



CSU44061 Machine Learning

Lab 2

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1 Introduction

In this assignment, the dataset used in part 'i' has the ID of 19-19-19-0 and the dataset used in part 'ii' has the ID of 19-38-19-0 .

2 Part i

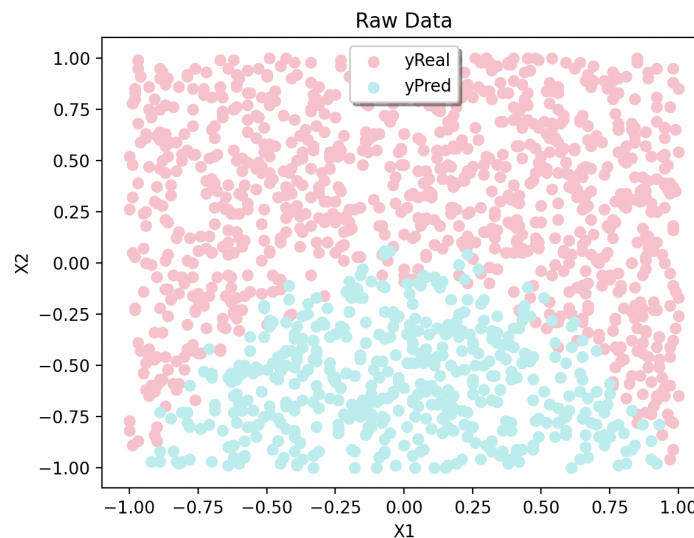


Figure 1: A scatter plot graph visualizing the first dataset.

2.1 (i)(a)

In (i)(a) we first read in the raw data and then visualize it on a graph as seen in figure one using circular markers. Each data point is placed depending on the value of its two features, with the X-axis corresponding to X_1 and the Y-axis corresponding to X_2 . The color of the marker depends on the target value y , if the marker is red then $y=1$ and if blue then $y=-1$. As seen in figure one there is a clear decision boundary between the two classifications.

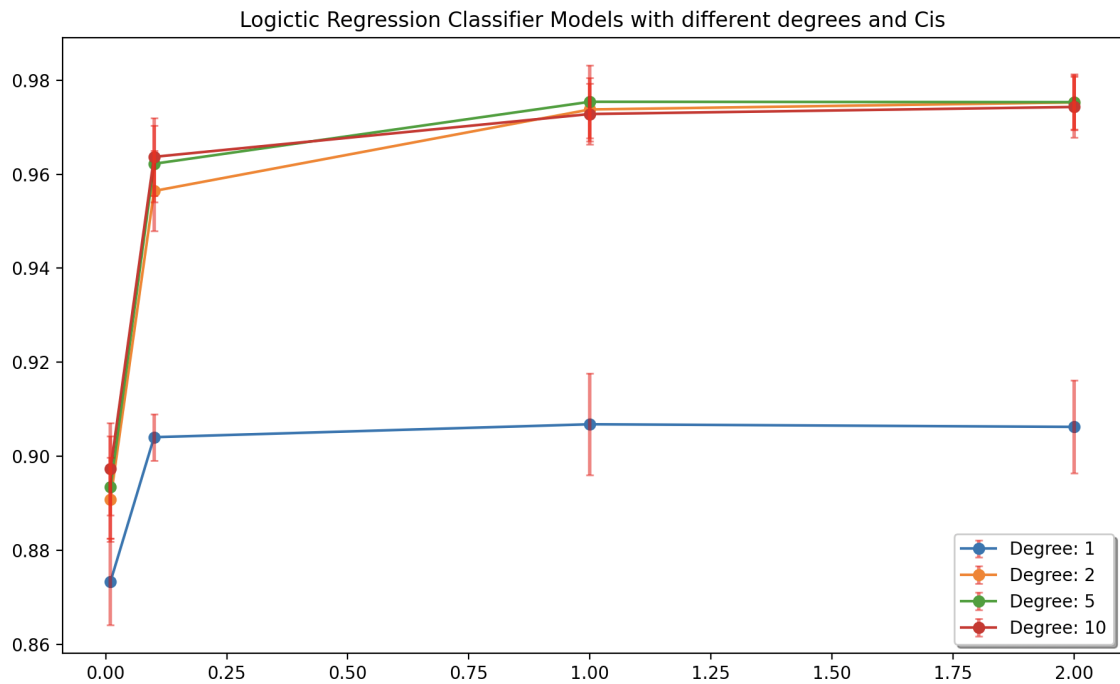


Figure 2: A plot with four lines, each representing a Logistic model trained with a different polynomial degree of X. Each line has four points with an error bar, each of them represent the f1 score mean and standard deviation of a model with a different C value.

In order to then train a logistic regression classifier on the data, we first have to use cross validation in order to choose the right polynomial degree of X and the correct weight for C. These are important to get right as the accuracy of a model can change drastically depending on the values.

During cross validation the range of polynomial degrees used was [1, 2, 5, 10]. I chose these values as they represent a good spread and represent the typical range of degrees used in logistic regression classifiers (which the addition of 1 and 10 as outliers). The range of C values used were [0.01, 0.1, 1, 2], chosen for the same reasons as the degrees. The default C used is typically 1, and then I added greater and lesser values to have a good spread.

The accuracy metric used in the following cross validation was the F1 score. The higher the score the better precision and recall a model has. The F1 score is calculated as:

$$P = \frac{\# \text{ True Positives}}{\# \text{ True Positives} + \# \text{ False Positives}}$$

$$R = \frac{\# \text{ True Positives}}{\# \text{ True Positives} + \# \text{ False Negative}}$$

$$\text{F1 Score} = 2 * (P * R) / (P + R)$$

F1 scores were chosen as it combines both precision and recall and gives good results when the dataset is imbalanced (as ours is, see figure 1). Also, MSE cannot be used as a metric for classification as it cannot compare discrete classes.

The graph in figure two represents the outcomes of cross validation. A model was trained on each combination of C values and degrees, with a total of 16 models. A five-fold cross validation is performed on each model, the f1 score of each iteration is calculated and a mean and standard deviation f1 scores taken for each model. Five-fold cross validation was chosen as it is commonly used.

