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Exercise 2 | TKO_7092 Evaluation of Machine Learning Methods 2024

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/neighbors.html
- The data should be standarized using z-score (using sklearn.preprocessing.StandardScaler is
advised).
- Implement Leave-One-Out cross-validation and calculate the C-index for each output (c_total, Cd,
Pb).
- Implement Leave-Replicas-Out cross-validation and calculate the C-index for each output (c_total,
Cd, Pb).
- 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 include
your full name in the filename.
- 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.

Import libraries

In [1]:
```
# In this cell import all libraries you need. For example:
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split,  LeaveOneOut, KFold, LeaveOneGroupOut
from sklearn.neighbors import KNeighborsRegressor
import matplotlib.pyplot as plt
```

Read and visualize the dataset

In [2]:
```
# In this cell read the file Water_data.csv
# Print the dataset dimesions (i.e. number of rows and columns)
# Print the first 5 rows of the dataset
water_data = pd.read_csv('water_data.csv')
print(water_data.shape)
print(water_data.head(5))
```

```
(268, 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
```

Standardization of the dataset

In [3]:
```
# 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 made my own function to calculate the z-score in a given data and column
def zstand(data, col, x):
    mean = data[col].mean()
    std = np.std(data[col])
    return (x-mean)/std

# a function to change the values to standardized form
def cols_to_z(data,cols):
    for col in cols:
        data[col] = data[col].apply(lambda x: zstand(data, col, x))

standardized = water_data.copy()
cols_to_z(standardized, ['Mod1', 'Mod2', 'Mod3'])
standardized.head(5)
```

Out[3]:

	Mod1	Mod2	Mod3	c_total	Cd	Pb
0	-0.972283	-0.670482	-0.358179	0	0.0	0.0
1	-0.975878	-0.670482	0.259488	0	0.0	0.0
2	-0.963351	-0.670394	0.066333	0	0.0	0.0
3	-0.963619	-0.670657	-0.186137	0	0.0	0.0
4	-0.965885	-0.671447	0.677776	14	0.0	14.0

C-index code

In [4]:
```
# In this cell, implement the C-index function. You may use the implementation from the first exercise.
def cindex(true_labels, pred_labels):
    n = 0
    h_num = 0
    for i in range(len(true_labels)):
        for j in range(i+1, len(true_labels)):
            if (true_labels[i] != true_labels[j]):
                n += 1
                if (pred_labels[i] < pred_labels[j] and true_labels[i] < true_labels[j]) or (pred_labels[i] > pred_labe
                    h_num += 1
                elif (pred_labels[i] == pred_labels[j]):
                    h_num += 0.5
    # just for errorhandling
    if n == 0:
        return 0
    cindx = h_num/n
    """Returns C-index between true labels and predicted labels"""
    return cindx
```

In [5]:
```
# 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) #For this example, a correct C-index implementation will result in 0.75
```

```
0.75
```

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.

In [6]:
```
k_values = [1,3,5,7]
col_names = ['c_total', 'Cd', 'Pb']

n = len(standardized)
loo_df = pd.DataFrame(columns=['variable', 'k', 'C-index'])
for col in col_names:

    X = standardized.drop(col_names, axis=1)
    y = standardized[col]

    for k in k_values:

        knn = KNeighborsRegressor(n_neighbors=k, metric= 'euclidean')
        c_index_values = []
        loo = LeaveOneOut()

        y_value_arr = []
        y_pred_arr = []

        for train_ind, test_ind in loo.split(X):
            X_train = X.iloc[train_ind]
            X_test = X.iloc[test_ind]
            y_train, y_test = y.iloc[train_ind], y.iloc[test_ind]

            knn.fit(X_train, y_train)
            y_pred = knn.predict(X_test)
            y_pred_arr.extend(y_pred)
            y_value_arr.extend(y_test.values)
            #print(f"true: {y_test}, pred: {y_pred}")
        c_index_values.append(cindex(y_value_arr, y_pred_arr))

        temp_df = pd.DataFrame({'variable': [col], 'k': [k], 'C-index': [np.mean(c_index_values)]})

        loo_df = pd.concat([loo_df, temp_df], ignore_index=True)
grouped_loo_df = loo_df.groupby('variable')

for name, group in grouped_loo_df:
    print(f"Group: {name}")
    print(group)
    print("\n")
```

```
Group: Cd
  variable  k   C-index
4       Cd  1  0.913592
5       Cd  3  0.912488
6       Cd  5  0.866349
7       Cd  7  0.831597


Group: Pb
   variable  k   C-index
8        Pb  1  0.879590
9        Pb  3  0.884710
10       Pb  5  0.860935
11       Pb  7  0.841043


Group: c_total
  variable  k   C-index
0  c_total  1  0.908098
1  c_total  3  0.920363
2  c_total  5  0.896185
3  c_total  7  0.883905
```

