KNN regression experiments

In class we learned about how KNN regression works, and tips for using KNN. For example, we learned that data should be scaled when using KNN, and that extra, useless predictors should not be used with KNN. Are these tips really correct?

In this notebook we run a bunch of tests to see how KNN is affect by the choice of k, scaling of the predictors, presence of useless predictors, and other things.

One experiment we do not run, and which would be interesting, is to see how KNN performance changes as a function of the size of the training set.

INSTRUCTIONS

Out[3]: Click here to display/hide the code.

Enter code wherever you see # YOUR CODE HERE in code cells, or YOU TEXT HERE in markup cells.

```
In [1]:
        import numpy as np
        import pandas as pd
        from sklearn.model_selection import train_test_split
        from sklearn.preprocessing import StandardScaler
        from sklearn.neighbors import KNeighborsRegressor
        import matplotlib.pyplot as plt
In [2]: # set default figure size
        plt.rcParams['figure.figsize'] = [8.0, 6.0]
In [3]: # code in this cell from:
        # https://stackoverflow.com/questions/27934885/how-to-hide-code-from-cells-in-ipyth
        from IPython.display import HTML
        HTML('''<script>
        code_show=true;
        function code_toggle() {
         if (code_show){
         $('div.input').hide();
         } else {
         $('div.input').show();
         code_show = !code_show
        $( document ).ready(code_toggle);
        <form action="javascript:code_toggle()"><input type="submit" value="Click here to d</pre>
```

Read the data and take a first look at it

The housing dataset is good for testing KNN because it has many numeric features. See Aurélien Géron's book titled 'Hands-On Machine learning with Scikit-Learn and TensorFlow' for information on the dataset.

```
In [4]: df = pd.read_csv("https://raw.githubusercontent.com/grbruns/cst383/master/housing.c
```

In [5]: | df.info()

<class 'pandas.core.frame.DataFrame'> RangeIndex: 20640 entries, 0 to 20639 Data columns (total 10 columns):

```
Non-Null Count Dtype
# Column
                               _____
---
0 longitude 20640 non-null float64
1 latitude 20640 non-null float64
 2 housing_median_age 20640 non-null float64
3 total_rooms 20640 non-null float64
4 total_bedrooms 20433 non-null float64
5 population 20640 non-null float64
6 households 20640 non-null float64
7 median_income 20640 non-null float64
     median_house_value 20640 non-null float64
 9 ocean_proximity 20640 non-null object
dtypes: float64(9), object(1)
```

memory usage: 1.6+ MB

Note that numeric features have different ranges. For example, the mean value of 'total_rooms' is over 2,500, while the mean value of 'median_income' is about 4. 'median_house_value' has a much greater mean value, over \$200,000, but we will be using it as the target variable.

```
In [6]: from IPython.display import Image
        from IPython.core.display import HTML
        Image(url= "data:image/jpeg;base64,/9j/4AAQSkZJRgABAQAAAQABAAD/2wCEAAoHCBIVFRgVFRYY
        #Flickr source for "Houses going down" : https://www.flickr.com/photos/59937401@N07
```

Out[6]:



```
In [7]: df.describe()
```

Out[7]:		longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population
	count	20640.000000	20640.000000	20640.000000	20640.000000	20433.000000	20640.0000
	mean	-119.569704	35.631861	28.639486	2635.763081	537.870553	1425.4767
	std	2.003532	2.135952	12.585558	2181.615252	421.385070	1132.4621
	min	-124.350000	32.540000	1.000000	2.000000	1.000000	3.0000
	25%	-121.800000	33.930000	18.000000	1447.750000	296.000000	787.0000
	50%	-118.490000	34.260000	29.000000	2127.000000	435.000000	1166.0000
	75%	-118.010000	37.710000	37.000000	3148.000000	647.000000	1725.0000
	max	-114.310000	41.950000	52.000000	39320.000000	6445.000000	35682.0000

Missing Data

Notice that 207 houses are missing their total_bedroom info:

```
In [8]:
        print(df.isnull().sum())
         df[df['total_bedrooms'].isnull()]
                                  0
        longitude
        latitude
                                 0
        \verb|housing_median_age|
        total_rooms
                                  0
        total_bedrooms
                               207
                                 0
        population
        households
                                 0
                                 0
        median_income
        median_house_value
                                 0
        ocean_proximity
        dtype: int64
```