As seen in figure two, the polynomial degree which consistently gives the higher f1 scores is five, and the C value which does the same is 1. Both of these outcomes make sense as these values are commonly the default for a logistic regression classifier.

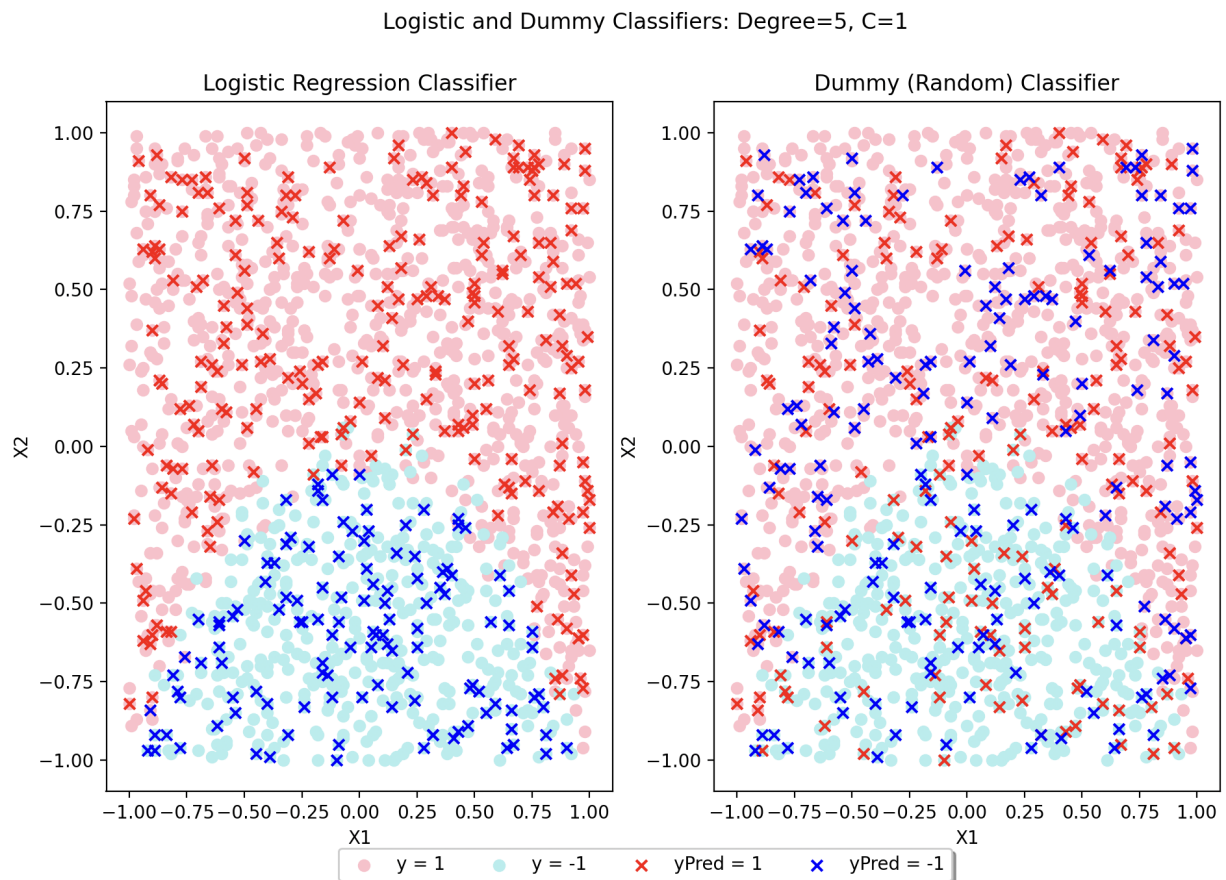


Figure 3: A figure with two scatter plots, the left one representing the predictions of the logistic regression classifier and the right being a random dummy model.

The data is then split between training and testing and the features are brought to an order of five. A logistic regression model (with a C of 1) and a dummy model (using an uniform random classification) are then trained and told to predict the testing data. The outcome of this is seen in figure 3. The LRC performed much better than the dummy classifier, with the f1 scores of each being 0.97899 and 0.58095 respectively.

2.2 (i)(b)

We then train a K-nearest neighbors classifier on the data. Knn, a point is predicted based on the most frequent classification of the points around it. The parameter 'k' defines the number of neighbors to use, we will use cross validation to choose this value. It is important to choose the correct k as too small of a k leads to overfitting while a too big k leads to under-fitting.

The values of k chosen for cross validation were [2, 5, 9, 14]. This spread was chosen as it represents both high, low, and 'typical' k's. Once again I used f1 scores and 5-fold cross validation. As there was only one value to cross validate instead of 2, there are only 4 models total. The outcome is shown in figure 4, from this graph we can see that a k of 5 and 9 produced the highest f1 scores, but 5 had a much lower standard deviation. As such we will be using a k of five in our optimal model.

The data is then split between training and testing sections. A knn model (with a k of 5) and a dummy model (using an uniform random classification) are then trained and told to predict the testing data. The outcome of this is seen in figure 5. The knn classifier performed much better than the dummy classifier, with the f1 scores of each being 0.97991 and 0.607305 respectively.

