Assignment 1 Task 1: KNN Regressor

Student ID = 31237223

Name = Yee Darren Jer Shien

Question 1.1: KNN Regressor

1.1 Preprocess Diabetes and California Housing Data

In [232…

```
from sklearn.datasets import load_diabetes, fetch_california_housing

diabetes = load_diabetes()
diabetes.data.shape, diabetes.target.shape, diabetes.feature_names
california_housing = fetch_california_housing()
```

In [233…

```
import numpy as np

# Splits data set according to method used in lab
def train_test_split(x, y, train_size=0.6, random_state=None):
    RNG = np.random.default_rng(random_state)
    N = len(x)
    N_train = round(N*train_size)
    idx_train = RNG.choice(N, N_train, replace=False)
    idx_test = np.setdiff1d(np.arange(N), idx_train)
    RNG.shuffle(idx_test)
    x_train = x[idx_train]
    y_train = y[idx_train]
    x_test = x[idx_test]
    y_test = y[idx_test]
    return x_train, x_test, y_train, y_test


x_train_diabetes, x_test_diabetes, y_train_diabetes, y_test_diabetes = train_test_s
x_train_cali, x_test_cali, y_train_cali, y_test_cali = train_test_split(california_
```

1.1 KNN Regressor Method

In [234…

```
from sklearn.base import BaseEstimator
from scipy.spatial import KDTree
from scipy.stats import pmean
from sklearn.metrics import mean_squared_error


class KnnRegressor(BaseEstimator):
    def __init__(self,k):
        self.k = k

    def fit(self, x, y):
        self.y_train_ = y
        self.x_train_kdtree_ = KDTree(x)
        return self

    # Predict method adapted from lab, we take the mean of each neighbouring values
    def predict(self, x):
        _, neighbours = self.x_train_kdtree_.query(x, k=self.k)
        neighbours = neighbours.reshape(len(x), self.k)
        neighbour_labels = self.y_train_[neighbours]
        m = pmean(neighbour_labels, axis=1, keepdims=False, p = 1)
        return m
```

Question 1.2: Training using Diabetes dataset

In [235…

```
knn1 = KnnRegressor(3)
knn1.fit(x_train_diabetes,y_train_diabetes)
y_hat_test_diabetes = knn1.predict(x_test_diabetes)
```

Question 1.2: Training using California housing dataset

In [236…

```
knn2 = KnnRegressor(3)
knn2.fit(x_train_cali,y_train_cali)
y_hat_test_cali = knn2.predict(x_test_cali)
```

Question 1.2: Error Rate for Training and Test Error Calculation

In [237…

```
from sklearn.metrics import mean_squared_error
import math
def error_rate(y, y_hat):
    error = mean_squared_error(y,y_hat)
    return math.sqrt(error)
```

Question 1.2: Error Rate of Diabetes dataset

In [238…

```
y_hat_train_diabetes = knn1.predict(x_train_diabetes)
error_rate(y_train_diabetes, y_hat_train_diabetes), error_rate(y_test_diabetes, y_h
```

Out[238]:

```
(48.50558333074415, 65.71185841590591)
```

Question 1.2: Error Rate of California Housing dataset

In [239…

```
y_hat_train_cali = knn2.predict(x_train_cali)
error_rate(y_train_cali, y_hat_train_cali), error_rate(y_test_cali, y_hat_test_cali
```

Out[239]:

```
(0.7560985377778375, 1.121240738220602)
```

Question 1.2: Default Bootstrap Splitter CV method adapted from lab, used for testing KNN Regressor Model

In [240…

```
import numpy as np
from sklearn.metrics import make_scorer, mean_squared_error

class BootstrapSplitter:

    def __init__(self, reps, train_size, random_state=None):
        self.reps = reps
        self.train_size = train_size
        self.RNG = np.random.default_rng(random_state)

    def get_n_splits(self):
        return self.reps

    def split(self, x, y=None, groups=None):
        for _ in range(self.reps):
            N = len(x)
            N_train = round(N*self.train_size)
            train_idx = self.RNG.choice(N, N_train, replace=True)
            test_idx = np.setdiff1d(np.arange(len(x)), train_idx)
            np.random.shuffle(test_idx)
            yield train_idx, test_idx
```

Question 1.2: Evaluation method adapted from lab, used to evaluate performance of KNN Regressor Diabetes Model

In [241...

```
from sklearn.model_selection import cross_validate

def evaluation(max_k, cv, data, target):
    r = cv.get_n_splits()
    test_results = np.zeros(shape=(r, max_k))
    train_results = np.zeros(shape=(r, max_k))
    for k in range(1, max_k+1):
        knn = KnnRegressor(k)
        cv_res = cross_validate(knn,data,target, cv=cv, return_train_score=True, sc
        test_results[:, k-1] = cv_res['test_score']
        train_results[:, k-1] = cv_res['train_score']

    return train_results, test_results
```

