ROB313 Intro to Learning from Data - Assignment 1

Objectives

The objective of this assignment is to familiarize one with the applications and varying implementations of the k-NN algorithm. In this respect, the k-NN algorithm will be used for both regression and classification of several datasets. Additionally, various parameters of the algorithm will be simulated to analyze the effect on the k-NN's performance (e.g. distance metrics, feature space dimensions). In doing so, one will also become familiar with the available linear algebra tools/libraries for various computations. The performance of the k-NN algorithm will be compared to the Linear Regression Model for deeper understanding. Altogether, this assignment serves to provide a first-hand experience in applying theoretical machine learning knowledge by implementing two introductory level algorithms

Code Structure and Strategies

The code structure was designed to be modular and easily understandable. To run the code for each question, the only modifications needed to be made to the file is to uncomment the corresponding section outlined in the main block. The remaining code is structured as follows:

 $Q1: ff_regression(data) - 5-fold\ regression\ function, ff_regression_test(data) - regression\ test$

Q2: one_fold_classification(data), classification_test(data) - classification validation and test

Questions 1 and 2 each share a common function called **run_model**(model_type, dataset) from which the Q1 and Q2 functions are called from, depending on the *model_type* parameter. The *run_model* function is called directly from the main block.

O3: regression performance(data, method) – Modified k-NN algorithms

This function is called many times to compute the Test RMSE for the provided dataset. However, the method parameter specifies what type of computation should take place (e.g. method = 'a' will compute predictions using the double loop over test points). This function is called directly from the main block.

Q4: linear_regression(*data*, *model_type*) – *Linear regression function*

This function is called directly from the main block and will compute predictions and Test RMSE/Test Accuracy Ratio using a linear model for either regression or classification datasets. The parameter, *model_type*, specified whether to run classification or regression.

The first strategy deployed was to make the code very modular. Thus, easily interchangeable functions are run directly from the main block for each question. The functions were designed to be generalizable so that they can be re-used for datasets with differing feature space dimensions. Furthermore, the final code has gone through several iterations to optimize the runtime of each function. Originally, performing regression and classification for the larger datasets would take several hours at a time. Changes such as inverting the loop structure of the function significantly decreased the overall runtime. For example, in Q1 and Q2, the distances between a given test

point and all training points are computed only once, and then used to obtain the k-nearest neighbours for many of k values. Finally, print statements are neatly organized throughout the main block so that the results can be easily obtained by the operator when executing the code. Neatness and organization aided in the debugging process so that little time was wasted searching for incorrect results.

Q1 - k-NN Algorithm for Regression

1-a) Implement k-NN Algorithm for Regression Datasets and use 5-fold Cross Validation:

The results of running the k-NN regression on all regression datasets are provided below. A *Cross-Validation RMSE*, *Test RMSE*, *Estimated k*, *and preferred Distance Metric* is reported for each dataset. Note that for each dataset, k values on a range (1, 30) were simulated. From these results, we can see a correspondence between the dimensionality of the feature space to the estimated k value. Additionally, we see that datasets with close feature space dimensions prefer the same distance metric.

Dataset	Estimated k	Distance Metric	CV RMSE	Test RMSE
mauna_loa	2	L2-norm	0.0318041026269	0.440704890355
rosenbrock	2	L2-norm	0.330741584025	0.247598644133

L-inf-norm

0.87221127042

0.832480142444

Table 1 – k-NN Regression Results

25

pumadyn32nm

1-b) Cross-Validation Loss Curve and Prediction on Test Set for Mauna Loa (L2-norm)

Figure 1 illustrates the cross-validation loss (merging predictions from all splits) across increasing values of k for the Mauna Loa dataset. As expected, we see that the loss is minimized for a k value of 2. Th corresponds to the Mauna Loa result shown in *Table 1*. Further, we see that the loss rapidly increases for higher k values which suggests that computing an estimate with more neighbours negatively effects the accuracy of predictions.