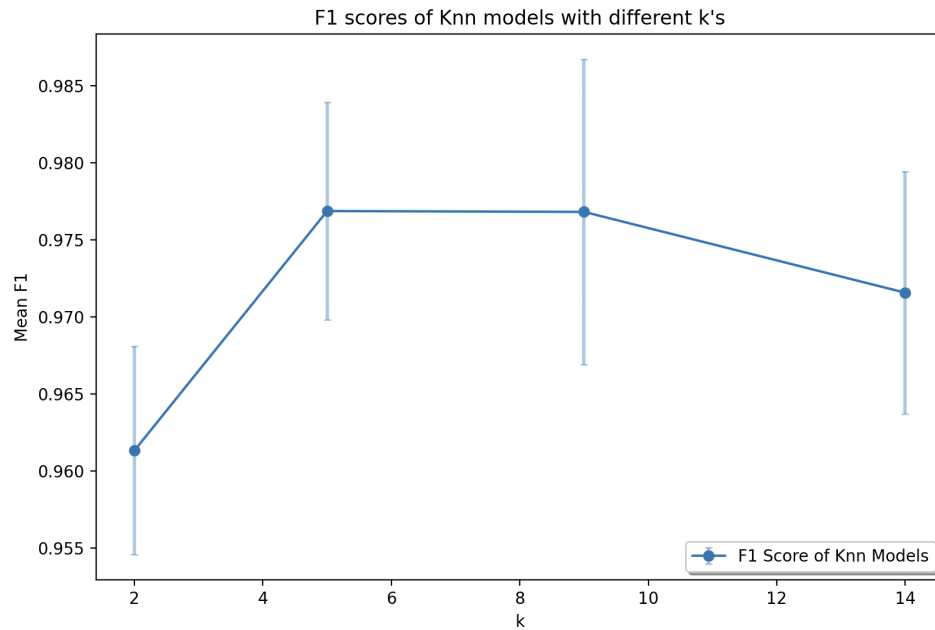


Figure 4: A plot with a singular line with four points, each point has an error bar. It represents the mean f1 scores of a knn model with different values of k.

Knn and Dummy Classifiers: k=5

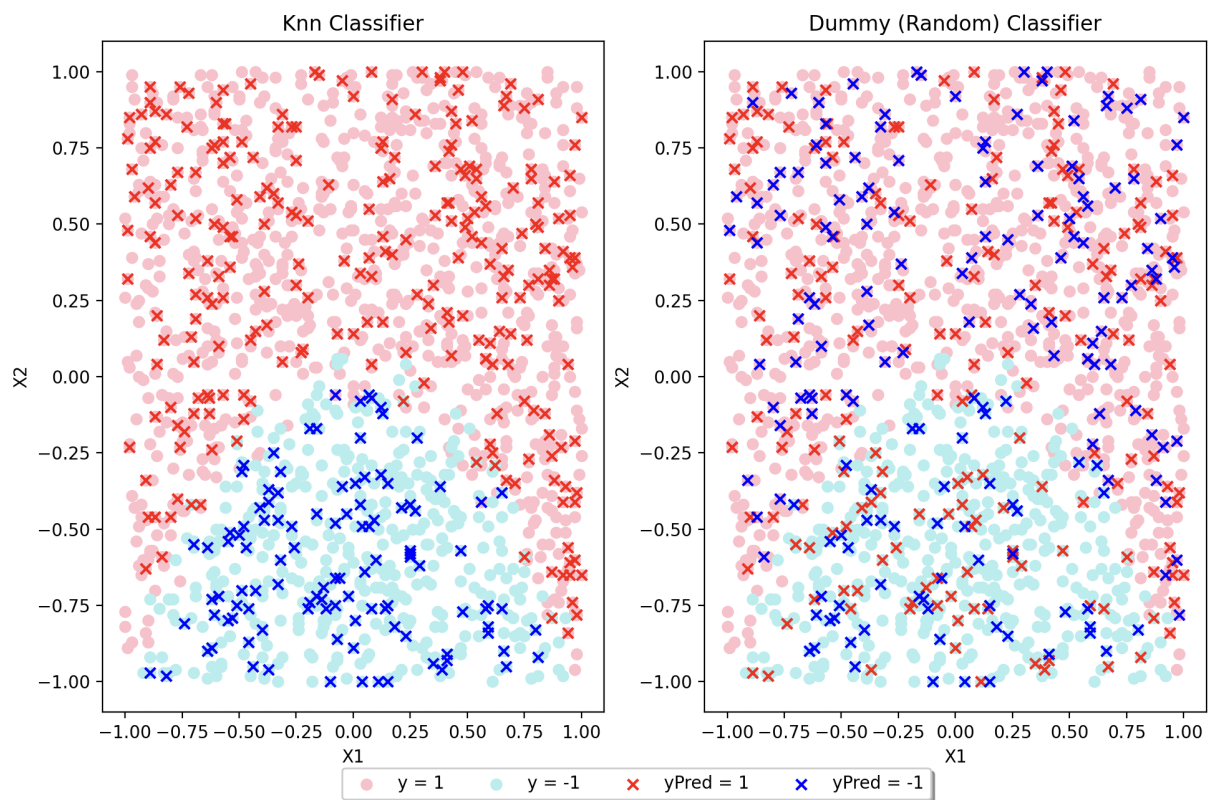


Figure 5: A figure with two scatter plots, the left one representing the predictions of the knn classifier and the right being a random dummy model.

2.3 (i)(c)

A confusion matrix is another type of performance metric that visualized the recall and precision in a table format. Data was split again between training and testing, and a LCR(C=1), Knn(k=5), and dummy (random) classifiers were all trained (with the LCR being trained with polynomial features to a degree of 5). They then made predictions based on the testing features and a confusion matrix was made by comparing those predictions to the real y values.

LCR	Predicted Positive	Predicted Negative		Dummy	Predicted Positive	Predicted Negative
True Positive	238	2		True Positive	109	131
True Negative	1	110		True Negative	58	63
Knn	Predicted Positive	Predicted Negative				
True Positive	236	4				
True Negative	7	114				

Figure 6: An image with 3 tables, each table being a confusion matrix for one of three models: LCR, Knn, and a dummy.

2.4 (i)(d)

An ROC curve is line that plots the true positive rate of a model against the false positive rate of a model at different classification thresholds. A classification threshold is the threshold that must be reached for a model to classify a point as positive. The formula for each rate are as follows:

$$\text{TPR} = \text{TP} / (\text{TP} + \text{FN})$$

$$\text{FPR} = \text{FP} / (\text{FP} + \text{TN})$$

Using the same data split and models as part C, the ROC curves of an LCR, Knn, and dummy model were plotted on the graph seen in figure 7.

