Aprendizagem 2023 Homework I — Group 003 (ist1107028, ist1107137)

Part I: Pen and paper

We collected four positive (P) observations,

$$\{x_1 = (A,0), x_2 = (B,1), x_3 = (A,1), x_4 = (A,0)\}$$

and four negative (N) observations,

$$\{x_5 = (B,0), x_6 = (B,0), x_7 = (A,1), x_8 = (B,1)\}$$

Consider the problem of classifying observations as positive or negative.

1. Compute the F1-measure of a kNN with k=5 and Hamming distance using a leave-one-out evaluation schema. Show all calculus.

We start by calculating Hamming distance between observations. The Hamming distance is the number of positions at which the corresponding symbols are different.

Since we are workin with k = 5, we will consider the 5 nearest neighbors of each observation (written in blue).

	$ x_1 $	$x_2$	$x_3$	$x_4$	$x_5$	$x_6$	$x_7$	$x_8$
$x_1$	-	2	1	0	1	1	1	2
$x_2$	2	-	1	2	1	1	1	0
$x_3$	1	1	-	1	2	2	0	1
$x_4$	0	2	1	-	1	1	1	2
$x_5$	1	1	2	1	-	0	2	1
$x_6$	1	1	2	1	0	-	2	1
$x_7$	1	1	0	1	2	2	-	1
$x_8$	2 1 0 1 1 1 2	0	1	2	1	1	1	-

Table 1: Hamming distance between observations

Now that we have the Hamming distance between all observations, we must identify if the prediction is correct or not. We will consider the majority class of the 5 nearest neighbors for each observation.

Example: For  $x_1$ , the 5 nearest neighbors are  $x_3$  and  $x_4$  (which are positive),  $x_5$ ,  $x_6$  and  $x_7$  (which are negative). The majority class is negative, therefore the prediction is incorrect.

We apply the same logic for the rest of the classes, ending up with the following table:

Observation	True Value	Prediction	Confusion Matrix Terminology
$\overline{x_1}$	Р	N	FN
$x_2$	Р	N	FN
$x_3$	Р	Р	TP
$x_4$	Р	N	FN
$x_5$	N	Р	$\operatorname{FP}$
$x_6$	N	Р	$\operatorname{FP}$
$x_7$	N	Р	FP
$x_8$	N	N	$\operatorname{TN}$

P - Positive observation; N - Negative observation

TP - True Positive; TN - True Negative; FP - False Positive; FN - False Negative

Table 2: Predictions for each observation - k = 5

With this table, we can know calculate the Precision, Recall and F1-measure using the following formulas:

$$Precision = \frac{True \ Positives}{True \ Positives + False \ Positives}$$
 (1)

$$Recall = \frac{True \ Positives}{True \ Positives + False \ Negatives}$$
 (2)

$$F1-measure = 2 \times \frac{Precision \times Recall}{Precision + Recall}$$
 (3)

Replacing the corresponding values in the formulas, we get:

for Precision (1) and Recall (2):

Precision = 
$$\frac{1}{1+3} = 0.25$$
 Recall =  $\frac{1}{1+3} = 0.25$ 

F1-measure (3):

F1-measure = 
$$2 \times \frac{0.25 \times 0.25}{0.25 + 0.25} = 0.25$$

2. Propose a new metric (distance) that improves the latter's performance (i.e., the F1-measure) by three fold.

To improve the F1-measure, we propose using K=3 instead of k=5. This way, we will consider the 3 nearest neighbors of each observation.

Simply by looking at the Hamming distance table, we can produce a new prediton table, like in the first exercise:

Observation	True Value	Prediction	Confusion Matrix Terminology
$\overline{x_1}$	P	Р	TP
$x_2$	P	N	FN
$x_3$	Р	N	FN
$x_4$	P	Р	TP
$x_5$	N	N	${ m TN}$
$x_6$	N	N	${ m TN}$
$x_7$	N	P	$\operatorname{FP}$
$x_8$	N	P	FP

P - Positive observation; N - Negative observation

TP - True Positive; TN - True Negative; FP - False Positive; FN - False Negative

Table 3: Predictions for each observation - k = 3

Precision = 
$$\frac{2}{2+2} = 0.5$$
 Recall =  $\frac{2}{2+2} = 0.5$  F1-measure =  $2 \times \frac{0.5 \times 0.5}{0.5 + 0.5} = 0.5$ 

An additional positive observation was acquired,  $x_9 = (B, 0)$ , and a third variable  $y_3$  was independently monitored, yielding estimates,

$$y_3|P=\{1.1,0.8,0.5,0.9,0.8\}$$
 and  $y_3|N=\{1,0.9,1.2,0.9\}$ 

3. Considering the nine training observations, learn a Bayesian classifier assuming: (i)  $y_1$  and  $y_2$  are dependent; (ii)  $y_1$ ,  $y_2$  and  $y_3$  variable sets are independent and equally important; and (iii)  $y_3$  is normally distributed. Show all parameters.

