
```
# Convert results_dict to a df for plotting
results_df = pd.DataFrame(results_dict)
```

```
num_rows = 1
num_cols = 3

fig, axs = plt.subplots(num_rows, num_cols, figsize=(15, 5))

# Iterate over each variable and plot its c-index values and k-values
for i, target_col in enumerate(y.columns):
    target_df = results_df[results_df['variable'] == target_col]
    ax = axs[i] if num_cols > 1 else axs

    # Separate plots for LOOCV and LRO
    loocv_df = target_df[target_df['type'] == 'loocv']
    lro_df = target_df[target_df['type'] == 'lro']

    # Plot the LOOCV data
    ax.plot(loocv_df['k'], loocv_df['cindex'], color='blue', label='LOOCV')

    # Plot the LRO data
    ax.plot(lro_df['k'], lro_df['cindex'], color='orange', label='LRO')

    ax.set_title(target_col)
    ax.set_xlabel("K-value")
    ax.set_ylabel("C-index")
    ax.set_ylim(0, 1)
    ax.set_yticks(np.arange(0, 1.1, step=0.1))
    ax.legend()

# Adjust layout
plt.tight_layout()
plt.show()
```



1.8 Interpretation of results

Answer the following questions based on the results obtained

- Which cross-validation method had more optimistic results?
- Explain the reason for the optimistic results produced by the cross-validation method.
- Which cross-validation method generalized better on unseen data? Why?

Leave-One-Out had noticably more optimistic C-index results for "unseen" test data compared to Leave-Replicas-Out. The reason for this is that the dataset had multiple similar datapoints, so when one data point was left out its copies caused overfitting on test data. Leave-Group-Out in this scenario was better on unseen data, since less information "leaked" from the training process.