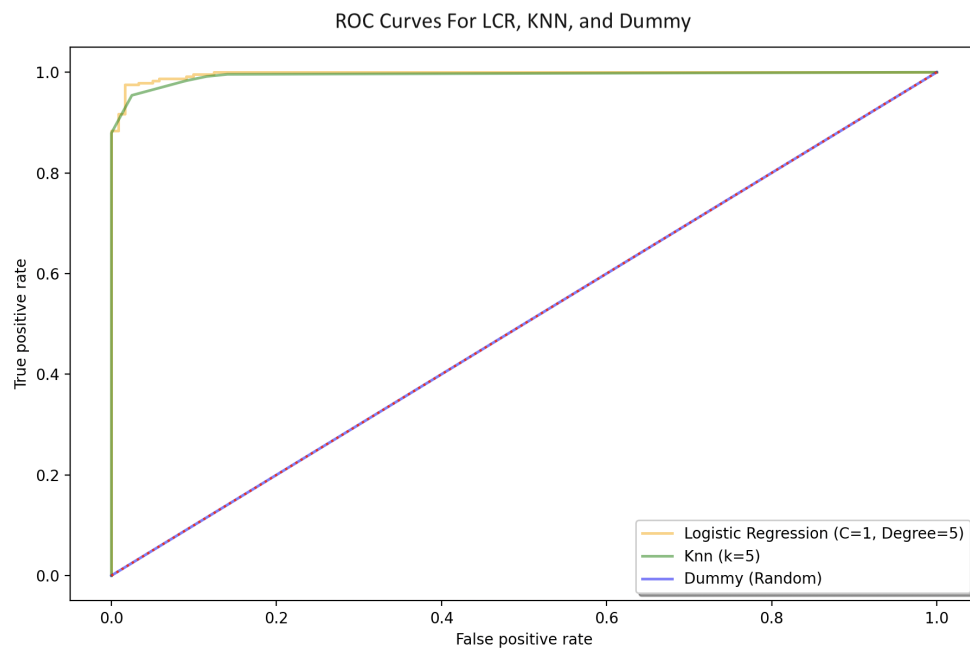


Figure 7: A graph with four lines, each representing the roc curve of a LCR, knn, and dummy model with a baseline 1-1 also plotted.

2.5 (i)(e)

The baseline dummy classifier performed far worse than both the LCR and Knn, as to be expected. It's confusion matrix had the most FPs and FNs and its ROC curve was practically the same as the baseline 1-1 line. The LCR performed slightly better than the Knn in the confusion matrix, as the number of FPs and FNs was only three, while Knn had 11 total. An ROC curve is considered better the closer the line is to an upside down L as it would mean that when the classification threshold is 1 the false positive rate is 0. The LCR again performs slightly better as it gets closer to the upper left corner than the Knn line does.

The f1 scores of each model are as follows: LCR = 0.97863, Knn = 0.97844, Dummy = 0.56937.

I would not be able to recommend a model for classification between the choice of LCR and Knn as the difference in the two in this example is not significant enough to be able to say for certain which is inherently better.

3 Part ii

3.1 (ii)(a)

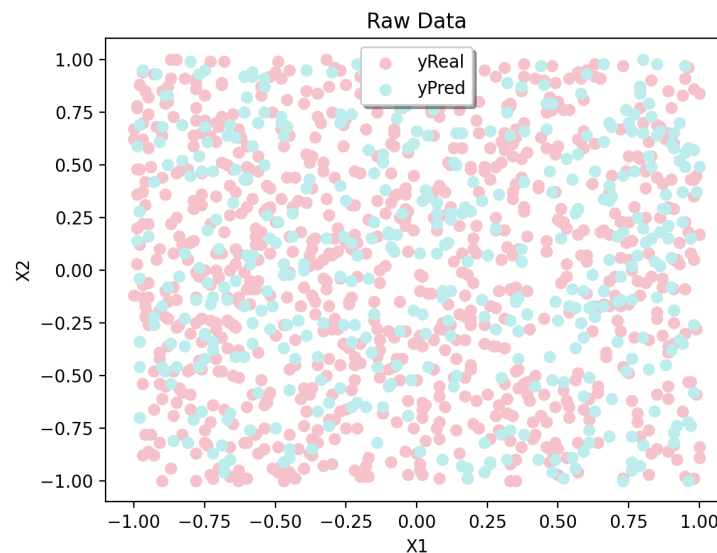


Figure 8: A scatter plot graph visualizing the second dataset.

In (ii)(a) we first read in the raw data and then visualize it on a graph as seen in figure one using circular markers. Each data point is placed depending on the value of its two features, with the X-axis corresponding to X1 and the Y-axis corresponding to X2. The color of the marker depends on the target value y, if the marker is red then $y=1$ and if blue then $y=-1$. As seen in figure 8, there is no clear decision boundary between the two classifications.

As in part (i)(a) we use the same form of cross validation with the same range of polynomial degrees and C values. The graph in figure 9 shows the outcomes of this cross validation. It is obvious from looking at the graph that this dataset does not seem to capture the same relationship as part i. Contrary to part (i) where the optimal degree was 5, for this dataset it seems to be 2. Though just barely as every combination of degree and C have extremely high standard deviations and have lower means than those in part (i)(a). The optimal C is either 0.1 or 1, we will use 1 as it is typically standard.

In figure 10 we can see the outcome of a LCR model with a C of 1 and degree 2 against a baseline random dummy model. It is interesting to note that the LCR model only ever predicted positive. The f1 scores were as follows: LCR = 0.81904, Dummy = 0.59893. The LCR still performed better than the dummy, but was much worse than in part i.