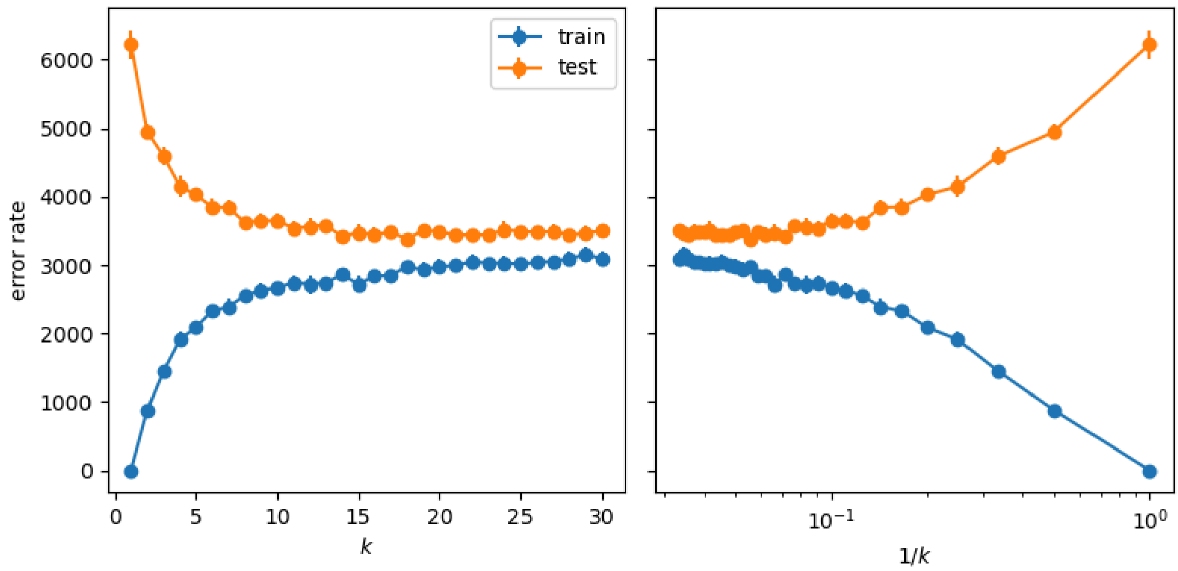
In [242...

```
import matplotlib.pyplot as plt

def plot (max_k,train_results,test_results):
    ks = np.arange(1, max_k+1)
    _, axs = plt.subplots(1, 2, figsize=(8,4), tight_layout=True, sharey=True)
    z = (reps**0.5)/1.96
    axs[0].errorbar(ks, train_results.mean(axis=0), yerr=train_results.std(axis=0)/
    axs[0].errorbar(ks, test_results.mean(axis=0), yerr=test_results.std(axis=0)/z,
    axs[0].legend()
    axs[0].set_xlabel('$k$')
    axs[0].set_ylabel('error rate')
    axs[1].errorbar(1/ks, train_results.mean(axis=0), yerr=train_results.std(axis=0
    axs[1].errorbar(1/ks, test_results.mean(axis=0), yerr=test_results.std(axis=0)/
    axs[1].set_xscale('log')
    axs[1].set_xlabel('$1/k$')
    plt.show()
```

In [243...

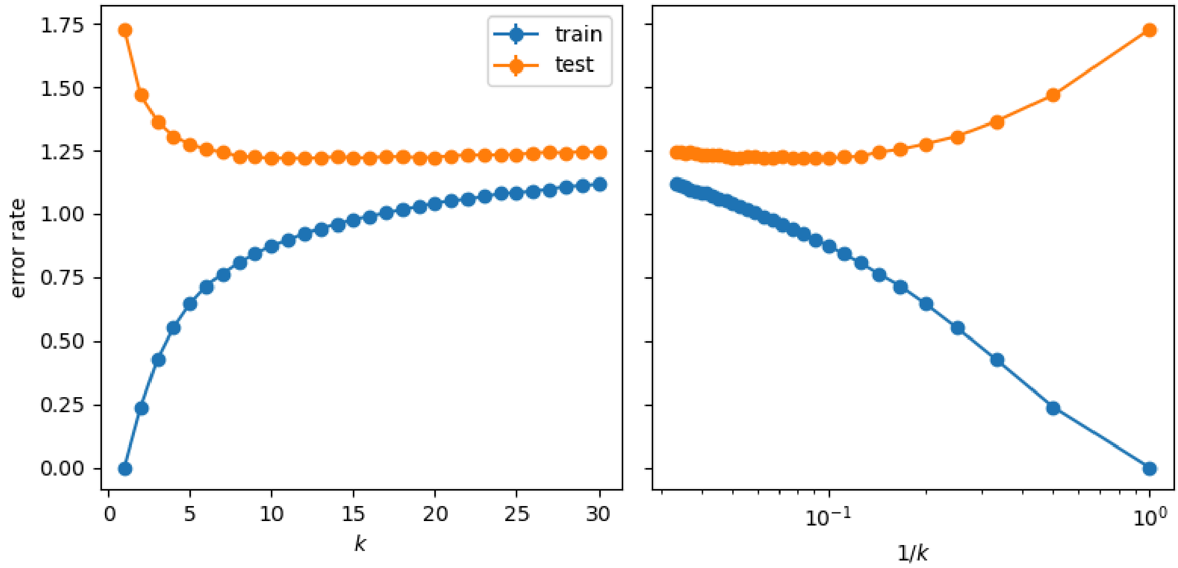
```
reps=25
max_k=30
train_results, test_results = evaluation(max_k=max_k, cv=BootstrapSplitter(reps, 0.
plot (max_k,train_results,test_results)
```



Question 1.2: Evaluation for KNN Regressor California Housing Model

In [244…

```
reps=25
max_k=30
train_results, test_results = evaluation(max_k=max_k, cv=BootstrapSplitter(reps, 0.
plot (max_k,train_results,test_results)
```



Question 1.2 Justification

From both graphs, we can see that our model performs as intended with testing error starting high and training error starting low, before both converging to an optimal level that balances between model's performance on seen and unseen data

Question 2.1: L Fold Cross Validation Model

In [245…

```
class LFold:
    def __init__(self, k, random_state=None): # ADD PARAMETERS AS REQUIRED
        self.k = k
        self.RNG = np.random.default_rng(random_state)

    def get_n_splits(self, x=None, y=None, groups=None):
        return self.k

    def split(self, x, y=None, groups=None):
        # size per fold
        per_fold = len(x) // self.k
        # creates the array contaning [0..len(x)-1] which represents all indices av
        indices_arr = np.arange(len(x))
        np.random.shuffle(indices_arr)
        for i in range (self.k):
            # slice the test idx based on the current fold
            test_idx = indices_arr [i*per_fold : i*per_fold + per_fold]
            # take every index before the current fold
            head = indices_arr [:i*per_fold]
            # take every index after the current fold
            tail = indices_arr [i*per_fold + per_fold:]
            # concatenate the leftover array into our train idx array
            train_idx = np.concatenate((head,tail))
            yield train_idx, test_idx
```

