Project 1: Predicting Metal Ion Concentration from Multi-Parameter Water Samples using KNN Regression and Cross-Validation

Import libraries ¶

In [67]:
```
import pandas as pd
from scipy.stats import kendalltau
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import LeaveOneOut
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import somersd
```

Read and visualize the dataset

Note: This dataset differs slightly from the one used in the video lectures.
In this dataset, some mixtures have 3 replicas, while others have 4 replicas.

In the following cell:

- Read the file water_data.csv
- Print the dimesions of the dataset (i.e. number of rows and columns) and display the first 5 rows.
- Identify the inputs and the outputs columns.
- Provide the number of mixtures with 3 replicas and 4 replicas, respectively.

In [68]:
```
# Here we are reading the dataset
file_path = 'water_data.csv'
df = pd.read_csv(file_path)
```

In [54]:
```
df
```

Out[54]:

	c_total	Cd	Pb	Mod1	Mod2	Mod3
0	0.0	0.0	0.0	-0.999216	-0.714208	-0.414911
1	0.0	0.0	0.0	-0.990800	-0.714373	-0.238335
2	0.0	0.0	0.0	-0.990539	-0.714125	0.020788
3	14.0	0.0	14.0	-1.001247	-0.713546	0.945465
4	14.0	0.0	14.0	-1.013727	-0.714125	0.569631
...	...	...	...	...	...	...
220	5000.0	4000.0	1000.0	-0.874613	-0.584157	-1.515186
221	5000.0	4000.0	1000.0	-0.875954	-0.604495	-1.516845
222	5000.0	5000.0	0.0	-0.872241	-0.349768	0.499810
223	5000.0	5000.0	0.0	-0.872021	-0.354729	0.777301
224	5000.0	5000.0	0.0	-0.865256	-0.373414	0.712840

225 rows × 6 columns

In [55]:
```
df.head()
```

Out[55]:

	c_total	Cd	Pb	Mod1	Mod2	Mod3
0	0.0	0.0	0.0	-0.999216	-0.714208	-0.414911
1	0.0	0.0	0.0	-0.990800	-0.714373	-0.238335
2	0.0	0.0	0.0	-0.990539	-0.714125	0.020788
3	14.0	0.0	14.0	-1.001247	-0.713546	0.945465
4	14.0	0.0	14.0	-1.013727	-0.714125	0.569631

In [69]:
```
# Print dataset dimensions and first 5 rows
print(f"Dataset Dimensions: {df.shape}")
df.head()
```

```
Dataset Dimensions: (225, 6)
```

Out[69]:

	c_total	Cd	Pb	Mod1	Mod2	Mod3
0	0.0	0.0	0.0	-0.999216	-0.714208	-0.414911
1	0.0	0.0	0.0	-0.990800	-0.714373	-0.238335
2	0.0	0.0	0.0	-0.990539	-0.714125	0.020788
3	14.0	0.0	14.0	-1.001247	-0.713546	0.945465
4	14.0	0.0	14.0	-1.013727	-0.714125	0.569631

In [71]:
```
# Identifying unique mixtures based on the first three columns (output colu
grouped = df.groupby(['c_total', 'Cd', 'Pb'])

# Counting the number of replicas for each unique mixture
replica_counts = grouped.size().reset_index(name='Replica_Count')

# Merging back with the original dataset to retain the replica count inform
df = df.merge(replica_counts, on=['c_total', 'Cd', 'Pb'], how='left')

# Print number of mixtures with 3 and 4 replicas
num_3_replicas = (df['Replica_Count'] == 3).sum()
num_4_replicas = (df['Replica_Count'] == 4).sum()
print(f"Number of mixtures with 3 replicas: {num_3_replicas}")
print(f"Number of mixtures with 4 replicas: {num_4_replicas}")
```

```
Number of mixtures with 3 replicas: 129
Number of mixtures with 4 replicas: 96
```

In [58]:
```
# Define input and output variables
X = df[['Mod1', 'Mod2', 'Mod3']].values
y = df[['c_total', 'Cd', 'Pb']].values
```

C-index code

In [59]:
```
# In this cell is the fuction that computes the c-index value based on Some
# Use this fuction as the evaluation metric in the Leave-One-Out (LOOCV) an

def cindex(true, pred):
    s_d = somersd(true, y=pred, alternative='two-sided')
    c_index = (s_d.statistic + 1.0)/2.0
    return c_index
```

Functions

In [60]:
```
# In this cell add the functions that you need for the data analysis part.
```

Results for Leave-One-Out cross-validation

In [61]:
```
# Here run your script for Leave-One-Out cross-validation and print the cor
```