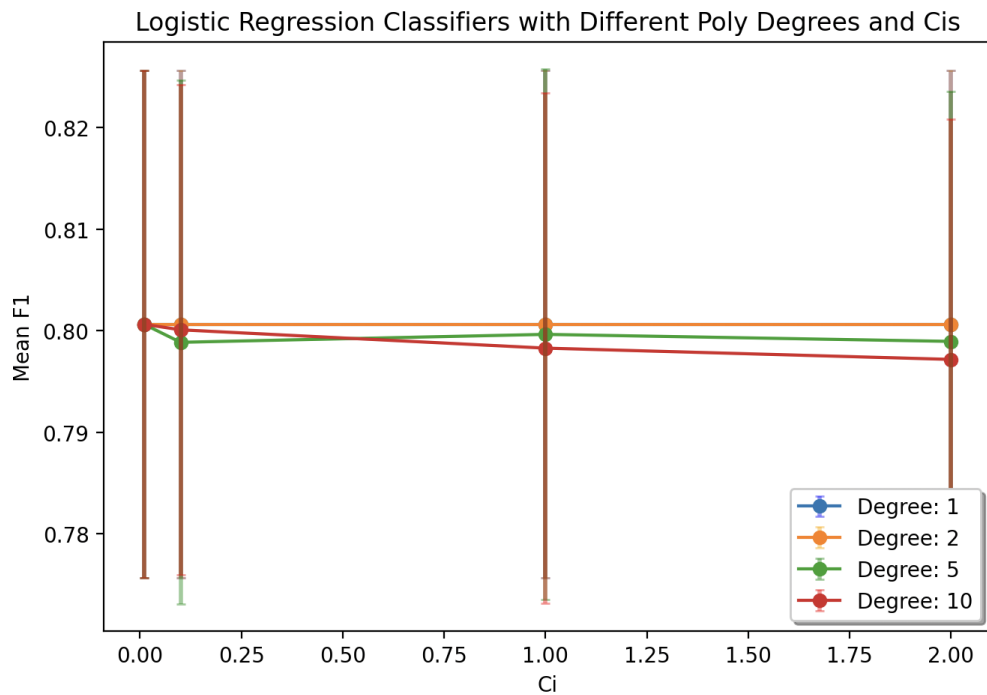


Figure 9: A plot with four lines, each representing a Logistic model trained with a different polynomial degree of X . Each line has four points with an error bar, each of them represent the f1 score mean and standard deviation of a model with a different C value.

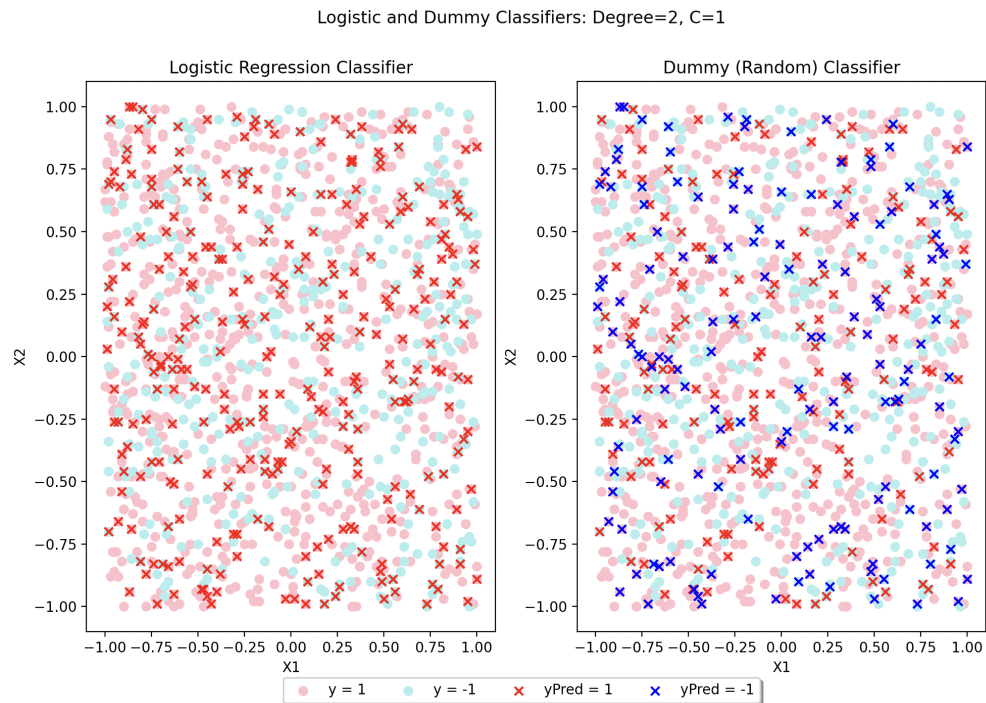


Figure 10: A figure with two scatter plots, the left one representing the predictions of the logistic regression classifier and the right being a random dummy model.

3.2 (ii)(b)

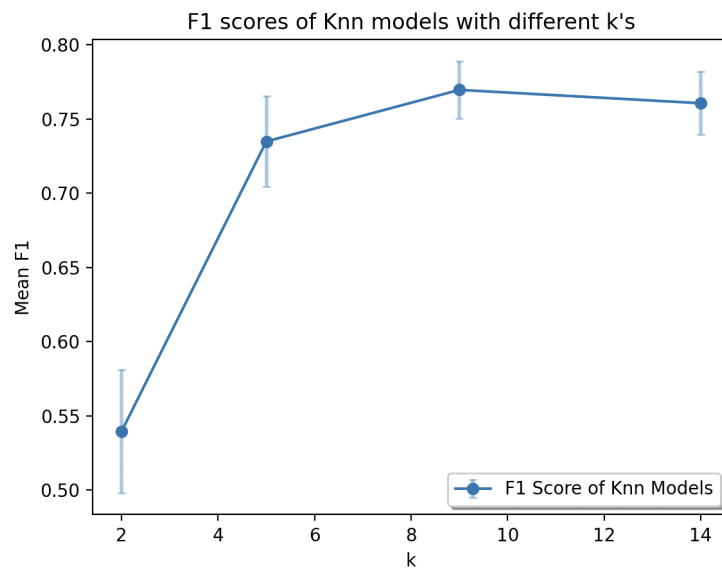


Figure 11: A plot with a singular line with four points, each point has an error bar. It represents the mean f1 scores of a knn model with different values of k.