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.

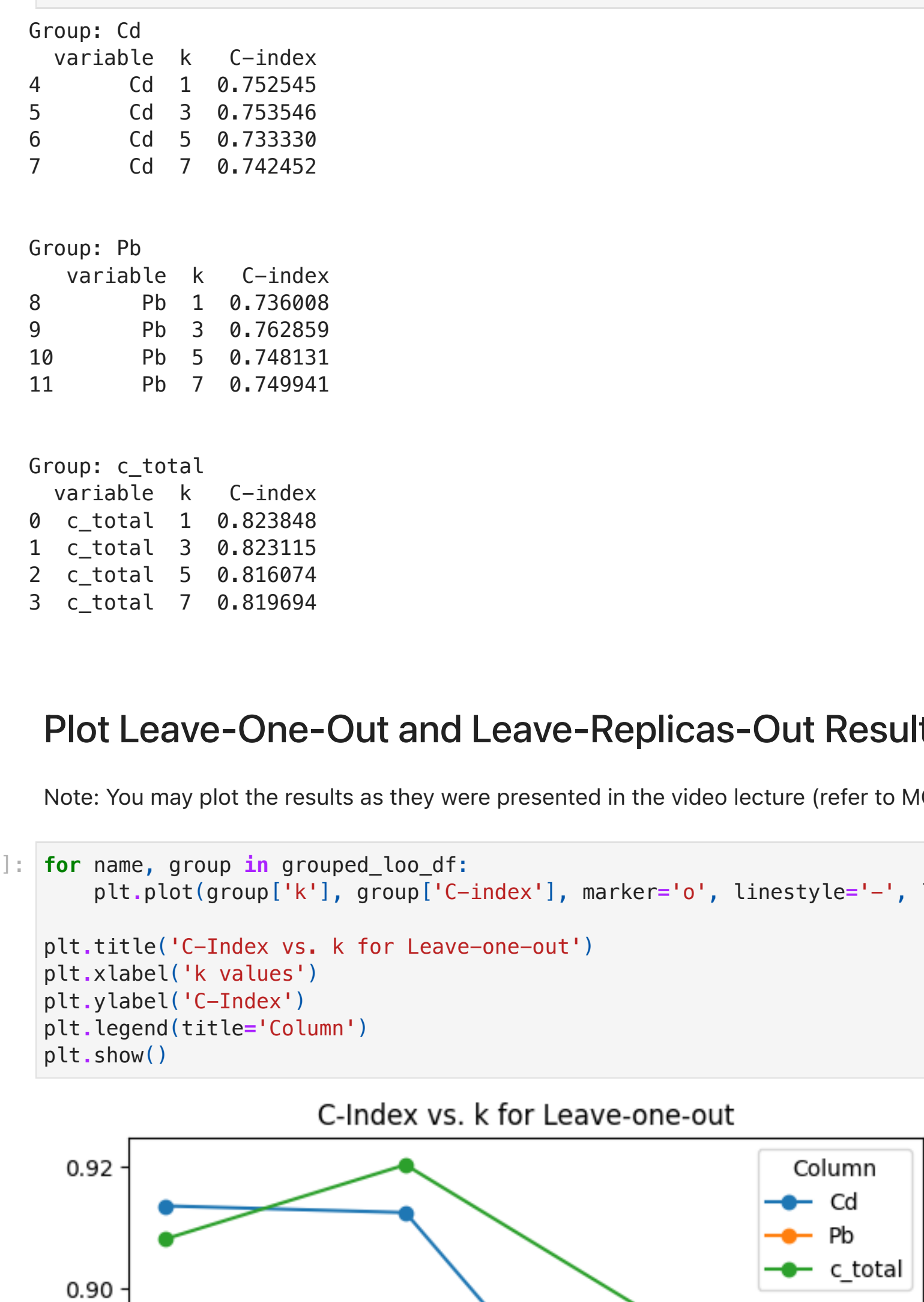
In [7]:
```
col_names = ['c_total', 'Cd', 'Pb']
target = standardized[col_names]


group = target.groupby(list(target.columns)).apply(lambda x: x.index.tolist()).tolist()
groups = []
for i in range(len(group)):
    for j in range(len(group[i])):
        groups.append(i)
logo_groups = np.array(groups)

logo_df = pd.DataFrame(columns=['variable', 'k', 'C-index'])
k_values = [1,3,5,7]
n = len(standardized)
features = ['Mod1', 'Mod2', 'Mod3']
Scores_logo = {
    'c_total': [],
    'Cd': [],
    'Pb': []
}
for col in col_names:
    X = standardized[features].values
    y = standardized[col].values
    col_values = []
    for k in k_values:

        knn = KNeighborsRegressor(n_neighbors=k, metric= 'euclidean')
        logo = LeaveOneGroupOut()

        c_index_values = []
        y_value_arr = []
        y_pred_arr = []

        for train_ind, test_ind in logo.split(X, y, groups=logo_groups):

            X_train, X_test = X[train_ind], X[test_ind]
            y_train, y_test = y[train_ind], y[test_ind]


            knn.fit(X_train, y_train)
            y_pred = knn.predict(X_test)
            y_pred_arr.extend(y_pred)
            y_value_arr.extend(y_test)

        c_index_values.append(cindex(y_value_arr, y_pred_arr))

        temp_df = pd.DataFrame({'variable': [col], 'k': [k], 'C-index': [np.mean(c_index_values)]})

        logo_df = pd.concat([logo_df, temp_df], ignore_index=True)
grouped_logo_df = logo_df.groupby('variable')

for name, group in grouped_logo_df:
    print(f"Group: {name}")
    print(group)
    print("\n")
```

```