Out[8]:		longitude	latitude	housing_median_age	total_rooms	total_bedrooms	population	househ
	290	-122.16	37.77	47.0	1256.0	NaN	570.0	2
	341	-122.17	37.75	38.0	992.0	NaN	732.0	2
	538	-122.28	37.78	29.0	5154.0	NaN	3741.0	12
	563	-122.24	37.75	45.0	891.0	NaN	384.0	1
	696	-122.10	37.69	41.0	746.0	NaN	387.0	1
	•••							
	20267	-119.19	34.20	18.0	3620.0	NaN	3171.0	7
	20268	-119.18	34.19	19.0	2393.0	NaN	1938.0	7
	20372	-118.88	34.17	15.0	4260.0	NaN	1701.0	6
	20460	-118.75	34.29	17.0	5512.0	NaN	2734.0	8
	20484	-118.72	34.28	17.0	3051.0	NaN	1705.0	4

207 rows × 10 columns

Let's drop these instances for now

```
In [9]: df = df.dropna()
```

Prepare data for machine learning

We will use KNN regression to predict the price of a house from its features, such as size, age and location.

We use a subset of the data set for our training and test data. Note that we keep an unscaled version of the data for one of the experiments we will run.

```
In [10]: # for repeatability
    np.random.seed(42)

In [11]: # select the predictor variables and target variables to be used with regression
    predictors = ['longitude','latitude','housing_median_age','total_rooms', 'total_bed
    #dropping categortical features, such as ocean_proximity, including spatial ones su
    target = 'median_house_value'
    X = df[predictors].values
    y = df[target].values

In [12]: # KNN can be slow, so get a random sample of the full data set
    indexes = np.random.choice(y.size, size=10000)
    X_mini = X[indexes]
    y_mini = y[indexes]
```

```
In [13]: # Split the data into training and test sets, and scale
       scaler = StandardScaler()
       # unscaled version (note that scaling is only used on predictor variables)
       X_train_raw, X_test_raw, y_train, y_test = train_test_split(X_mini, y_mini, test_si
       # scaled version
       X_train = scaler.fit_transform(X_train_raw)
       X_test = scaler.transform(X_test_raw)
In [14]: # sanity check
       print(X_train.shape)
       print(X_train[:3])
       (7000, 8)
       [[\ 1.22783551\ -1.3492796\ \ 0.34639424\ -0.16627017\ \ 0.11697691\ -0.15874461
          0.18687025 -0.74984935]
        -0.14171346 1.12877289]
        -0.04890738 -0.10303138]]
```

Baseline performance

For regression problems, our baseline is the "blind" prediction that is just the average value of the target variable. The blind prediction must be calculated using the training data. Calculate and print the test set root mean squared error (test RMSE) using this blind prediction. I have provided a function you can use for RMSE.

```
In [15]: def rmse(predicted, actual):
    return np.sqrt(((predicted - actual)**2).mean())

In [16]: blind_prediction = y_train.mean()
    test_rmse = rmse(blind_prediction, y_test)
    print('test, rmse baseline: {:0.1f}'.format(test_rmse))
    test, rmse baseline: 112909.3
```

Performance with default hyperparameters

Using the training set, train a KNN regression model using the ScikitLearn KNeighborsRegressor, and report on the test RMSE. The test RMSE is the RMSE computed using the test data set.

When using the KNN algorithm, use algorithm='brute' to get the basic KNN algorithm.

```
In [17]: #train knn regression model using scikit kneighborsregressor
knn = KNeighborsRegressor(algorithm = 'brute')
knn.fit(X_train, y_train)

#predict
predictions = knn.predict(X_test)

#calculate RMSE
predicted_test_rmse = rmse(predictions, y_test)

#report RMSE
print('test RMSE, default hyperparameters: {:0.1f}'.format(predicted_test_rmse))
```

test RMSE, default hyperparameters: 62448.9

Impact of K

In class we discussed the relationship of the hyperparameter k to overfitting.