Knn and Dummy Classifiers: k=9

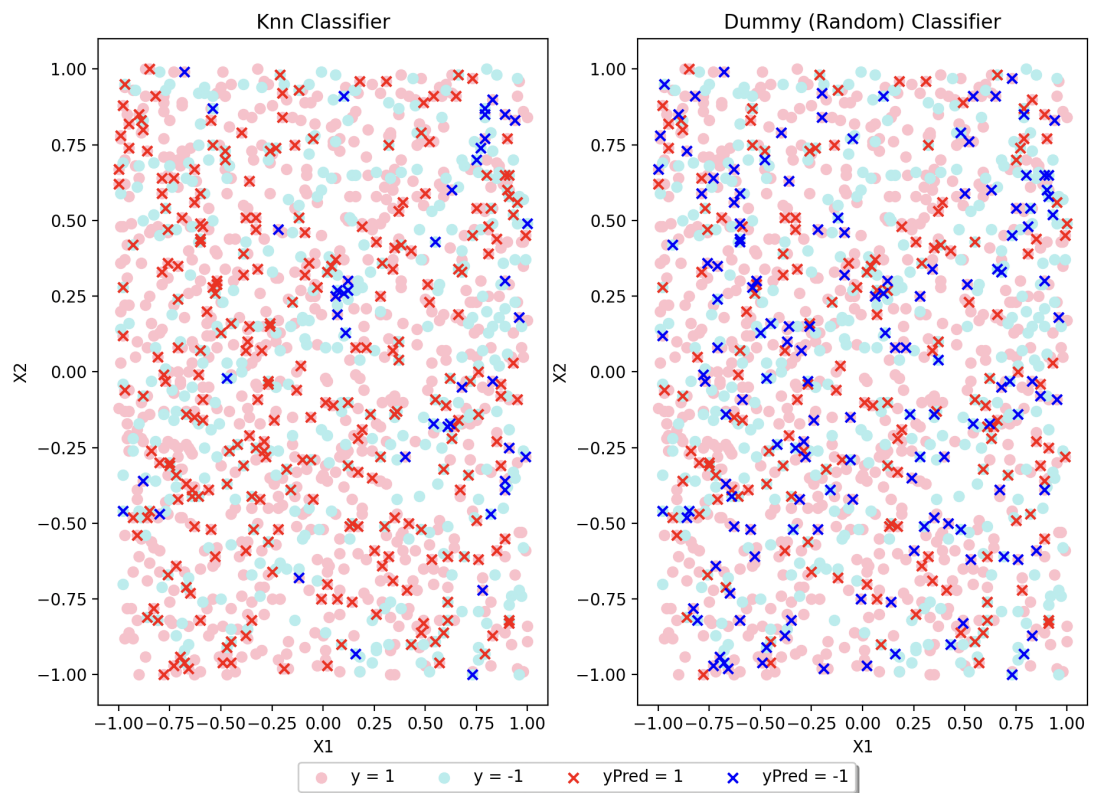


Figure 12: A figure with two scatter plots, the left one representing the predictions of the knn classifier and the right being a random dummy model.

As in part (i)(b) we use the same form of cross validation with the same range of k values. The graph in figure 11 shows the outcome. The optimal K for this dataset seems to be 9, not 5 like in the previous part. Once again we split the data and train a Knn model with a k of nine and a dummy model and then ask them to predict the test X 's. The outcome of which is shown on figure 12. The $f1$ scores were as follows: Knn = 0.75213, Dummy = 0.5589. The Knn still performed better than the dummy, but was much worse than in part i.

3.3 (ii)(c)

Confusion matrices were made for the LCR (degree=2, $C=1$), Knn ($k=9$), and dummy models in the same way as in part i. They can be seen in figure 13.

LCR	Predicted Positive	Predicted Negative		Dummy	Predicted Positive	Predicted Negative
True Positive	206	0		True Positive	114	92
True Negative	104	0		True Negative	49	55

Knn	Predicted Positive	Predicted Negative
True Positive	179	27
True Negative	86	18

Figure 13: An image with 3 tables, each table being a confusion matrix for one of three models: LCR, Knn, and a dummy.

3.4 (ii)(d)

Using the same data split and models as part C, the ROC curves of an LCR, Knn, and dummy model were plotted on the graph seen in figure 14.

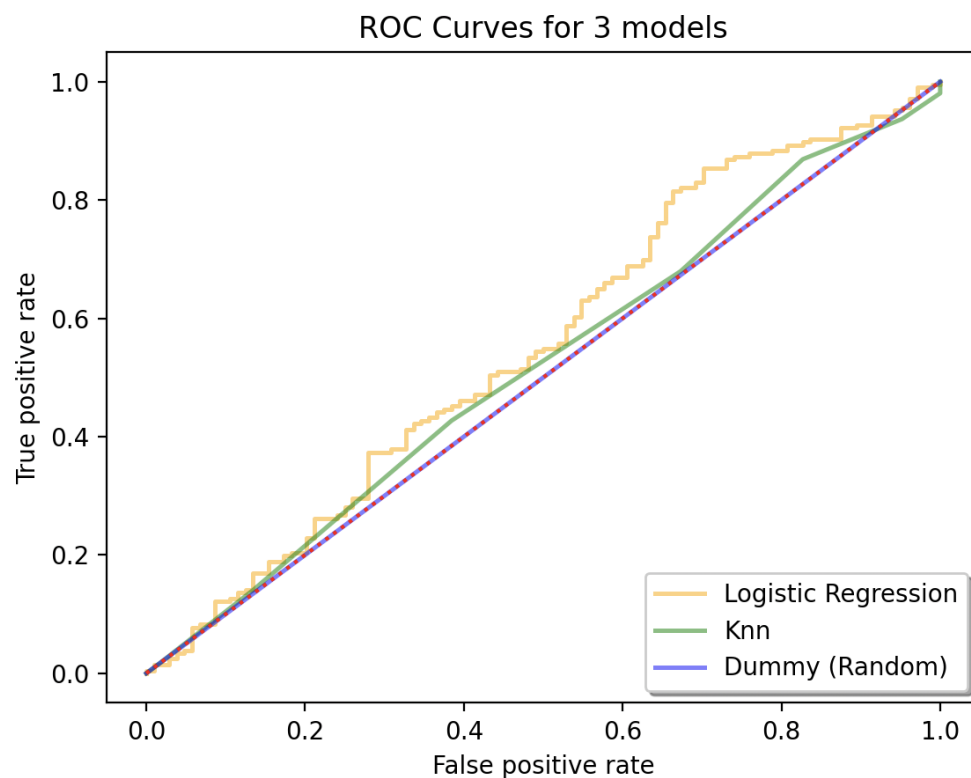


Figure 14: A graph with four lines, each representing the roc curve of a LCR, knn, and dummy model with a baseline 1-1 also plotted.

3.5 (ii)(e)

The baseline dummy classifier performed worse than both the LCR and Knn, as to be expected. It's confusion matrix had the most FPs and FNs and its ROC curve was practically the same as the baseline 1-1 line. Both the LCR and Knn model performed far worse than in the previous parts, this is because the dataset is not useful and there wasn't any clear decision boundary between the two classifications. The LCR performed slightly better than the Knn in the confusion matrix, as the number of FPs and FNS was 104, while Knn had 113 total. Though it should be noted that the LCR strangely only predicted positive. The LCR again performs slightly better in the ROC graph as it gets closer to the upper left corner than the Knn line does.