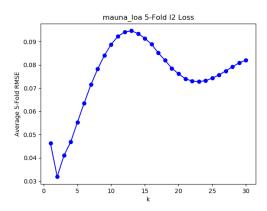


Figure 1 – Cross Validation Loss Curve for Mauna Loa

In *Figure* 2, we have the prediction of the k-NN regression on the test set for Mauna Loa. Notice that for all test points, the predicted values are identical. Intuitively, this makes sense as the Mauna Loa dataset represents data taken over *time*. The 1-dimensional feature space of time values for the test set contains data points that were collected after all the data points in the training and validation set, chronologically. Thus, the k nearest neighbours for all test points are the same, yielding identical predictions. It is for this reason that the Test RMSE shown in *Table 1* is significantly larger than the Cross-Validation RMSE for this particular dataset.

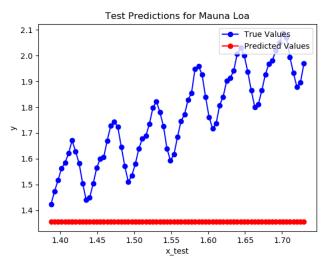


Figure 2 – Prediction on Test Set for Mauna Loa

Q2 - k-NN Algorithm for Classification

A similar k-NN algorithm was used as a classification model and was applied to two classification datasets. The results are summarized in *Table 2*, containing the *Estimated k*, *preferred Distance Metric*, *Validation Accuracy Ratio*, *and the Test Accuracy Ratio* for each dataset.

Dataset	Estimated k	Distance Metric	Validation Ratio	Test Ratio
iris	15	L1-norm	0.9032258064516129	1.0
mnist_small	1	L2-norm	0.95	0.959

Table 2 – k-NN Classification Results

Q3 - k-NN Performance with Varying Computational Modifications

Four versions of the k-NN algorithm were implemented to compute predictions on the rosenbrock (k=5, $n_{train}=5000$) regression test set over increasing values of d (dimension of feature space). The four versions were: brute force double loop (a), half-vectorized method (b), fully-vectorized method (c), k-d tree method (d). Using the L2-norm to compute distances, the

performance metrics *Run-time and Test RMSE*, were tracked over d values on a range (2, 9). The quantities are summarized in *Table 3* and displayed in *Figures 3-4*.

Table 3 – k-NN Performance Results with	Various Computational Modifications (plotted on Figures 3-4)

d	Methods (a, b, c, d)							
	Double	Loop (a)	Half-Vect	orized (b)	Fully-Vec	torized (c)	k-d Tı	ree (d)
	Time [s]	RMSE	Time [s]	RMSE	Time [s]	RMSE	Time [s]	RMSE
2	172.363	0.267	2.505	0.267	0.157	0.267	0.003	0.267
3	106.918	0.379	2.873	0.379	0.155	0.379	0.005	0.379
4	109.243	0.420	2.899	0.420	0.171	0.420	0.007	0.420
5	305.698	0.521	3.007	0.521	0.158	0.521	0.011	0.521
6	290.247	0.611	3.012	0.611	0.164	0.611	0.018	0.611
7	129.156	0.689	3.485	0.689	0.170	0.689	0.029	0.689
8	310.322	0.747	6.338	0.747	0.204	0.747	0.174	0.747
9	153.278	0.800	3.904	0.800	0.180	0.800	0.064	0.800

Figure 3 depicts the prediction runtimes of all four methods over increasing feature space dimension. As we can see, the Double Loop method take significantly longer than the vectorized and k-d tree methods. Analyzing Table 3, we can see that the k-d tree implementation is consistently the best performer in terms of time, followed by the fully-vectorized and half-vectorized methods, although the k-d tree and fully-vectorized methods come quite close. An interesting observation is that the double loop method seems to be extremely sensitive to the size of the feature space, while the other three methods stay quite consistent in runtimes. Overall, vectorizing the code significantly reduced the runtime of the algorithm, and using a k-d data structure further improves the computational performance in comparison to the brute-force method.