_I provided code to test KNN on k=1, k=3, k=5, ..., k=29. For each value of k, compute the training RMSE and test RMSE. The training RMSE is the RMSE computed using the training data. Use the 'brute' algorithm, and Euclidean distance, which is the default. You need to add the get_train_testrmse() function.

```
In [ ]:
In [18]:
         def get_train_test_rmse(regr, X_train, X_test, y_train, y_test):
             regr.fit(X_train, y_train)
             knn_predictions_train = regr.predict(X_train)
             knn_predictions_test = regr.predict(X_test)
             tr_rmse = rmse(y_train,knn_predictions_train)
             te_rmse = rmse(y_test, knn_predictions_test)
             return(tr_rmse, te_rmse)
In [19]: n = 30
         test_rmse = []
         train_rmse = []
         ks = np.arange(1, n+1, 2)
         for k in ks:
             print(k, ' ', end='')
             regr = KNeighborsRegressor(n_neighbors=k, algorithm='brute')
             rmse_tr, rmse_te = get_train_test_rmse(regr, X_train, X_test, y_train, y_test)
             train_rmse.append(rmse_tr)
             test_rmse.append(rmse_te)
         print('done')
         print(test_rmse)
         1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 done
```

[68169.22068133096, 64167.06662829433, 62448.852862157735, 62421.49844854768, 63020 .39551718987, 63671.29567276784, 63778.65866649261, 64058.43829650595, 64158.772794 491975, 64505.40182570007, 64626.24530464219, 64842.6353245348, 65072.84618154924, 65177.24405433061, 65250.508334697806]

```
In [20]: # sanity check
print('Test RMSE when k = 3: {:0.1f}'.format(np.array(test_rmse)[ks==3][0]))
Test RMSE when k = 3: 64167.1
```

Using the training and test RMSE values you got for each value of k, find the k associated with the lowest test RMSE value. Print this k value and the associated lowest test RMSE value. In other words, if you found that k=11 gave the lowest test RMSE, then print the value 11 and the test RMSE value obtained when k=11.

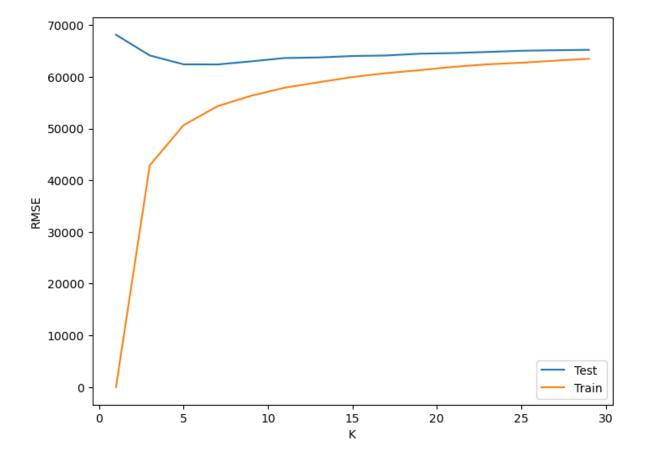
```
In [21]: def get_best(ks, rmse):
    return (ks[(np.array(rmse)) == (np.array(rmse)).min()][0], (np.array(rmse)).min

best_k, best_rmse = get_best(ks, test_rmse)
print('best k = {}, best test RMSE: {:0.1f}'.format(best_k, best_rmse))

best k = 7, best test RMSE: 62421.5
```

Plot the test and training RMSE as a function of k, for all the k values you tried.

Out[22]: <matplotlib.legend.Legend at 0x1e126f5d190>



In the markup cell below, write about what you learned from your plot. I would expect two or three sentences, but what's most important is that you write something thoughtful.

Training error is increasing as K increases. Testing error appeared to be decreasing until just before k=5, then is started increasing and it appears it will continue to increase as k increases.

Impact of noise predictors

In class we heard that the KNN performance goes down if useless "noisy predictors" are present. These are predictor that don't help in making predictions. In this section, run KNN regression by adding one noise predictor to the data, then 2 noise predictors, then three, and then four. For each, compute the training and test RMSE. In every case, use k=10 as the k value and use the default Euclidean distance as the distance function.