Question 2.2 Evaluation Model for L Fold Cross Validation Model

In [246…

```
from sklearn.model_selection import cross_validate

def evaluation_l_fold(max_k, cv,data,target):

    r = cv.get_n_splits()
    test_mean = np.zeros(max_k)
    test_std = np.zeros(max_k)
    test_con = np.zeros(max_k)
    train_mean = np.zeros(max_k)
    train_std = np.zeros(max_k)
    train_con = np.zeros(max_k)

    for k in range(1, max_k+1):
        knn = KnnRegressor(k)
        current_fold_test_score = []
        current_fold_train_score = []
        test_scores = []
        train_scores = []

        for train_index, test_index in cv.split(data):
            X_train, X_test = data[train_index], data[test_index]
            y_train, y_test = target[train_index],target[test_index]

            knn.fit(X_train, y_train)
            y_train_pred = knn.predict(X_train)
            y_test_pred = knn.predict(X_test)

            train_scores.append(mean_squared_error(y_train, y_train_pred))
            test_scores.append(mean_squared_error(y_test, y_test_pred))

        test_mean[k - 1] = np.mean(test_scores)
        test_std[k - 1] = np.std(test_scores)
        test_con[k - 1] = (1.96 * test_std[k - 1]) / (np.sqrt(r))

        train_mean[k - 1] = np.mean(train_scores)
        train_std[k - 1] = np.std(train_scores)
        train_con[k - 1] = (1.96 * train_std[k - 1]) / (np.sqrt(r))

    return test_mean, test_std , test_con, train_mean, train_std, train_con
```

In [247…

```
def l_fold_plot (max_k, plot, test_mean, test_std , test_con, train_mean, train_std

    if plot == 1:
        plt.errorbar(range(1, max_k + 1), train_mean, yerr=train_std, label='Train'
        plt.errorbar(range(1, max_k + 1), test_mean, yerr=test_std, label='Test')
        plt.xlabel('Value of k')
        plt.ylabel('Mean Squared Error with std deviation error bar')
        plt.title('Mean Squared Error vs k')
        plt.legend()
        plt.show()

    elif plot == 2:
        plt.errorbar(range(1, max_k + 1), train_std, label='Train')
        plt.errorbar(range(1, max_k + 1), test_std, label='Test')
        plt.xlabel('Value of k')
        plt.ylabel('Standard Deviation')
        plt.title('Standard Deviation vs k')
        plt.legend()
        plt.show()

    else:
        plt.errorbar(range(1, max_k + 1), train_mean, yerr=train_con, label='Train'
        plt.errorbar(range(1, max_k + 1), test_mean, yerr=test_con, label='Test')
```

```
        plt.xlabel('Value of k')
        plt.ylabel('Mean Squared Error with confidence interval error bar')
        plt.title('Mean Squared Error vs k')
        plt.legend()
        plt.show()
```

Question 2.2 Running L Fold evaluation on Diabetes data set

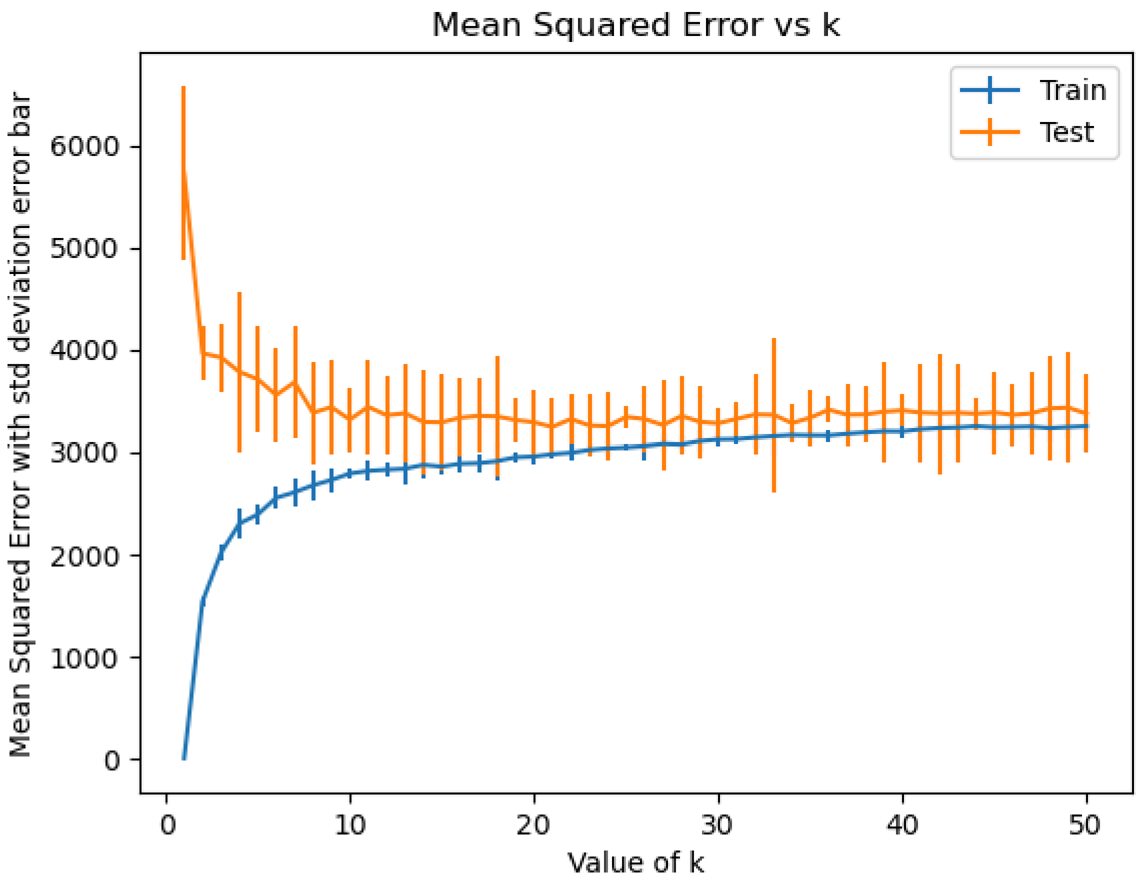
In [248…

```
max_k = 50
test_mean_diabetes, test_std_diabetes , test_con_diabetes, train_mean_diabetes, tra
```