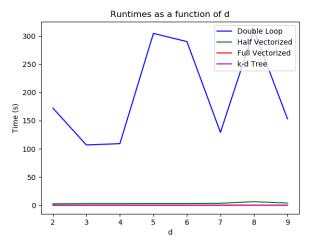


Figure 3 – Prediction Runtimes for all k-NN Methods

Figure 4 displays the Test RMSE values for all methods over the increasing feature space dimension. As expected, all versions of the k-NN algorithm predict the same values, and hence their test RMSE values should be identical. This corresponds to the overlapping curves below.

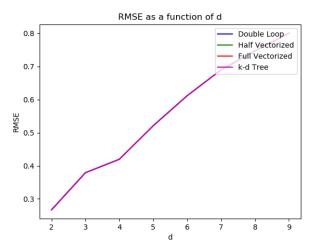


Figure 4 – Test RMSE for all k-NN Methods

Q4 - Linear Regression Model for Regression and Classification

Two versions of a linear regression model were implemented for regression and classification of all datasets. The test RMSE values (regression) and test accuracy ratios (classification) are reported in *Table 4*. Comparing the results of the linear model to the k-NN algorithm we see several things. For the regression sets, the test RMSE values suffered a significant increase for rosenbrock and a minor increase pumadyn32nm. However, the test RMSE value decreased for the Mauna Loa dataset. The result for Mauna Loa is expected, as the linear regression model is able to better fit the data with an increasing slope, which the k-NN algorithm was unable to do (see *Figure 2*). For classification, the linear regression model slight underperformed in comparison to the k-NN algorithm for both iris and mnist_small datasets. Thus, the k-NN algorithm outperforms the linear regression model over all datasets except for Mauna Loa.