_The add_noise_predictor() method makes it easy to add a predictor variable of random values to X_train or Xtest.

```
In [23]: def add_noise_predictor(X):
    """ add a column of random values to 2D array X """
    noise = np.random.normal(size=(X.shape[0], 1))
    return np.hstack((X, noise))
```

_Hint: In each iteration of your loop, add a noisy predictor to both X_train and X_test. You don't need to worry about rescaling the data, as the new noisy predictor is already scaled. Don't modify X_train and Xtest however, as you will be using them again.

```
In [24]: rmse_train_noisy = []
rmse_test_noisy = []

for i in range(0,5):
    print(i, ' ', end='')

    X_train_noisy = add_noise_predictor(X_train)
    X_test_noisy = add_noise_predictor(X_test)

    regr = KNeighborsRegressor(n_neighbors=10)

    rmse_tr_noisy, rmse_te_noisy = get_train_test_rmse(regr, X_train_noisy, X_test_rmse_train_noisy.append(rmse_tr_noisy)
    rmse_test_noisy.append(rmse_te_noisy)

print('done')
```

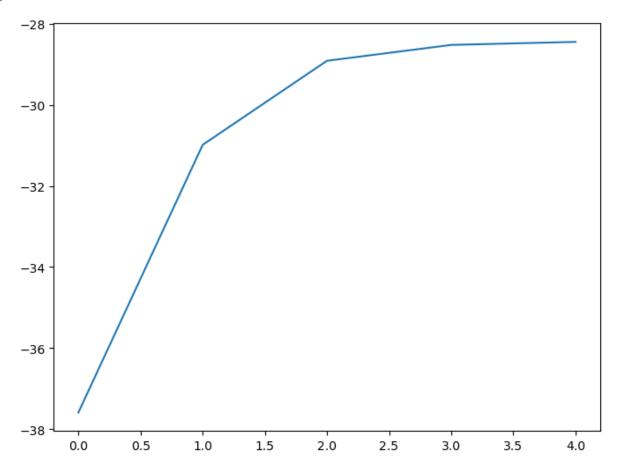
0 1 2 3 4 done

Plot the percent increase in test RMSE as a function of the number of noise predictors. The x axis will range from 0 to 4. The y axis will show a percent increase in test RMSE.

_To compute percent increase in RMSE for n noise predictors, compute 100 * (rmse - base_rmse)/base_rmse, where basermse is the test RMSE with no noise predictors, and rmse is the test RMSE when n noise predictors have been added.

```
In [74]:
         # perc inc.append((100*(rmse test noisy-test rmse))/test rmse)
         # print('rmse test noisy: ',type(rmse_test_noisy), rmse_test_noisy)
         # print('test rmse: ',type(test_rmse), test_rmse)
         # #print('rmse test noisy: ',type(np.array(rmse_test_noisy)), rmse_test_noisy)
         #print('test rmse: ',type(test_rmse), test_rmse)
         #print( (100*(rmse_test_noisy-test_rmse)/test_rmse) )
         # print( type(np.array(rmse_test_noisy)) )
         # print( type(np.array(test_rmse)) )
         # for i in range(0,5):
                # print( (np.array(rmse_test_noisy))[i]-(np.array(test_rmse)))
                print( (((np.array(rmse_test_noisy))[i]-(np.array(test_rmse))[i])/(np.array(t
         perc_inc = []
         for i in range(0,5):
               perc_inc.append((((np.array(rmse_test_noisy))[i]-(np.array(test_rmse))[i])/(np
         x = range(0,5)
         y = perc_inc
         plt.plot(x, y)
         # print(type(perc_inc), perc_inc)
         # print('rmse test noisy: ',type(rmse_test_noisy), rmse_test_noisy)
         # print('test remse: ',type(test_rmse))
         # print(np.array(rmse_test_noisy) - 5)
```

Out[74]: [<matplotlib.lines.Line2D at 0x1e12da18090>]



Look at the results you obtained and add some thoughtful commentary.

YOUR TEXT HERE

Impact of scaling

In class we learned that we should scaled the training data before using KNN. How important is scaling with KNN? Repeat the experiments you ran before (like in the impact of distance metric section), but this time use unscaled data.