Question 2.2 Mean MSE vs k plot for diabetes data

In [249…

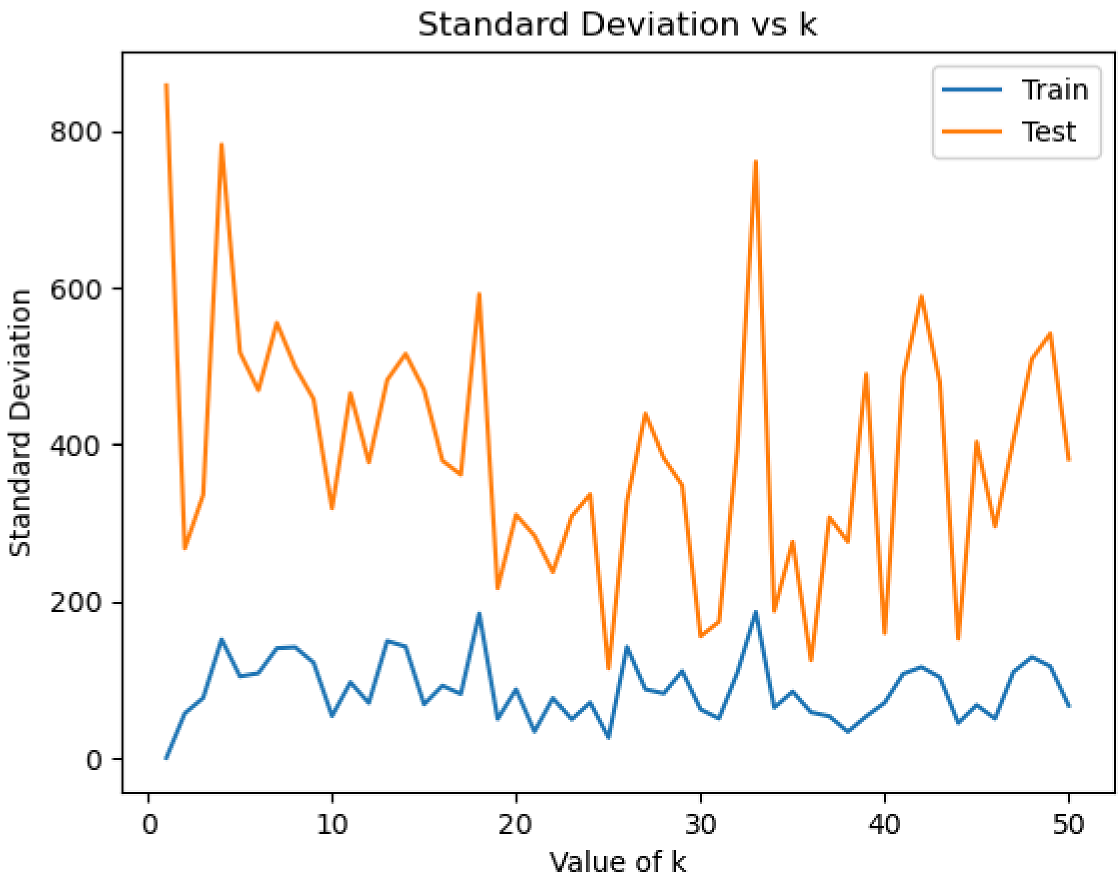
```
l_fold_plot (max_k, 1, test_mean_diabetes, test_std_diabetes , test_con_diabetes, t
```



Question 2.2 Standard Deviation vs k plot for diabetes data

In [250…

```
l_fold_plot (max_k, 2, test_mean_diabetes, test_std_diabetes , test_con_diabetes, t
```



Question 2.2 Reporting best K according to testing performance

In [251…

```
best_test_diabetes = np.argmin(test_mean_diabetes)
print ("Best K for Diabetes data set according to testing performance = ", best_tes
```

```
Best K for Diabetes data set according to testing performance =  21
```

Question 2.2 Running L Fold evaluation on California Housing data set

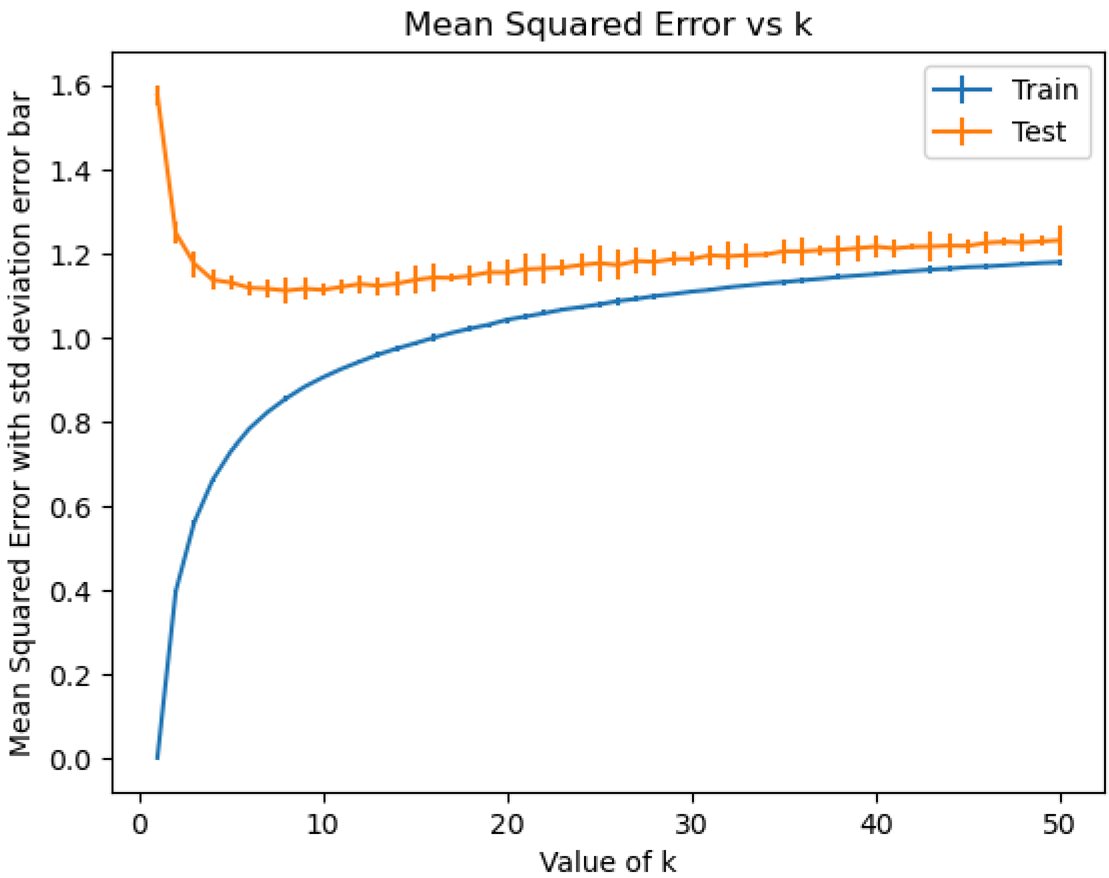
In [252…

```
max_k = 50
test_mean_ch, test_std_ch , test_con_ch, train_mean_ch, train_std_ch, train_con_ch=
```