The f1 scores of each model are as follows: LCR = 0.79844, Knn = 0.76008, Dummy = 0.572207.

I would not be able to recommend a model for classification between the choice of LCR and Knn as they both performed poorly and the difference in the two in this example is not significant enough to be able to say for certain which is better. This dataset is useless for classification and no classification model would be able to perform well.

4 Appendix

```

1 # id:19-19-19-0
2 # id:19--38-19-0
3 import numpy as np
4 import pandas as pd
5 import matplotlib.pyplot as plt
6 from sklearn.dummy import DummyClassifier
7 from sklearn.linear_model import LogisticRegression
8 from sklearn.metrics import confusion_matrix, f1_score, roc_curve
9 from sklearn.model_selection import KFold, train_test_split
10 from sklearn.neighbors import KNeighborsClassifier
11 from sklearn.preprocessing import PolynomialFeatures
12
13 ##Function to do a-e for each dataset
14 def partsatoc(filename):
15
16     if filename=="week4a.csv":
17         optimalk= 5
18         optimaldegree= 5
19     else:
20         optimalk= 9
21         optimaldegree= 2
22
23     #Part A
24     ##Read in data
25     df = pd.read_csv(filename)
26     X1=df.iloc[:,0]
27     X2=df.iloc[:,1]
28     X=np.column_stack((X1,X2))
29     y=df.iloc[:,2]
30
31     ##Graph data
32     plt.scatter(X1[y == 1], X2[y == 1], color='pink', marker='o')
33     plt.scatter(X1[y == -1], X2[y == -1], color='paleturquoise', marker='o')
34
35     plt.xlabel("X1")
36     plt.ylabel("X2")
37     plt.legend(["yReal", "yPred"], loc='upper center', fancybox=True, shadow=True)
38     plt.title("Raw Data")
39     plt.show()
40

```

```

41  ##Cross Validation for polynomial and C values
42  plt.title("Logistic Regression Classifiers with Different Poly Degrees and Cis")
43
44  polyRange = [1, 2, 5, 10]
45  cRange = [0.01, 0.1, 1, 2]
46  color = ['b', 'orange', 'g', 'r']
47  counter = 0
48  for i in polyRange:
49      mean_f1=[]; std_f2=[]
50      for c in cRange:
51          model = LogisticRegression(C=c)
52          temp=[]
53          kf = KFold(n_splits=5)
54          polyX = PolynomialFeatures(i).fit_transform(np.array(X))
55          for train, test in kf.split(polyX):
56              model.fit(polyX[train], y[train])
57              ypred = model.predict(polyX[test])
58              temp.append(f1_score(y[test], ypred))
59          mean_f1.append(np.array(temp).mean())
60          std_f2.append(np.array(temp).std())
61      ##Graph
62      markers, caps, bars = plt.errorbar(cRange, mean_f1, barsabove=True, yerr=std_f2,
63      ecolor=color[counter], capsize=2, elinewidth=2, fmt="-o")
64      [bar.set_alpha(0.4) for bar in bars]
65      [cap.set_alpha(0.4) for cap in caps]
66      counter = counter + 1
67
68  plt.legend(["Degree: 1", "Degree: 2", "Degree: 5", "Degree: 10"], loc='lower right',
69  fancybox=True, shadow=True)
70  plt.xlabel("Ci")
71  plt.ylabel("Mean F1")
72  plt.show()
73
74  ##Train optimal model
75  polyX = PolynomialFeatures(optimaldegree).fit_transform(np.array(X))
76  X_train, X_test, y_train, y_test = train_test_split(polyX, y)
77  fig, (ax1, ax2) = plt.subplots(1, 2)
78
79  logreg = LogisticRegression()
80  logreg.fit(X_train, y_train)
81  ypred = logreg.predict(X_test)
82
83  ##Train dummy
84  dclf = DummyClassifier(strategy = 'uniform')
85  dclf.fit(X_train, y_train)
86  ydummy = dclf.predict(X_test)
87
88  ##Graph
89  ax1.scatter(X1[y == 1], X2[y == 1], color='pink', marker='o')
90  ax1.scatter(X1[y == -1], X2[y == -1], color='paleturquoise', marker='o')
91  ax1.scatter(X_test[ypred == 1,1], X_test[ypred == 1,2], color='r', marker='x')
92  ax1.scatter(X_test[ypred == -1,1], X_test[ypred == -1,2], color='b', marker='x')
93
94  ax1.set_xlabel='X1', ylabel='X2'
95  ax1.set_title("Logistic Regression Classifier")
96
97  ax2.scatter(X1[y == 1], X2[y == 1], color='pink', marker='o')
98  ax2.scatter(X1[y == -1], X2[y == -1], color='paleturquoise', marker='o')
99  ax2.scatter(X_test[ydummy == 1,1], X_test[ydummy == 1,2], color='r', marker='x')
100  ax2.scatter(X_test[ydummy == -1,1], X_test[ydummy == -1,2], color='b', marker='x')
101
102  ax2.set_xlabel='X1', ylabel='X2'
103  ax2.set_title("Dummy (Random) Classifier")
104
105  if filename=="week4a.csv":
106      fig.suptitle("Logistic and Dummy Classifiers: Degree=5, C=1")
107  else:
108      fig.suptitle("Logistic and Dummy Classifiers: Degree=2, C=1")