Run KNN as before but use the unscaled version of the data. You will vary k as before. Use algorithm='brute' and Euclidean distance.

```
In [26]: 
    n = 30
    test_rmse = []
    train_rmse = []
    ks = np.arange(1, n+1, 2)
    for k in ks:
        print(k, ' ', end='')
        regr = KNeighborsRegressor(n_neighbors=k, algorithm='brute')
        rmse_tr, rmse_te = get_train_test_rmse(regr, X_train_raw, X_test_raw, y_train, train_rmse.append(rmse_tr)
        test_rmse.append(rmse_te)
    print('done')
```

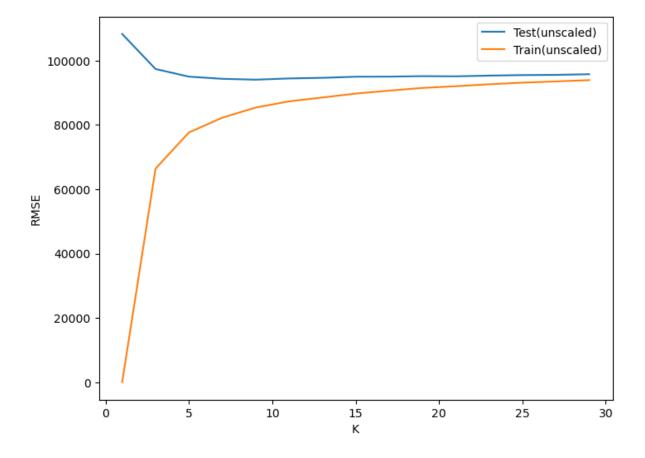
1 3 5 7 9 11 13 15 17 19 21 23 25 27 29 done

Print the best k and the test RMSE associated with the best k.

```
In [27]: best_k, best_rmse = get_best(ks, test_rmse)
print('best k = {}, best test RMSE: {:0.1f}'.format(best_k, best_rmse))
best k = 9, best test RMSE: 94057.4
```

Plot training and test RMSE as a function of k. Your plot title should note the use of unscaled data.

```
In [28]: x = ks
y = test_rmse
plt.plot(x, y)
x = ks
y=train_rmse
plt.plot(x, y)
plt.xlabel('K')
plt.ylabel('RMSE')
plt.legend(['Test(unscaled)','Train(unscaled)'])
Out[28]: 
cmatplotlib.legend.Legend at 0x1e128ea8190>
```



Reflect on what happened and provide some short commentary, as in previous sections.

The general shape of the graph is the same, but because the data is now unscaled, the y range runs from 0 to 100,000 instead of from 0 to 70,000.

Since the plot automatically adjusted, it hides the fact that the raw data is much more spread out than the scaled data was.

Impact of algorithm

We didn't discuss in class that there are variants of the KNN algorithm. The main purpose of the variants is to be faster and to reduce that amount of training data that needs to be stored.

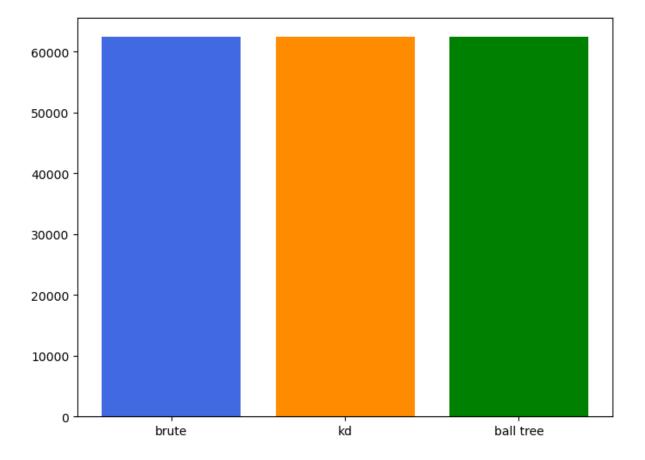
_Run experiments where you test each of the three KNN algorithms supported by Scikit-Learn: ball_tree, kdtree, and brute. In each case, use k=10 and use Euclidean distance.

```
In [29]: n = 9
         #train_rmse_ball_tree= np.array([])
         test_rmse_ball_tree= np.array([])
         #train_rmse_kd= np.array([])
         test_rmse_kd= np.array([])
         #train_rmse_brute= np.array([])
         test_rmse_brute= np.array([])
         algs = ['ball_tree', 'kd_tree', 'brute']
         ks = np.arange(1, n+1, 2)
         for alg in algs:
             train_rmse_alg= []
             test_rmse_alg= []
             for k in ks:
                  print(k, ' ', end='')
                  regr = KNeighborsRegressor(n_neighbors=k, algorithm= alg)
                 rmse_tr, rmse_te = get_train_test_rmse(regr, X_train, X_test, y_train, y_te
                 if alg == 'ball_tree':
                     test_rmse_ball_tree = np.append(test_rmse_ball_tree, rmse_te)
                  elif alg == 'kd_tree':
                     test_rmse_kd = np.append(test_rmse_kd,rmse_te)
                  elif alg == 'brute':
                     test_rmse_brute = np.append(test_rmse_brute, rmse_te)
                  else:
                      print('invalid algorithm')
             print(alg, 'done')
         1 3 5 7 9 ball_tree done
```

Print the name of the best algorith, and the test RMSE achieved with the best algorithm.