Question 2.2 Mean MSE vs k plot for California Housing data

In [253…

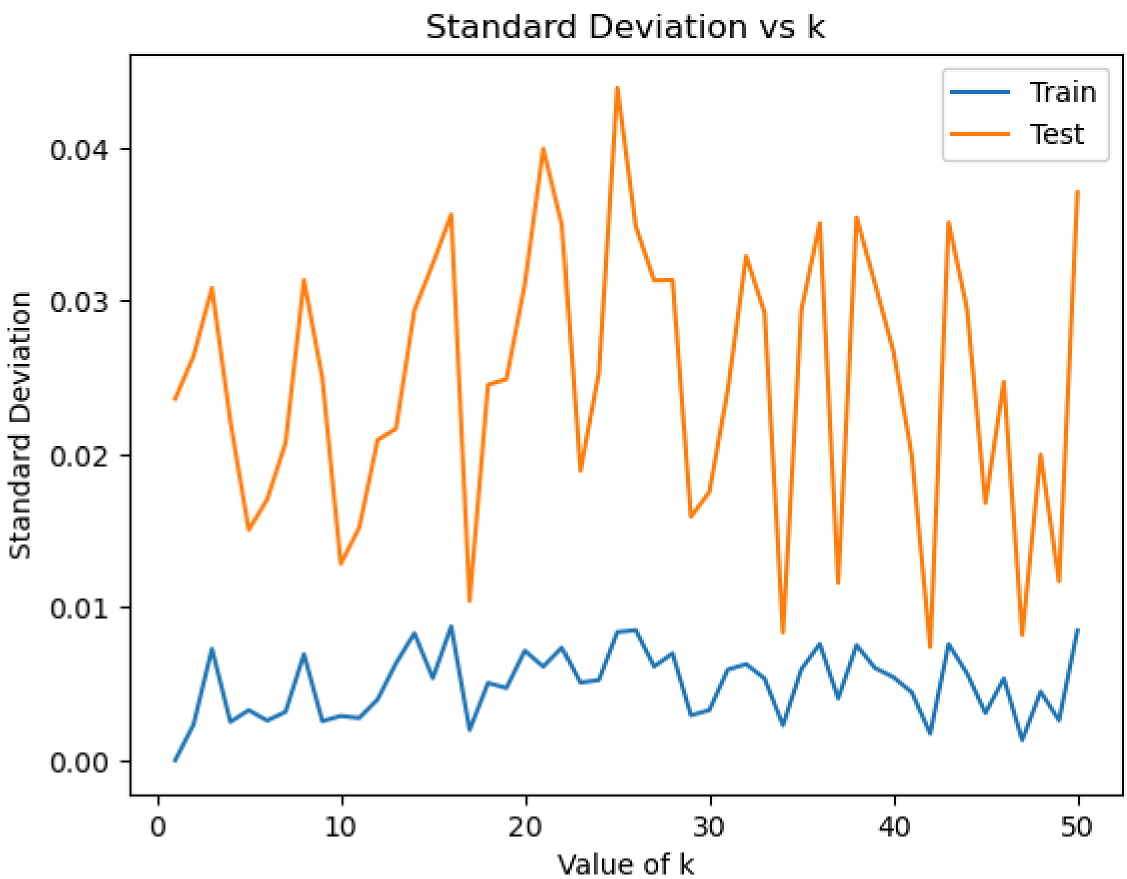
```
l_fold_plot (max_k, 1, test_mean_ch, test_std_ch , test_con_ch, train_mean_ch, trai
```



Question 2.2 Standard Deviation vs k plot for California Housing data

In [254…

```
l_fold_plot (max_k, 2, test_mean_ch, test_std_ch , test_con_ch, train_mean_ch, trai
```