In [62]:
```
# Initialize Leave-One-Out cross-validation
loo = LeaveOneOut()

# Evaluate C-index for different k values
k_values = [1, 3, 5, 7]
c_index_results = []

for k in k_values:
    # Initialize lists to store true and predicted values for each output
    y_true_all = [[] for _ in range(3)]
    y_pred_all = [[] for _ in range(3)]

    for train_index, test_index in loo.split(X):
        X_train, X_test = X[train_index], X[test_index]
        y_train, y_test = y[train_index], y[test_index]

        # Train Nearest Neighbors Regression model
        model = KNeighborsRegressor(n_neighbors=k)
        model.fit(X_train, y_train)

        # Make predictions
        y_pred = model.predict(X_test)

        # Store true and predicted values for each output
        for i in range(3):
            y_true_all[i].append(y_test[:, i][0])  # Ensure scalar values
            y_pred_all[i].append(y_pred[:, i][0])

    # Compute C-index for each output variable
    c_indices = [cindex(y_true_all[i], y_pred_all[i]) for i in range(3)]
    c_index_results.append([k] + c_indices)

# Convert results to a DataFrame and display
c_index_df = pd.DataFrame(c_index_results, columns=['k', 'C-index c_total',
print(c_index_df)
```

```
   k  C-index c_total  C-index Cd  C-index Pb
0  1         0.908283    0.921869    0.880549
1  3         0.914191    0.899591    0.874452
2  5         0.894101    0.861966    0.854261
3  7         0.873729    0.814152    0.835533
```

Results for Leave-Replicas-Out cross-validation

In [63]:
```
# Here run your script for Leave-Replicas-Out cross-validation and print th
```

In [64]:
```
c_index_results_lro = []

for k in k_values:
    y_true_all = [[] for _ in range(3)]
    y_pred_all = [[] for _ in range(3)]

    for mixture, group in df.groupby(['c_total', 'Cd', 'Pb']):
        if len(group) > 1:  # Ensure there are replicas
            test = group  # Use all replicas as test data
            train = df.drop(test.index)  # Exclude all replicas from traini

            X_train, y_train = train[['Mod1', 'Mod2', 'Mod3']], train[['c_t
            X_test, y_test = test[['Mod1', 'Mod2', 'Mod3']], test[['c_total

            model = KNeighborsRegressor(n_neighbors=min(k, len(X_train)))
            model.fit(X_train, y_train)
            y_pred = model.predict(X_test)

            for i in range(3):
                y_true_all[i].extend(y_test.iloc[:, i].values)
                y_pred_all[i].extend(y_pred[:, i])

    c_indices = [cindex(y_true_all[i], y_pred_all[i]) for i in range(3)]
    c_index_results_lro.append([k] + c_indices)

# Convert results to a DataFrame and display
c_index_df_lro = pd.DataFrame(c_index_results_lro, columns=['k', 'C-index c
print("Leave-Replicas-Out Cross-Validation Results:")
print(c_index_df_lro)
```

```
Leave-Replicas-Out Cross-Validation Results:
   k  C-index c_total  C-index Cd  C-index Pb
0  1         0.818413    0.778427    0.737775
1  3         0.818673    0.761452    0.768948
2  5         0.811702    0.739717    0.747839
3  7         0.816371    0.715309    0.761849
```

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

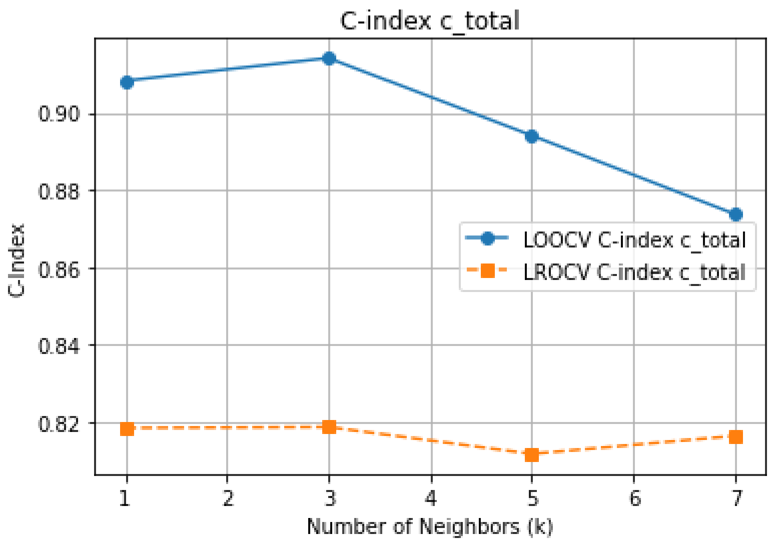
Note: You may plot the results as they were presented in the video lecture (refer to MOOC2-Module 2 .pptx slides).