1 3 5 7 9 kd_tree done 1 3 5 7 9 brute done

```
In [30]: b t min = test rmse ball tree.min()
         b t min index = np.where(test rmse ball tree == test rmse ball tree.min())
         b_t_min_index = b_t_min_index[0]
         k_d_min = test_rmse_kd.min()
         k d min index = np.where(test rmse kd == test rmse kd.min())
         k_d_min_index = k_d_min_index[0]
         brute_min = test_rmse_brute.min()
         brute_min_index = np.where(test_rmse_brute == test_rmse_brute.min())
         brute_min_index = brute_min_index[0]
         #{:0.1f}'.format(
         print('best ball tree k=', ks[b_t_min_index[0]], 'best ball tree test RMSE: {:0.3f}
         print('best kd tree k=', ks[k_d_min_index[0]], 'best kd test RMSE: {:0.3f}'.format(
         print('best brute k=', ks[brute_min_index[0]], 'best brute test RMSE: {:0.3f}'.form
         min_rmses = np.array([test_rmse_ball_tree.min(), test_rmse_kd.min(), test_rmse_brut
         min_of_all = min_rmses.min()
         if (min of all == test rmse brute.min() and min of all == test rmse kd.min() and mi
             print('All 3 have the best rmse with k=',ks[brute_min_index[0]])
         elif min_of_all == test_rmse_brute.min() and min_of_all == test_rmse_kd.min():
                  print('brute and kd tree have the best rmse with k=',ks[brute_min_index[0]]
         elif min_of_all == test_rmse_brute.min() and min_of_all == test_rmse_ball_tree.min()
             print('brute and ball tree have the best rmse with k=',ks[brute_min_index[0]])
         elif min of all == test rmse kd.min() and min of all == test rmse ball tree.min():
             print('kd tree and ball tree have the best rmse with k=',ks[k d min index[0]])
         elif min_of_all == test_rmse_ball_tree.min():
             print('ball tree has the best rmse with k=',ks[b_t_min_index[0]])
         elif min_of_all == test_rmse_kd.min():
             print('kd tree has the best rmse with k=',ks[k_d_min_index[0]])
         elif min of all == test rmse brute.min():
             print('brute has the best rmse with k=',ks[brute_min_index[0]])
         best ball tree k= 7 best ball tree test RMSE: 62421.498
         best kd tree k= 7 best kd test RMSE: 62421.498
         best brute k= 7 best brute test RMSE: 62421.498
         All 3 have the best rmse with k=7
         Plot the test RMSE for each of the three algorithms as a bar plot.
In [31]: | rmses = test_rmse_brute.min(), test_rmse_kd.min(), test_rmse_ball_tree.min()
         x= ['brute', 'kd', 'ball tree']
         colors = ['royalblue', 'darkorange', 'green']
         plt.bar(x, rmses, color = colors)
         <BarContainer object of 3 artists>
Out[31]:
```



As usual, reflect on the results and add comments.

In this case, the different algorithms all resulted in the same minimum RMSE at the same numbers of neighbors. So it seems that for this data, using the knn neighbors algorithm doesn't have a big effect on the best predictions, it's more about finding the right number of neighbors to use, and once that is found, they all perform equally well.

Impact of weighting

It was briefly mentioned in lecture that there is a variant of KNN in which training points are given more weight when they are closer to the point for which a prediction is to be made. The 'weight' parameter of KNeighborsRegressor() has two possible values: 'uniform' and 'distance'. Uniform is the basic algorithm.