```

```

107 fig.legend(["y = 1", "y = -1", "yPred = 1", "yPred = -1"], ncol=4, loc='lower center',
108 fancybox=True, shadow=True)
109 plt.show()
110
111 print("Logistic Regression F1 Score: ", f1_score(y_test, ypred))
112 print("Dummy (Random) F1 Score: ", f1_score(y_test, ydummy))
113
114 #Part B
115 kRange = [2, 5, 9, 14]
116 mean_f1=[]; std_f2=[]
117 for k in kRange:
118     model = KNeighborsClassifier(n_neighbors=k)
119     temp=[]
120     kf = KFold(n_splits=5)
121     for train, test in kf.split(X):
122         model.fit(X[train], y[train])
123         ypred = model.predict(X[test])
124         temp.append(f1_score(y[test], ypred))
125     mean_f1.append(np.array(temp).mean())
126     std_f2.append(np.array(temp).std())
127
128 ##Graph
129 markers, caps, bars = plt.errorbar(kRange, mean_f1, barsabove=True, yerr=std_f2, capsize
130 =2, elinewidth=2, fmt="-o")
131 [bar.set_alpha(0.4) for bar in bars]
132 [cap.set_alpha(0.4) for cap in caps]
133
134 plt.legend(["F1 Score of Knn Models"], loc='lower right', fancybox=True, shadow=True)
135 plt.title("F1 scores of Knn models with different k's")
136 plt.xlabel("k")
137 plt.ylabel("Mean F1")
138 plt.show()
139
140 ##Train optimal model
141 X_train, X_test, y_train, y_test = train_test_split(X, y)
142 fig, (ax1, ax2) = plt.subplots(1, 2)
143
144 knn = KNeighborsClassifier(n_neighbors=optimal_k)
145 knn.fit(X_train, y_train)
146 ypred = knn.predict(X_test)
147
148 ##Train dummy
149 dclf = DummyClassifier(strategy = 'uniform')
150 dclf.fit(X_train, y_train)
151 ydummy = dclf.predict(X_test)
152
153 ##Graph
154 ax1.scatter(X1[y == 1], X2[y == 1], color='pink', marker='o')
155 ax1.scatter(X1[y == -1], X2[y == -1], color='paleturquoise', marker='o')
156 ax1.scatter(X_test[ypred == 1,0], X_test[ypred == 1,1], color='r', marker='x')
157 ax1.scatter(X_test[ypred == -1,0], X_test[ypred == -1,1], color='b', marker='x')
158
159 ax1.set_xlabel('X1', ylabel='X2')
160 ax1.set_title("Knn Classifier")
161
162 ax2.scatter(X1[y == 1], X2[y == 1], color='pink', marker='o')
163 ax2.scatter(X1[y == -1], X2[y == -1], color='paleturquoise', marker='o')
164 ax2.scatter(X_test[ydummy == 1,0], X_test[ydummy == 1,1], color='r', marker='x')
165 ax2.scatter(X_test[ydummy == -1,0], X_test[ydummy == -1,1], color='b', marker='x')
166
167 ax2.set_xlabel('X1', ylabel='X2')
168 ax2.set_title("Dummy (Random) Classifier")
169
170 if filename=="week4a.csv":
171     fig.suptitle("Knn and Dummy Classifiers: k=5")
172 else:
173     fig.suptitle("Knn and Dummy Classifiers: k=9")
174 fig.legend(["y = 1", "y = -1", "yPred = 1", "yPred = -1"], ncol=4, loc='lower center',
175 fancybox=True, shadow=True)

```

```

173 plt.show()
174
175 print("Knn F1 Score: ", f1_score(y_test, ypred))
176 print("Dummy (Random) F1 Score: ", f1_score(y_test, ydummy))
177
178 #Part C
179 ##Using the models from the previous parts, test them all on the same y_test
180 X_train, X_test, y_train, y_test = train_test_split(X, y)
181 polyXtest = PolynomialFeatures(optimaldegree).fit_transform(np.array(X_test))
182 polyXtrain = PolynomialFeatures(optimaldegree).fit_transform(np.array(X_train))
183
184 logreg = LogisticRegression().fit(polyXtrain, y_train)
185 knn = KNeighborsClassifier(n_neighbors=optimalk).fit(X_train, y_train)
186 dclf = DummyClassifier(strategy='uniform').fit(X_train, y_train)
187
188 predlog = logreg.predict(polyXtest)
189 predknn = knn.predict(X_test)
190 preddummy = dclf.predict(X_test)
191
192 ##Print confusion matrices
193 print("Confusion matrix for Logistic Regression Classifier")
194 print(confusion_matrix(y_test, predlog))
195 print("Confusion matrix for Knn Classifier")
196 print(confusion_matrix(y_test, predknn))
197 print("Confusion matrix for Dummy Classifier (random)")
198 print(confusion_matrix(y_test, preddummy))
199
200 #Part D
201
202 ##Graph ROC curve for each model
203 logreg = LogisticRegression().fit(polyXtrain, y_train)
204 fpr, tpr, __ = roc_curve(y_test, logreg.predict_proba(polyXtest)[: , 1])
205 plt.plot(fpr, tpr, color='orange', alpha=0.5, linewidth=1.8)
206
207 knn = KNeighborsClassifier(n_neighbors=optimalk).fit(X_train, y_train)
208 fpr, tpr, __ = roc_curve(y_test, knn.predict_proba(X_test)[: , 1])
209 plt.plot(fpr, tpr, color='green', alpha=0.5, linewidth=1.8)
210
211 dummy = DummyClassifier(strategy='uniform').fit(X_train, y_train)
212 fpr, tpr, __ = roc_curve(y_test, dummy.predict_proba(X_test)[: , 1])
213 plt.plot(fpr, tpr, color='blue', alpha=0.5, linewidth=1.8)
214
215 plt.plot([0, 1], [0, 1], color='red', linestyle='dotted')
216
217 ##Specify graph details
218 plt.legend(['Logistic Regression', "Knn", "Dummy (Random)"], loc='lower right', fancybox=
True, shadow=True)
219 plt.xlabel('False positive rate')
220 plt.ylabel('True positive rate')
221 plt.title("ROC Curves for 3 models")
222 plt.show()
223
224 #Part E
225 ##Graph f1 scores of each model for comparison
226 classifiers = ["Logistic Regression", "Knn", "Dummy (Random)"]
227 fscores = [f1_score(y_test, logreg.predict(polyXtest)), f1_score(y_test, knn.predict(
X_test)), f1_score(y_test, dummy.predict(X_test))]
228 bar_colors = ['tab:orange', 'tab:green', 'tab:blue']
229
230 for i in range(3):
231     print(classifiers[i], " - ", fscores[i])
232
233 plt.bar(classifiers, fscores, color=bar_colors)
234 plt.title("F1 Scores of 3 different Classifiers")
235 plt.show()
236
237 partsatoe("week4a.csv")
238 partsatoe("week4b.csv")

```