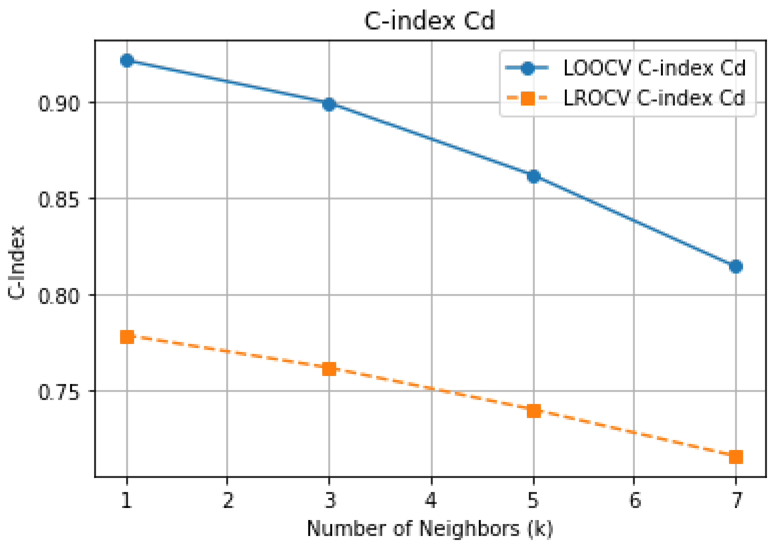
In [72]:
```python
# just to verify the variables
print(c_index_df)
print(c_index_df_lro)
```

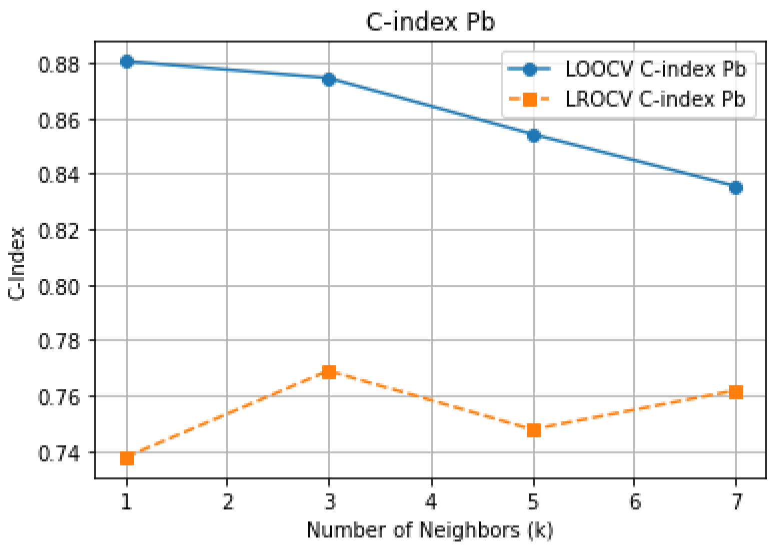
```
   k  C-index c_total  C-index Cd  C-index Pb
0  1         0.908283    0.921869    0.880549
1  3         0.914191    0.899591    0.874452
2  5         0.894101    0.861966    0.854261
3  7         0.873729    0.814152    0.835533
   k  C-index c_total  C-index Cd  C-index Pb
0  1         0.818413    0.778427    0.737775
1  3         0.818673    0.761452    0.768948
2  5         0.811702    0.739717    0.747839
3  7         0.816371    0.715309    0.761849
```

```
In [66]: #plotting the graphhs between k-valus and c-index for total, Cd and Pb
         outputs = ['C-index c_total', 'C-index Cd', 'C-index Pb']
         for output in outputs:
             plt.figure(figsize=(6, 4))
             plt.plot(k_values, c_index_df[output], marker='o', linestyle='-', label
             plt.plot(k_values, c_index_df_lro[output], marker='s', linestyle='--',

             plt.xlabel("Number of Neighbors (k)")
             plt.ylabel("C-Index")
             plt.title(f"{output}")
             plt.legend()
             plt.grid()
             plt.show()
```







Interpretation of results

Answer the following questions based on the results obtained

1. Which cross-validation approach produced more optimistic results, and why?
2. Which cross-validation method provides a better estimate of the model's performance on unseen mixtures? Explain your answer.

Answers:

Answer: 1 I think the Leave-One-Out cross-validation (LOOCV) generally produces more optimistic results compared to Leave-Replicas-Out cross-validation (LROCV). This is because LOOCV removes only one single sample at a time, which allows the model to train on almost the entire dataset, which leads to lower variability in predictions and often sometimes higher C-index values. On the other hand, LROCV removes entire sets of replicated measurements for a given mixture, which makes the test set more independent and which in turn prevents the model from relying on nearly identical training samples. This results in a more realistic evaluation of generalization performance, which often leads to lower C-index values compared to LOOCV.

Answer: 2 I think LROCV provides a better estimate of the model’s performance on unseen mixtures compared to LeaveLOOCV. I think this is because LROCV removes all replicas of a given mixture from the training set, which ensures that the model is tested on completely unseen data. on the other hand LOOCV only removes one single instance at a time, which means that the test sample often has very similar training samples available, which leads to an overestimation of the model’s performance. I think by ensuring that the test data is truly independent of the training set, LROCV is able to give a more realistic measure of the model’s generalization ability to new mixtures.