Table 4 – Linear Regression Model Test Results

Dataset	Test RMSE	Test Accuracy Ratio
mauna_loa	0.349388310499	
rosenbrock	0.984087203069	
pumadyn32nm	0.86225124366	
iris		0.866666666667
mnist_small		0.855

```
1 import numpy as np
 2 import time
 3 import math
 4 from matplotlib import pyplot as plt
5 from data_utils import load_dataset
 6 import heapq
 7 from sklearn import neighbors
    _author__ = 'Christopher Agia (1003243509)'
9
10 __date__ = 'February 12, 2019'
11
12
13 # Root Mean Squared Error Function
14 def rmse(y_test, y_estimates):
15
       return np.sqrt(np.average((y_test-y_estimates)**2))
16
17 # Norm Utility Functions
18 def l1_norm(x1, x2):
19
       return np.linalg.norm([x1-x2], ord=1)
20
21
22 def 12_norm(x1, x2):
23
       return np.linalg.norm([x1-x2], ord=2)
24
25
26 def linf_norm(x1, x2):
27
       return np.linalg.norm([x1-x2], ord=np.inf)
28
29
30 def ff_regression(x_train, x_valid, y_train, y_valid, distance_functions, k_list=None):
31
32
       assert((len(x_train)+len(x_valid)) == (len(y_train)+len(y_valid)))
33
34
       rmse vals = {}
35
       error = []
36
       x_total = np.vstack([x_train, x_valid])
37
38
       y_total = np.vstack([y_train, y_valid])
39
       np.random.seed(5)
40
       np.random.shuffle(x_total)
41
       np.random.seed(5)
42
       np.random.shuffle(y_total)
43
44
       ff_length = len(x_total)//5
45
       # Trial K values to try
46
47
       if not k_list:
48
           k_list = list(range(0, 30))
49
       # Iterate over 5-folds
50
51
       for i in range(5):
52
53
           # Obtain validation and train set associated with fold i
           y_valid = y_total[i * ff_length:(i + 1) * ff_length]
54
55
           y_train = np.vstack([y_total[:i * ff_length], y_total[(i + 1) * ff_length:]])
           x_valid = x_total[i * ff_length:(i + 1) * ff_length]
x_train = np.vstack([x_total[:i * ff_length], x_total[(i + 1) * ff_length:]])
56
57
58
           # Loop over distance functions (e.g. l1_norm, l2_norm, linf_norm)
59
60
           for func in distance functions:
61
               y_est = {}
62
                # Compute distances according to distance function for one validation point
63
                for j in range(ff_length):
64
                    d = []
                    for t in range(len(x_train)):
65
                        d.append((func(x_train[t], x_valid[j]), y_train[t]))
67
68
                    # Sort distances to take the nearest k-values
                    d.sort(key=lambda x: x[0])
69
70
71
                    # Compute y_estimate for validation point j
72
                    for k in k_list:
                        y = 0
                        for elem in d[:k+1]:
74
75
                            y += elem[1]
76
77
                        if k not in y_est:
78
                            y_est[k] = []
```

```
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                           C:\Users\Christopher Agia\Desktop\Year 3\Term 2\ROB313 Intro to Learning from Data\Assignment 1\knn main.py
  80
                           y_{est[k].append(y/(k+1))}
  81
                  # Compute root mean squared error for each k-value
  82
                  for k in k list:
  83
  24
                       if (func, k) not in rmse_vals:
  85
                           rmse_vals[(func, k)] = []
  86
                       rmse_vals[(func, k)].append(rmse(y_valid, y_est[k]))
  87
  88
  89
          # Error will contain 30 rmse-error values as per k for each function
          for func, k in rmse_vals:
  90
  91
              ff_error = sum(rmse_vals[(func, k)]) / 5
              error.append((k+1, func, ff_error))
  92
  93
  94
          return error
  95
  96
  97 def ff_regression_test(x_train, x_valid, x_test, y_train, y_valid, y_test, k, func, plot=False):
  98
  99
          # Create total training set (no validation)
 100
          x total = np.vstack([x train, x valid])
          y_total = np.vstack([y_train, y_valid])
 101
 102
          # Predictions for each test data point will be stored in this list
 103
 104
          predictions = []
 105
 106
          # Iterate over test points
 107
          for elem in x_test:
 108
 109
              # Compute distances between all training points and test point
 110
              d = []
 111
              for i in range(len(x total)):
 112
                  d.append((func(elem, x_total[i]), y_total[i]))
 113
              # Sort in terms of increasing distance
 114
              d.sort(key=lambda x: x[∅])
 115
 116
 117
              # Average over k nearest y values
              y_est = 0
 118
 119
              for item in d[:k]:
 120
                  y_{est} += item[1]
 121
              avg = y_est/k
 122
 123
              # Append to predictions
 124
              predictions.append(avg)
 125
 126
          test error = rmse(y test, predictions)
 127
          if plot:
 128
 129
              # Predictions on test set
 130
              plt.figure(2)
              plt.plot(x_test, y_test, '-bo', label='True Values')
plt.plot(x_test, predictions, '-ro', label='Predicted Values')
 131
 132
              plt.title('Test Predictions for Mauna Loa')
 133
 134
              plt.xlabel('x_test')
              plt.ylabel('y')
 135
 136
              plt.legend(loc='upper right')
 137
              plt.savefig('mauna_loa_prediction.png')
 138
 139
          return test_error
 140
 141
 142 def one_fold_classification(x_train, y_train, x_valid, y_valid, distance_functions, k_list=None):
 143
          assert ((len(x_train) + len(x_valid)) == (len(y_train) + len(y_valid)))
 144
 145
 146
          tally = \{\}
 147
 148
          if not k list:
 149
              k_list = list(range(0, 30))
 150
 151
          # Loop over distance functions (e.g. L1_norm, L2_norm, Linf_norm)
 152
          for func in distance functions:
 153
              # Compute distances according to distance function for one validation point
 154
 155
              for j in range(len(x_valid)):
                  d = []
 156
 157
                  for t in range(len(x_train)):
                       \label{eq:dappend} $$d.append((func(x\_train[t], x\_valid[j]), y\_train[t]))$
 158
```

```
160
                # Sort distances to take the nearest k-values
161
                d.sort(key=lambda x: x[0])
162