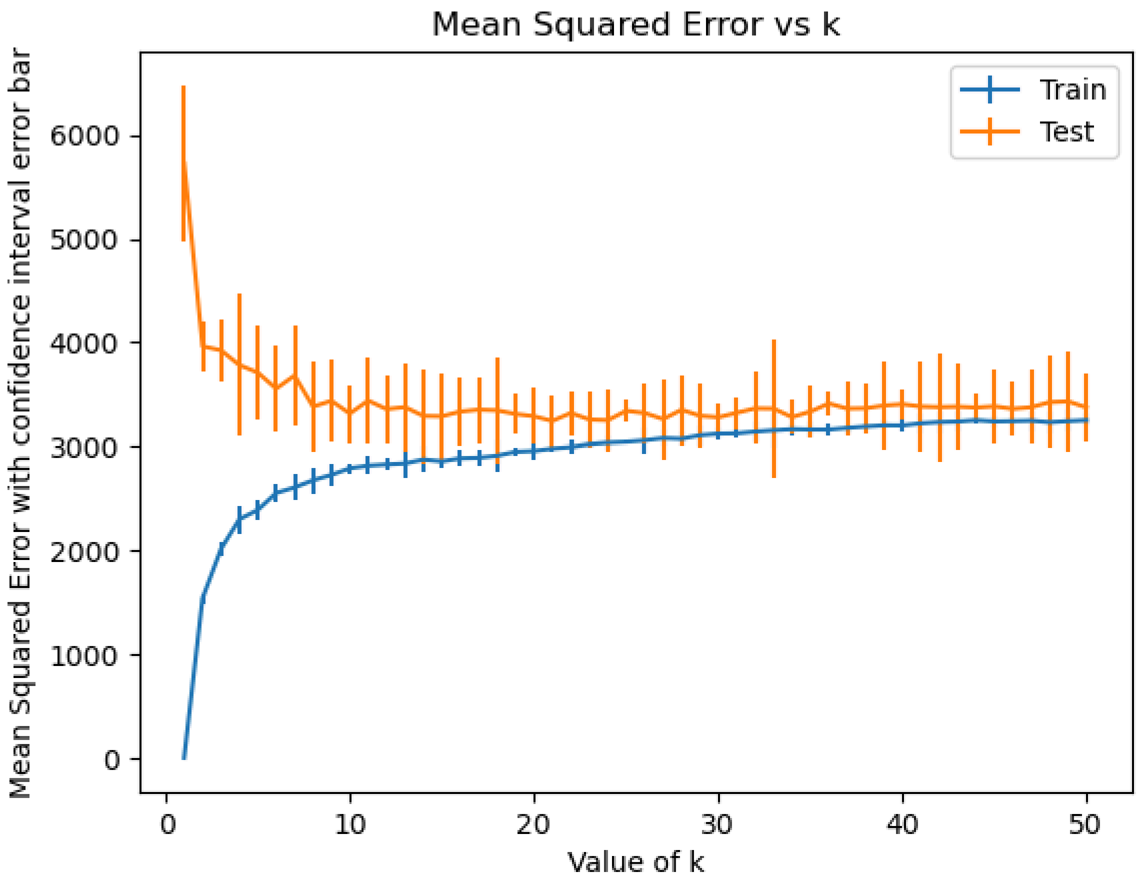
Question 2.2 Reporting best K according to testing performance

In [255…
```
best_test_ch = np.argmin(test_mean_ch)
print ("Best K for California Housing data set according to testing performance = "
```

```
Best K for California Housing data set according to testing performance =  8
```

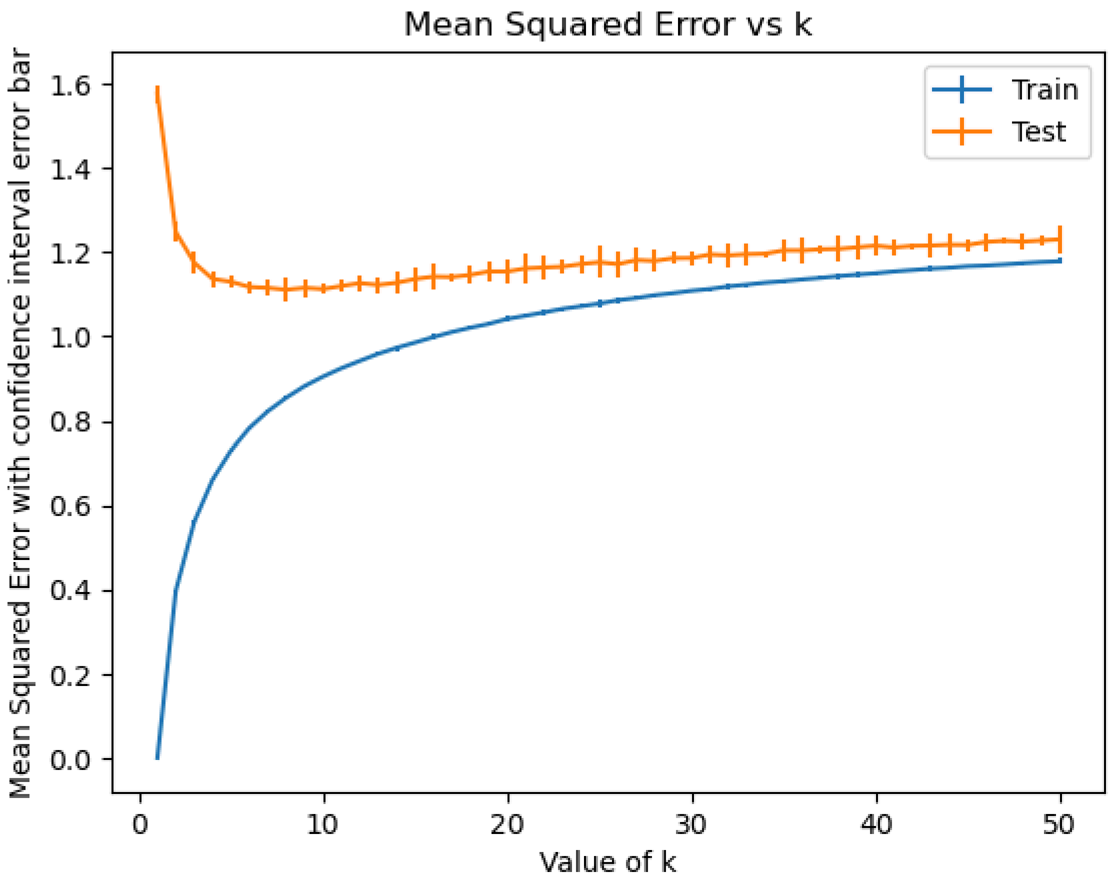
Question 2.3 MSE plot against K using confidence interval error bar with L = 5 for Diabetes data set

In [256…
```
l_fold_plot (max_k, 3, test_mean_diabetes, test_std_diabetes , test_con_diabetes, t
```



Question 2.3 MSE plot against K using confidence interval error bar with L = 5 for California Housing data set

In [257…
```
l_fold_plot (max_k, 3, test_mean_ch, test_std_ch , test_con_ch, train_mean_ch, trai
```



Question 2.3 Running both datasets with different L value

In [258…

```
max_k = 50
fold = 20
test_mean_diabetes, test_std_diabetes , test_con_diabetes, train_mean_diabetes, tra
```