Run an experiment similar to the previous one. Compute the test RMSE for uniform and distance weighting. Using k = 10, the brute algorithm, and Euclidean distance.

```
In [32]: n = 9
         #train rmse uniform= np.array([])
         test_rmse_uniform= np.array([])
         #train_rmse_distance= np.array([])
         test_rmse_distance= np.array([])
         weights = ['uniform', 'distance']
         ks = np.arange(1, n+1, 2)
         for weight in weights:
             train_rmse_alg= []
             test_rmse_alg= []
             for k in ks:
                  print(k, ' ', end='')
                  regr = KNeighborsRegressor(n_neighbors=k, algorithm = 'brute', weights = we
                 rmse_tr, rmse_te = get_train_test_rmse(regr, X_train, X_test, y_train, y_te
                  if weight == 'uniform':
                     test_rmse_uniform = np.append(test_rmse_uniform, rmse_te)
                  elif weight == 'distance':
                     test_rmse_distance = np.append(test_rmse_distance,rmse_te)
                  else:
                      print('invalid weight')
             print(weight, 'done')
```

1 3 5 7 9 uniform done 1 3 5 7 9 distance done

Print the weighting the gave the lowest test RMSE, and the test RMSE it achieved.

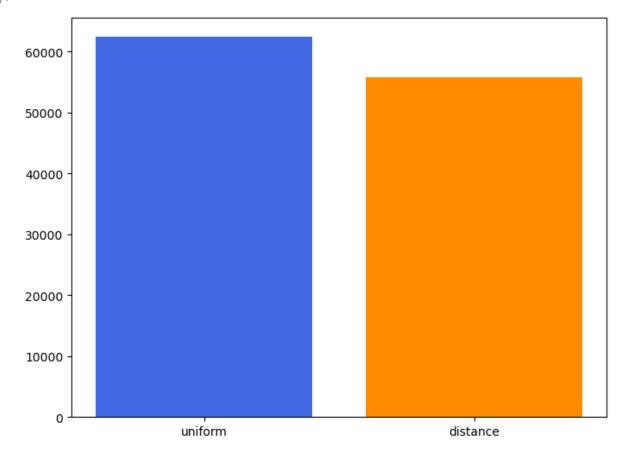
```
uniform min = test rmse uniform.min()
In [33]:
         uniform_min_index = np.where(test_rmse_uniform == test_rmse_uniform.min())
         uniform_min_index = uniform_min_index[0]
         #print(uniform_min, uniform_index)
         distance_min = test_rmse_distance.min()
         distance_min_index = np.where(test_rmse_distance == test_rmse_distance.min())
         distance_min_index = distance_min_index[0]
         print('best uniform k=', ks[uniform_min_index[0]], 'best uniform test RMSE: {:0.3f}
         print('best distance k=', ks[distance_min_index[0]], 'best distance test RMSE: {:0.
         min_rmses = np.array([test_rmse_uniform.min(), test_rmse_distance.min()])
         min_of_all = min_rmses.min()
         if (min_of_all == test_rmse_uniform.min() and min_of_all == test_rmse_distance.min()
             print('Both have the best rmse with k=',ks[brute_min_index[0]])
         elif min_of_all == test_rmse_uniform.min():
             print('uniform has the best rmse with k=',ks[b_t_min_index[0]])
         elif min_of_all == test_rmse_distance.min():
             print('distance has the best rmse with k=',ks[k_d_min_index[0]])
```

```
best uniform k=7 best uniform test RMSE: 62421.498 best distance k=7 best distance test RMSE: 55800.710 distance has the best rmse with k=7
```

Create a bar plot showing the test RMSE for the uniform and distance weighting options.

```
In [34]: rmses = test_rmse_uniform.min(), test_rmse_distance.min()
x = ['uniform', 'distance']
colors = ['royalblue', 'darkorange', 'green']
plt.bar(x, rmses, color = colors)
```

Out[34]: <BarContainer object of 2 artists>



Comments

As usual, reflect and comment.

While the uniform data is the same as the previous example, since uniform is the default, we do see an improvment in the RMSE when the algorithm gives weight by the distance of the neighbor. The optimal number of neighbors is still 7, but in this case it does appear our predictions may be more accurate if the algorithm weights by distance.

Conclusions

Please provide at least a few sentences of commentary on the main things you've learned from the experiments you've run.

I enjoyed getting the practice of training data, making predictions, and calculating RMSE. I found it intersting that, at least from these exercises on kNN, it seems like the first step is finding out the optimal number of neigbors, and then you can experiment with algorithm and weights to see if you can improve the accuracy further.