                classes = {}
163
164
                # Identify k-nearest neighbours for x_valid[j]
165
                for k in k list:
166
                     classes[k] = []
167
                     for elem in d[:k + 1]:
168
                         classes[k].append(elem[1])
169
170
                for k in k_list:
171
                    occurance = {}
172
                     for point in classes[k]:
173
                         if str(point) not in occurance:
                             occurance[str(point)] = (point, 0)
174
175
                         occurance[str(point)] = (point, occurance[str(point)][1] + 1)
176
177
                     occur_list = list(occurance.values())
178
                    occur_list.sort(key=lambda x: x[1], reverse=True)
179
180
                    if np.all(occur_list[0][0] == y_valid[j]):
                         if (k + 1, func) not in tally:
181
182
                             tally[(k + 1, func)] = 0
                         tally[(k + 1, func)] += 1
183
184
185
        results = []
186
        for k, func in tally:
187
            ratio = tally[(k, func)]/len(y_valid)
188
            result = (k, func, ratio)
189
            results.append(result)
190
191
        return results
192
193
194 def classification_test(x_train, x_valid, x_test, y_train, y_valid, y_test, k, func):
195
        # Create total training set (no validation)
196
197
        x_total = np.vstack([x_train, x_valid])
198
        y_total = np.vstack([y_train, y_valid])
199
        tally = 0
200
201
        # Iterate over test points
202
        for i in range(len(x_test)):
203
            # Compute distances between all training points and test point
204
205
            d = []
206
            for j in range(len(x_total)):
207
                d.append((func(x_test[i], x_total[j]), y_total[j]))
208
            # Sort in terms of increasing distance
209
            d.sort(key=lambda x: x[0])
210
211
212
            occurance = {}
213
            for item in d[: k]:
214
                if str(item[1]) not in occurance:
                    occurance[str(item[1])] = (item[1], 0)
215
216
                occurance[str(item[1])] = (item[1], occurance[str(item[1])][1] + 1)
217
218
            occur_list = list(occurance.values())
219
            occur_list.sort(key=lambda x: x[1], reverse=True)
220
            if np.all(occur_list[0][0] == y_test[i]):
221
222
                tally += 1
223
224
        return tally/len(x_test)
225
226
227 def run_model(model_type, dataset):
228
229
        functions = [l1_norm, l2_norm, linf_norm]
230
231
        if model_type == 'regression':
232
            if dataset == 'rosenbrock':
233
234
                x_train, x_valid, x_test, y_train, y_valid, y_test = load_dataset(dataset, n_train=1000, d=2)
235
            else.
236
                x_train, x_valid, x_test, y_train, y_valid, y_test = load_dataset(dataset)
237
238
            if dataset == 'mauna_loa':
                result = ff_regression(x_train, x_valid, y_train, y_valid, [12_norm])
```

```
240
241
                # Result = (k, Function, RMSE Error)
242
                result.sort(key=lambda x: x[0])
243
244
                k_vals = []
245
                error vals = []
246
                for k, func, error in result:
247
                    k_vals.append(k)
248
                    error_vals.append(error)
249
250
                plt.figure(1)
                plt.plot(k_vals, error_vals, '-bo')
251
252
                plt.xlabel('k')
253
                plt.ylabel('Average 5-Fold RMSE')
                plt.title(dataset + ' 5-Fold 12 Loss')
254
                plt.savefig(dataset +'12_loss.png')
255
256
257
                result.sort(key=lambda x: x[2])
258
                k_min = result[0][0]
259
                func = result[0][1]
260
                test error = ff regression test(x train, x valid, x test, y train, y valid, y test, k min, func, plot=True)
261
262
                print('Results for Mauna Loa with L2 Norm :')
263
                print('')
print('Optimal k: ' + str(k_min))
264
265
266
                print('Optimal Distance Metric: ' + str(func))
                print('Five fold RMSE: ' + str(result[0][2]))
267
                print('Test RMSE: ' + str(test_error))
268
                print('')
269
270
271
            result = ff_regression(x_train, x_valid, y_train, y_valid, functions)
272
            result.sort(key=lambda x: x[2])
273
            k_min = result[0][0]
274
            func = result[0][1]
            test error = ff regression test(x train, x valid, x test, y train, y valid, y test, k min, func)
275
276
277
            return result[0][0], result[0][1], result[0][2], test_error
278
279
        elif model_type == 'classification':
280
281
            x_train, x_valid, x_test, y_train, y_valid, y_test = load_dataset(dataset)
282
            one_fold_result = one_fold_classification(x_train, y_train, x_valid, y_valid, functions)
283
            one_fold_result.sort(key=lambda x: x[2], reverse=True)
            # ff_result = (k, func, ratio)
284
285
            k_min = one_fold_result[0][0]
286
            func = one fold result[0][1]
287
            test_ratio = classification_test(x_train, x_valid, x_test, y_train, y_valid, y_test, k_min, func)
288
289
            return k_min, func, one_fold_result[0][2], test_ratio
290
        return 0
291
292
293
294 def regression_performance(x_total, x_test, y_total, y_test, k, f, method):
295
296
        start = time.time()
297
        # Predictions for each test data point will be stored in this list
298
299
        predictions = []
300
301
        # Brute-force Double For Loop Method
        if method == 'a':
302
303
304
            # Iterate over test points
305
            for elem in x_test:
306
307
                # Compute distances between all training points and test point
308
                d = []
309
                for j in range(len(x_total)):
310
                    d.append((f(elem, x_total[j]), y_total[j]))
311
312
                # Sort in terms of increasing distance
313
                d.sort(key=lambda x: x[0])
314
315
                # Average over k nearest y values
316
                y_est = 0
                for item in d[:k]:
317
318
                    y_est += item[1]
                avg = y_est/k
```