With the nine training observations, we can calculate the parameters for the Bayesian classifier. We will refer to the outcome, which can be positive or negative, as P and N respectively, and 'class' or 'c' when we mean both.

To estimate  $P(\text{class}|y_1, y_2, y_3)$ , we can use Bayes' theorem:

$$P(\text{class}|y_1, y_2, y_3) = \frac{P(y_1, y_2, y_3|\text{class}) \times P(\text{class})}{P(y_1, y_2, y_3)}$$
(4)

Since we know  $\{y_1, y_2\}$  and  $\{y_3\}$  are independent, we can rewrite  $P(y_1, y_2, y_3)$  as  $P(y_1, y_2) \times P(y_3)$ . Rewriting (4) with this, results in:

$$P(\operatorname{class}|y_1, y_2, y_3) = \frac{P(y_1, y_2|\operatorname{class})P(y_3|\operatorname{class}) \times P(\operatorname{class})}{P(y_1, y_2) \times P(y_3)}$$
(5)

Given a new observation O, we are able to classify it by calculating P(class|O) for all classes and selecting the class with the highest probability as our prediction.

$$\hat{z} = \underset{c \in \{P,N\}}{\operatorname{arg max}} \left\{ P(c|O) \right\} \\
= \underset{c \in \{P,N\}}{\operatorname{arg max}} \left\{ \frac{P(y_1, y_2|c)P(y_3|c) \times P(c)}{P(y_1, y_2)P(y_3)} \right\} \\
= \underset{c \in \{P,N\}}{\operatorname{arg max}} \left\{ P(y_1, y_2|c)P(y_3|c) \times P(c) \right\} \quad \text{(we can remove parameters that do not depend on } c \right)$$

We can now begin to compute these parameters.

Priors: 
$$P(P) = \frac{5}{9}$$
  $P(N) = 1 - P(P) = \frac{4}{9}$ 

To get the likelihoods, we start by calculating the joint probabilities for the categorical variables  $y_1$  and  $y_2$ :

$$P((y_1 = A, y_2 = 0)|P) = \frac{2}{5} \quad P((y_1 = A, y_2 = 1)|P) = \frac{1}{5}$$

$$P((y_1 = A, y_2 = 0)|N) = \frac{0}{4} \quad P((y_1 = A, y_2 = 1)|N) = \frac{1}{4}$$

$$P((y_1 = B, y_2 = 0)|P) = \frac{1}{5} \quad P((y_1 = B, y_2 = 1)|P) = \frac{1}{5}$$

$$P((y_1 = B, y_2 = 0)|N) = \frac{2}{4} \quad P((y_1 = B, y_2 = 1)|N) = \frac{1}{4}$$

For the third variable, we know that it is normally distributed, so we start by calculating the mean and variance for each class:

mean: 
$$\mu = \frac{1}{n} \sum_{i=1}^{n} y_i$$
 variance:  $\sigma^2 = \frac{1}{n-1} \sum_{i=1}^{n} (y_i - \mu)^2$ 

Positive class:

$$\mu_P = \frac{1.1 + 0.8 + 0.5 + 0.9 + 0.8}{5} = 0.82$$

$$\sigma_P^2 = \frac{(1.1 - 0.82)^2 + (0.8 - 0.82)^2 + (0.5 - 0.82)^2 + (0.9 - 0.82)^2 + (0.8 - 0.82)^2}{4} = 0.47$$

Negative class:

$$\mu_N$$
 =  $\frac{1+0.9+1.2+0.9}{4} = 1.0$   
 $\sigma_N^2$  =  $\frac{(1-1)^2+(0.9-1)^2+(1.2-1)^2+(0.9-1)^2}{3} = 0.02$ 

Since  $y_3$  is normally distributed, we can calculate the likelihood for each class using the normal distribution formula:

$$P(y_z|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_z-\mu)^2}{2\sigma^2}\right)$$
 (7)

We must now replace  $y_3$  with each value in the set  $\{1.1, 0.8, 0.5, 0.9, 0.8\}$  and  $\{1, 0.9, 1.2, 0.9\}$  to calculate the likelihoods for each class. Having the parameters for the normal distribution, we can calculate the likelihoods for  $y_3$  as per (7):