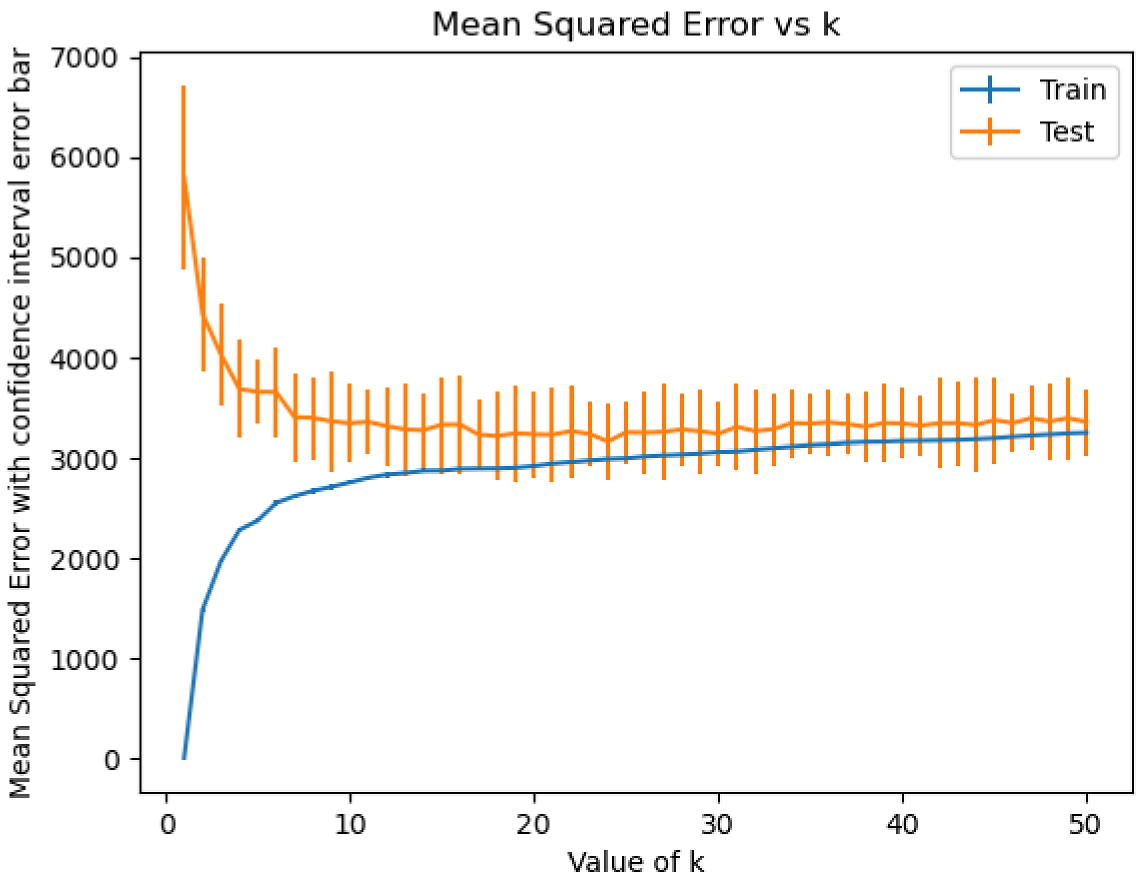
In [259…

```
test_mean_ch, test_std_ch , test_con_ch, train_mean_ch, train_std_ch, train_con_ch=
```

Question 2.3 MSE plot against K using confidence interval error bar with L = 10 for Diabetes data set

In [260…

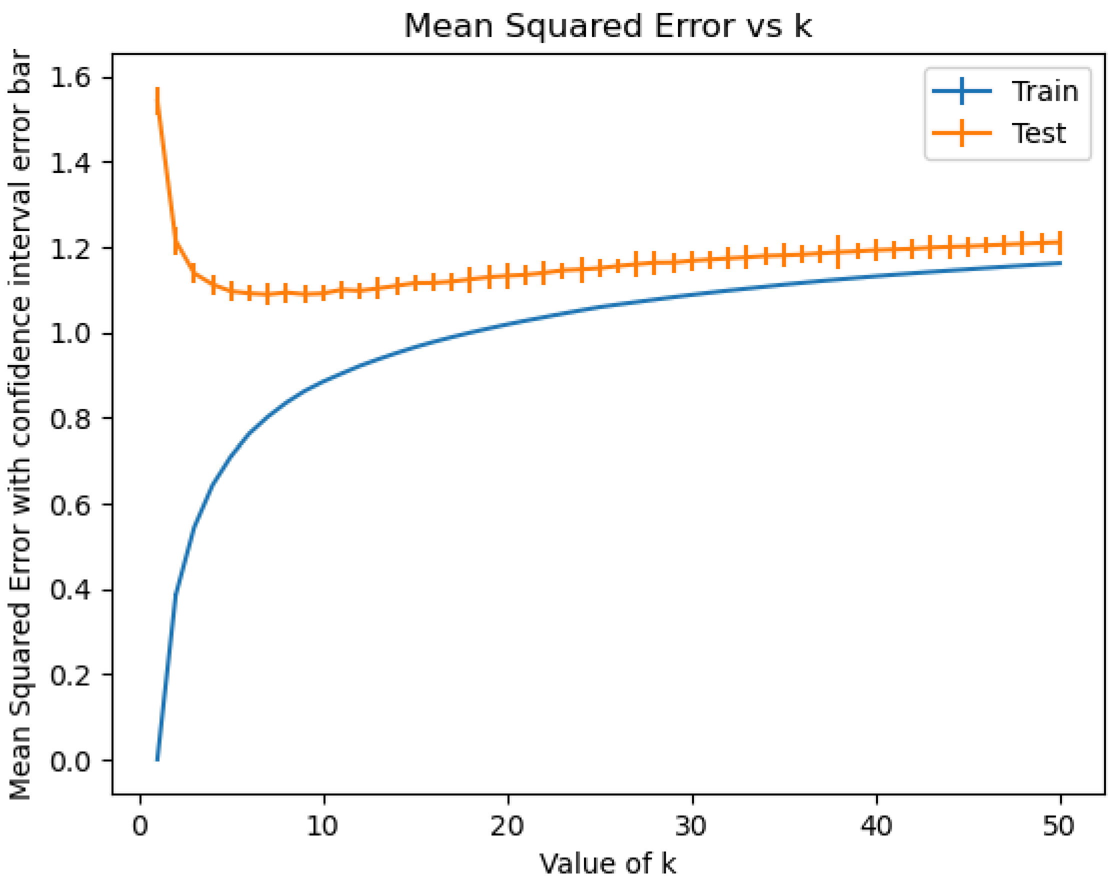
```
l_fold_plot (max_k, 3, test_mean_diabetes, test_std_diabetes , test_con_diabetes, t
```