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 320
 321
                  # Append to predictions
 322
                  predictions.append(avg)
 323
 324
              test_error = rmse(y_test, predictions)
 325
 326
          # Half-Vectorization Method
 327
          elif method == 'b':
 328
 329
              for j in range(len(x_test)):
                  d = np.sqrt(np.sum(np.square(x_total - x_test[j]), axis=1))
 330
                  k_nb = heapq.nsmallest(k, range(len(d)), d.take)
 331
                  predictions.append(np.array([(np.average(np.take(y\_total, k\_nb)))]))
 332
 333
              test_error = rmse(y_test, predictions)
 334
 335
 336
          # Full Vectorization Method
 337
          elif method == 'c':
 338
              d = np.sqrt(-2 * np.dot(x_test, x_total.T) + np.sum(x_total ** 2, axis=1) + np.sum(x_test ** 2, axis=1)[:, np.newaxis])
 339
 340
              k_nb = np.argpartition(d, kth=k, axis=1)[:, : k]
              predictions = np.sum(y_total[k_nb], axis=1) / k
 341
 342
 343
              test_error = rmse(y_test, predictions)
 344
 345
          # K-D Tree Method
 346
          elif method == 'd':
 347
 348
              kdt = neighbors.KDTree(x_total)
 349
              d, k_nb = kdt.query(x_test, k=k)
 350
              predictions = np.sum(y_total[k_nb], axis=1) / k
 351
 352
              test_error = rmse(y_test, predictions)
 353
          runtime = time.time() - start
 354
 355
          return runtime, test error
 356
 357
 358 def linear_regression(x_train, x_valid, x_test, y_train, y_valid, y_test, model_type):
 359
          if model_type == 'regression':
 360
 361
 362
              x_total = np.vstack([x_train, x_valid])
 363
              y_total = np.vstack([y_train, y_valid])
 364
 365
              # Create X matrix
 366
              X = np.ones((len(x_total), len(x_total[0]) + 1))
 367
              X[:, 1:] = x_{total}
 368
 369
              # Compute SVD
 370
              U, S, Vh = np.linalg.svd(X)
 371
 372
              # Invert Sigma
 373
              sig = np.diag(S)
 374
              filler = np.zeros([len(x_total)-len(S), len(S)])
 375
              sig_inv = np.linalg.pinv(np.vstack([sig, filler]))
 376
 377
              # Compute weights and predictions
              w = np.dot(Vh.T, np.dot(sig_inv, np.dot(U.T, y_total)))
 378
 379
 380
              X_{\text{test}} = \text{np.ones}((\text{len}(x_{\text{test}}), \text{len}(x_{\text{test}}[0]) + 1))
 381
              X_{test}[:, 1:] = x_{test}
 382
              predictions = np.dot(X_test, w)
 383
 384
              result = rmse(y_test, predictions)
 385
          elif model_type == 'classification':
 386
 387
 388
              x_total = np.vstack([x_train, x_valid])
 389
              y_total = np.vstack([y_train, y_valid])
 390
 391
              # Expand X matrix
 392
              X = np.ones([len(x_total), len(x_total[0]) + 1])
 393
              X[:, 1:] = x_{total}
 394
 395
              # Convert to integer
 396
              #y_test = 1 * y_test
 397
 398
              # Perform SVD
              U, S, Vh = np.linalg.svd(X)
```