Positive class:

$$P(y_3 = 1.1 | \mu_P, \sigma_P^2) = \frac{1}{\sqrt{2\pi \times 0.47}} \exp\left(-\frac{(1.1 - 0.82)^2}{2 \times 0.47}\right) \approx 0.535$$

$$P(y_3 = 0.8 | \mu_P, \sigma_P^2) = \frac{1}{\sqrt{2\pi \times 0.47}} \exp\left(-\frac{(0.8 - 0.82)^2}{2 \times 0.47}\right) \approx 0.582$$

$$P(y_3 = 0.5 | \mu_P, \sigma_P^2) = \frac{1}{\sqrt{2\pi \times 0.47}} \exp\left(-\frac{(0.5 - 0.82)^2}{2 \times 0.47}\right) \approx 0.522$$

$$P(y_3 = 0.9 | \mu_P, \sigma_P^2) = \frac{1}{\sqrt{2\pi \times 0.47}} \exp\left(-\frac{(0.9 - 0.82)^2}{2 \times 0.47}\right) \approx 0.578$$

Negative class:

$$P(y_3 = 1 | \mu_N, \sigma_N^2) = \frac{1}{\sqrt{2\pi \times 0.02}} \exp\left(-\frac{(1-1)^2}{2 \times 0.02}\right) \approx 2.821$$

$$P(y_3 = 0.9 | \mu_N, \sigma_N^2) = \frac{1}{\sqrt{2\pi \times 0.02}} \exp\left(-\frac{(0.9-1)^2}{2 \times 0.02}\right) \approx 2.197$$

$$P(y_3 = 1.2 | \mu_N, \sigma_N^2) = \frac{1}{\sqrt{2\pi \times 0.02}} \exp\left(-\frac{(1.2-1)^2}{2 \times 0.02}\right) \approx 1.038$$

Now we have all the parameters to apply the Bayesian classifier to new observations.

Consider now three testing observations,

$$\{(A, 1, 0.8), (B, 1, 1), (B, 0, 0.9)\}$$

## 4. Under a MAP assumption, classify each testing observation showing all your calculus.

MAP (Maximum A Posteriori) is defined as:

$$\hat{z} = \underset{c_i}{\operatorname{arg max}} \left\{ P(c_i|x) \right\}$$

$$= \underset{c_i}{\operatorname{arg max}} \left\{ \frac{P(x|c_i) \times P(c_i)}{P(x)} \right\}$$

$$= \underset{c_i}{\operatorname{arg max}} \left\{ P(x|c_i) \times P(c_i) \right\}$$
(8)

In order to apply this assumption we use the likelihoods and the priors calculated in the beginning of this report.

$$P(P) = \frac{5}{9} \qquad P(N) = 1 - P(P) = \frac{4}{9}$$

$$P((y_1 = A, y_2 = 1)|P) = \frac{1}{5} \qquad P((y_1 = A, y_2 = 1)|N) = \frac{1}{4}$$

$$P((y_1 = B, y_2 = 1)|P) = \frac{1}{5} \qquad P((y_1 = B, y_2 = 1)|N) = \frac{1}{4}$$

$$P((y_1 = B, y_2 = 0)|P) = \frac{1}{5} \qquad P((y_1 = B, y_2 = 0)|N) = \frac{2}{4}$$

$$P(y_3 = 0.8|\mu_P, \sigma_P^2) \approx 0.582 \qquad P(y_3 = 1.0|\mu_N, \sigma_N^2) \approx 2.821$$

$$P(y_3 = 0.9|\mu_N, \sigma_N^2) \approx 2.197 \qquad P(y_3 = 0.9|\mu_P, \sigma_P^2) \approx 0.578$$

Before using MAP assumption, we must calculate the missing values needed -  $P(y_3 = 0.8 | \mu_N, \sigma_N^2)$  and  $P(y_3 = 1 | \mu_P, \sigma_P^2)$ .

$$P(y_3 = 0.8 | \mu_N, \sigma_N^2) = \frac{1}{\sqrt{2\pi \times 0.02}} \exp\left(-\frac{(0.8 - 1)^2}{2 \times 0.02}\right) \approx 2.821$$
$$P(y_3 = 1 | \mu_P, \sigma_P^2) = \frac{1}{\sqrt{2\pi \times 0.47}} \exp\left(-\frac{(1 - 0.82)^2}{2 \times 0.47}\right) \approx 0.535$$

With this, we can just replace the values in the MAP formula (8) to get the predictions for each observation.