Question 2.3 MSE plot against K using confidence interval error bar with L = 10 for California Housing data set

In [261…

```
l_fold_plot (max_k, 3, test_mean_ch, test_std_ch , test_con_ch, train_mean_ch, trai
```



Question 2.3 Justification

Effects of parameter K

The parameter K is extremely important for our KNN regressor as it decides how many neighbours should we base our predictions on. As we can see from the graphs, the model starts off overfitting for both datasets due to their low initial mean squared error values for training but high values for testing. This is due to the phenomenon that the model captures more noise instead of learning the underlying pattern which means that it fails to generalise well. However, as we increase the amount of points within the neighbourhood, we start to see testing error going down and training error going up instead, which shows that the model is slowly capturing relavant underlying pattern to predict unseen data. However, for both datasets, we can see that once K gets to around 20-30, the model becomes too simple due to the large number of points within the neighbourhood which causes both testing and training error to either stagnate or rise because the model is unable to capture relevant information.

Effects of L

We performed the same evaluation with different L values on both datasets and in both cases, we are able to see the effects of the increased number of fold by observing the confidence intervals. The confidence intervals for our training error seemingly decreases significantly which seems to indicate that the increased folds are helping the CV process by decreasing variability different portions of the data are being used which allows for a more stable estimation of training performance

Question 3 KNN Regressor with nested CV

In [262…

```
from sklearn.base import BaseEstimator

class KnnRegressorCV(BaseEstimator):
    def __init__(self, ks=list(range(1, 21)), cv=LFold(5)):
    # YOUR CODE HERE
        self.ks = ks
        self.cv = cv
        self.inner_best_k =[]
        self.outer_best_k = []

    def fit(self, x, y):
    # YOUR CODE HERE
        self.k = 0
        r = self.cv.get_n_splits()
        current_best_k = 0
        current = 0
        for idx_train, idx_test in self.cv.split(x):
            best_test = math.inf
            current_best_k = 0
            # for every k, loop every fold combination of this current fold
            for i in range (len(self.ks)):
                knn = KnnRegressor(self.ks[i])
                # inner cross validation
                for idx_train_inner, idx_val in self.cv.split(x[idx_train]):
                    current_fold_test = []
                    current_fold_train = []
                    cv_res = cross_validate(knn, x[idx_train_inner], y[idx_train_ir
                    current_fold_train.append(cv_res['train_score'])
                    current_fold_test.append(cv_res['test_score'])
```

```
                current_fold_train_score = np.mean(current_fold_train)
                current_fold_test_score = np.mean(current_fold_test)
                if current_fold_test_score < best_test:
                    current_best_k = self.ks[i]
                    best_test = current_fold_test_score
            self.inner_best_k.append(current_best_k)
            current += 1

            # Outer cross validation for outer folds which includes the training se
            best_outer_k = 0
            best_outer_score = math.inf
            for k in self.ks:
                knn = KnnRegressor(k)
                knn.fit(x[idx_train], y[idx_train])
                y_pred = knn.predict(x[idx_test])
                outer_score = mean_squared_error(y[idx_test], y_pred)
                if outer_score < best_outer_score:
                    best_outer_score = outer_score
                    best_outer_k = k
            self.outer_best_k.append(best_outer_k)
        self.k = math.floor(np.mean(self.inner_best_k))
        self.y_train_ = y
        self.x_train_kdtree_ = KDTree(x)
        return self


    def predict(self, x):
        _, neighbours = self.x_train_kdtree_.query(x, k=self.k)
        neighbours = neighbours.reshape(len(x), self.k)
        neighbour_labels = self.y_train_[neighbours]
        m = pmean(neighbour_labels, axis=1, keepdims=False, p = 1)
        return m
```

In [263…

```
knn_cv = KnnRegressorCV()
knn_cv.fit(x_train_diabetes,y_train_diabetes)
y_hat_test_diabetes = knn_cv.predict(x_test_diabetes)
y_hat_train_diabetes = knn_cv.predict(x_train_diabetes)
error_rate(y_train_diabetes, y_hat_train_diabetes), error_rate(y_test_diabetes, y_h
```

Out[263]:

```
(57.82457620597039, 54.32521156685629)
```

In [264…

```
knn_cv2 = KnnRegressorCV()
knn_cv2.fit(x_train_cali,y_train_cali)
y_hat_test_cali = knn_cv2.predict(x_test_cali)
y_hat_train_cali = knn_cv2.predict(x_train_cali)
error_rate(y_train_cali, y_hat_train_cali), error_rate(y_test_cali, y_hat_test_cali
```

Out[264]:

```
(0.9599509799467973, 1.0894768645457906)
```

Question 3.2 Displaying the inner and outer CV across both datasets

In [265…

```
print ("KNN Regressor Diabetes Inner CV Best K = ", np.mean(knn_cv.inner_best_k))
print ("KNN Regressor Diabetes Outer CV Best K = ", np.mean(knn_cv.outer_best_k))
print ("KNN Regressor California Housing Inner CV Best K = ", np.mean(knn_cv2.inner
print ("KNN Regressor California Housing Outer CV Best K = ", np.mean(knn_cv2.outer
```

```
KNN Regressor Diabetes Inner CV Best K =  14.2
KNN Regressor Diabetes Outer CV Best K =  12.0
KNN Regressor California Housing Inner CV Best K =  10.0
KNN Regressor California Housing Outer CV Best K =  8.0
```

Question 3.2 Justification for inner and outer CV

For both datasets, we can see that the inner cross validation is consistently able to select an optimal K that is close to the outer cross validation step. This is crucial since the outer cross validation is done with the testing set included. This means that the inner CV is able to find hyperparameters that are close enough for the data to perform well for both training data as well as generalise well on unseen data