Group: Cd
  variable  k   C-index
4       Cd  1  0.752545
5       Cd  3  0.753546
6       Cd  5  0.733330
7       Cd  7  0.742452


Group: Pb
   variable  k   C-index
8        Pb  1  0.736008
9        Pb  3  0.762859
10       Pb  5  0.748131
11       Pb  7  0.749941


Group: c_total
  variable  k   C-index
0  c_total  1  0.823848
1  c_total  3  0.823115
2  c_total  5  0.816074
3  c_total  7  0.819694
```

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).

In [8]:
```
for name, group in grouped_loo_df:
    plt.plot(group['k'], group['C-index'], marker='o', linestyle='-', label=name)

plt.title('C-Index vs. k for Leave-one-out')
plt.xlabel('k values')
plt.ylabel('C-Index')
plt.legend(title='Column')
plt.show()
```



In [9]:
```
for name, group in grouped_logo_df:
    plt.plot(group['k'], group['C-index'], marker='o', linestyle='-', label=name)

plt.title('C-Index vs. k for Leave-replicas-out')
plt.xlabel('k values')
plt.ylabel('C-Index')
plt.legend(title='Column')
plt.show()
```

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?

In this cell write your answers to the questions.

1. Leave-one-out had more optimistic results.
2. Leave-one-out uses one data point as an test sample each iteration. We know that there are at least 3 identical data points as the one we are using as test sample. In leave-replicas-out method there migth be no identical samples in the train set as in the test set.
3. Leave-one-out might be too optimistic and overfitted so Leave-replicas-out method could generalze the unseen data better. The higher c-index values implicate LOO to be the better of these two methods but seems to be little overfitted.