```
400
401
            # Expand Sigma Matrix
402
            sig = np.diag(S)
403
            filler = np.zeros([len(x_total) - len(S), len(S)])
404
            sig_inv = np.linalg.pinv(np.vstack([sig, filler]))
405
406
            # Compute weights
            w = np.dot(Vh.T, np.dot(sig_inv, np.dot(U.T, y_total)))
407
408
409
            # Create Test Matrix
            X_{\text{test}} = \text{np.ones}([\text{len}(x_{\text{test}}), \text{len}(x_{\text{test}}[\emptyset]) + 1])
410
411
            X_{test}[:, 1:] = x_{test}
412
413
            # find prediction accuracy
            predictions = np.argmax(np.dot(X_test, w), axis=1)
414
415
            y_test = np.argmax(1 * y_test, axis=1)
416
417
            result = (predictions == y_test).sum() / len(y_test)
418
419
        return result
420
421
422 if __name__ == '__main__':
423
        # All Dataset Names
        all_datasets = ['mauna_loa', 'rosenbrock', 'pumadyn32nm', 'iris', 'mnist_small']
424
        regression_sets = ['mauna_loa', 'rosenbrock', 'pumadyn32nm']
classification_sets = ['iris', 'mnist_small']
425
426
427
        # ----- Question 1 -----
428
429
430
        # print('-----')
431
        # print('')
432
        # for d_set in regression_sets:
433
             k_min, metric_min, ff_rmse, test_rmse = run_model('regression', d_set)
434
              print('-----
             print('Results for ' + d_set + ' :')
print('')
435
436
        #
             print('Optimal k: ' + str(k_min))
437
             print('Optimal Distance Metric: ' + str(metric_min))
438
        #
439
             print('Five fold RMSE: ' + str(ff_rmse))
             print('Test RMSE: ' + str(test_rmse))
440
        #
             print('')
441
        #
442
443
        # ----- Question 2 -----
444
445
446
        # print('-----')
        # print('')
447
448
        # for d_set in classification_sets:
             k_min, metric_min, max_ratio, test_ratio = run_model('classification', d_set)
449
450
             print('Results for ' + d_set + ' :')
451
452
             print('')
             print('Optimal k: ' + str(k_min))
453
        #
             print('Optimal Distance Metric: ' + str(metric_min))
454
             print('Validation Ratio: ' + str(max_ratio))
455
             print('Test Ratio: ' + str(test_ratio))
456
457
              print('')
458
459
        # ------ Question 3 -----
460
461
        # result_table = {}
462
        # result_table['Double Loop'] = []
463
       # result_table['Half Vectorized'] = []
# result_table['Full Vectorized'] = []
# result_table['k-d Tree'] = []
464
465
466
467
468
        # for ind_d in range(2, 10):
469
470
              x_train, x_valid, x_test, y_train, y_valid, y_test = load_dataset('rosenbrock', n_train=5000, d=ind_d)
471
              x_total = np.vstack([x_train, x_valid])
472
        #
             y_total = np.vstack([y_train, y_valid])
473
        #
              run_time, test_rmse = regression_performance(x_total, x_test, y_total, y_test, 5, l2_norm, 'a')
474
475
        #
             result_table['Double Loop'].append((ind_d, run_time, test_rmse))
476
        #
477
        #
              run\_time, \ test\_rmse = regression\_performance(x\_total, \ x\_test, \ y\_total, \ y\_test, \ 5, \ l2\_norm, \ 'b')
478
              result_table['Half Vectorized'].append((ind_d, run_time, test_rmse))
```

```
480
       #
             run_time, test_rmse = regression_performance(x_total, x_test, y_total, y_test, 5, l2_norm, 'c')
481
       #
             result_table['Full Vectorized'].append((ind_d, run_time, test_rmse))
482
       #
             run\_time, \ test\_rmse = regression\_performance(x\_total, \ x\_test, \ y\_total, \ y\_test, \ 5, \ l2\_norm, \ 'd')
483
484
             result_table['k-d Tree'].append((ind_d, run_time, test_rmse))
485
486
       # print('-----')
       # print('')
487
488
       #
489
       # m = list(result_table.keys())
       # for r in range(8):
490
491
            print('--- Results for d = ' + str(r+2) + ' ---')
             print('')
print('Times-- ' + m[0] + ': ' + str(result_table[m[0]][r][1]) + ' ' + m[1] + ': ' + str(result_table[m[1]][r][1]))
492
       #
493
       #
            494
       #
495
496
             print('
                           ' + m[2] + ': ' + str(result_table[m[2]][r][2]) + ' ' + m[3] + ': ' + str(result_table[m[3]][r][2]))
       #
       #
             print('')
497
498
199
       # d_arr = list(range(2, 10))
500
       # plt.figure(3)
       # plt.title('Runtimes as a function of d')
501
       # plt.xlabel('d')
502
503
       # plt.ylabel('Time (s)')
504
       # plt.figure(4)
       # plt.title('RMSE as a function of d')
505
506
       # plt.xlabel('d')
507
       # plt.ylabel('RMSE')
508
       # count = 0
509
510
       # for m in result_table:
511
512
       #
             if count == 0:
                tab = '-b'
513
             elif count == 1:
514
       #
                 tab = '-q'
515
516
             elif count == 2:
       #
517
                tab = '-r'
518
       #
            else:
                tab = '-m'
519
       #
            count += 1
520
       #
521
       #
522
       #
            runtimes = []
523
       #
             rmses = []
             for i in range(len(result_table[m])):
524
525
       #
                runtimes.append(result_table[m][i][1])
526
       #
                rmses.append(result table[m][i][2])
527
       #
528
             plt.figure(3)
529
       #
             plt.plot(d_arr, runtimes, tab, label=m)
       #
530
531
       #
             plt.figure(4)
532
       #
             plt.plot(d_arr, rmses, tab, label=m)
533
       #
534
       # plt.figure(3)
       # plt.legend(loc='upper right')
535
536
       # plt.savefig('runtimes_vs_d.png')
537
538
       # plt.figure(4)
539
       # plt.legend(loc='upper right')
540
       # plt.savefig('rmses_vs_d.png')
541
542
       # ------ Ouestion 4 -----
543
544
       # print('-----')
       # print('')
545
546
       # for d_set in regression_sets:
547
548
       #
             if d set == 'rosenbrock':
549
       #
                x_{train}, x_{valid}, x_{test}, y_{train}, y_{valid}, y_{test} = load_dataset(d_set, n_train=1000, d=2)
550
551
       #
                 x_{train}, x_{valid}, x_{test}, y_{train}, y_{valid}, y_{test} = load_dataset(d_set)
552
       #
             final\_rmse = linear\_regression(x\_train, x\_valid, x\_test, y\_train, y\_valid, y\_test, 'regression')
553
       #
             print('Test RMSE for ' + d_set + ': ' + str(final_rmse))
554
555
       #
556
557
       # for d_set in classification_sets:
558
559
             x_train, x_valid, x_test, y_train, y_valid, y_test = load_dataset(d_set)
```

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```
560 #
```

561 # final_ratio = linear_regression(x_train, x_valid, x_test, y_train, y_valid, y_test, 'classification')
562 # print('Test Ratio for ' + d_set + ': ' + str(final_ratio))