(A, 1, 0.8)

$$P(y_1 = A, y_2 = 1, y_3 = 0.8|P) = P(y_1 = A, y_2 = 1|P) \cdot P(y_3 = 0.8|P) \cdot P(P)$$
  
=  $\frac{1}{5} \times 0.582 \times \frac{5}{9} \approx 0.065$ 

$$P(y_1 = A, y_2 = 1, y_3 = 0.8|N) = P(y_1 = A, y_2 = 1|N) \times P(y_3 = 0.8|N) \times P(N)$$
  
=  $\frac{1}{4} \times 2.197 \times \frac{4}{9} \approx 0.488$ 

$$\begin{split} \hat{z}_{(A,1,0.8)} &= \underset{c \in \{P,N\}}{\text{arg max}} \ \{P(y_1 = A, y_2 = 1 | c) P(y_3 = 0.8 | c) \times P(c)\} \\ &= \underset{c \in \{P,N\}}{\text{arg max}} \ \{P(y_1, y_2 | P) P(y_3 | P) \times P(P); P(y_1, y_2 | N) P(y_3 | N) \times P(N)\} \\ &= N \end{split}$$

(B, 1, 1)

$$P(y_1 = B, y_2 = 1, y_3 = 1|P) = P(y_1 = B, y_2 = 1|P) \times P(y_3 = 1|P) \times P(P)$$
  
=  $\frac{1}{5} \times 2.821 \times \frac{5}{9} \approx 0.313$ 

$$P(y_1 = B, y_2 = 1, y_3 = 1|N) = P(y_1 = B, y_2 = 1|N) \times P(y_3 = 1|N) \times P(N)$$
  
=  $\frac{1}{4} \times 0.535 \times \frac{4}{9} \approx 0.059$ 

$$\begin{split} \hat{z}_{(B,1,1)} &= \underset{c \in \{P,N\}}{\text{arg max}} \ \{P(y_1 = B, y_2 = 1 | c) P(y_3 = 1 | c) \times P(c)\} \\ &= \underset{c \in \{P,N\}}{\text{arg max}} \ \{P(y_1, y_2 | P) P(y_3 | P) \times P(P); P(y_1, y_2 | N) P(y_3 | N) \times P(N)\} \\ &= P \end{split}$$

(B, 0, 0.9)

$$P(y_1 = B, y_2 = 0, y_3 = 0.9|P) = P(y_1 = B, y_2 = 0|P) \times P(y_3 = 0.9|P) \times P(P)$$
  
=  $\frac{1}{5} \times 0.578 \times \frac{5}{9} \approx 0.064$ 

$$P(y_1 = B, y_2 = 0, y_3 = 0.9|N) = P(y_1 = B, y_2 = 0|N) \times P(y_3 = 0.9|N) \times P(N)$$
  
=  $\frac{2}{4} \times 2.197 \times \frac{4}{9} \approx 0.488$ 

$$\begin{split} \hat{z}_{(B,0,0.9)} &= \underset{c \in \{P,N\}}{\text{max}} \ \left\{ P(y_1 = B, y_2 = 0 | c) P(y_3 = 0.9 | c) \times P(c) \right\} \\ &= \underset{c \in \{P,N\}}{\text{max}} \ \left\{ P(y_1, y_2 | P) P(y_3 | P) \times P(P); P(y_1, y_2 | N) P(y_3 | N) \times P(N) \right\} \\ &= N \end{split}$$

Therefore, the predictions for each observation are N, P and N respectively.

At last, consider only the following sentences and their respective connotations,

$$\{("Amazing run", P), ("I \ like \ it", P), ("To \ tired", N), ("Bad \ run", N)\}$$

5. Using a naïve Bayes under a ML assumption, classify the new sentence "I like to run". For the likelihoods calculation consider the following formula,

$$P(T_i|c) = rac{freq(t_i) + 1}{N_c + V}$$

where  $t_i$  represents a certain term i, V the number of unique terms in the vocabulary, and  $N_c$  the total number of terms in class c. Show all calculus.

## Part II: Programming

Consider the heart-disease.csv dataset available at the course webpage's homework tab. Using sklearn, apply a 5-fold stratified cross-validation with shuffling (random\_state = 0) for the assessment of predictive models along this section.

- (1) Compare the performance of a kNN with k = 5 and a Naive Bayes with Gaussian assumption (consider all remaining parameters as default):
- a. Plot two boxplots with the fold accuracies for each classifier. Is there one more stable than the other regarding performance? Why do you think that is the case? Explain.

```
import matplotlib.pyplot as plt, pandas as pd
2 from sklearn.model_selection import StratifiedKFold, cross_val_score
3 from sklearn.neighbors import KNeighborsClassifier
4 from sklearn.naive_bayes import GaussianNB
6 # Read the dataset
7 df = pd.read_csv("./heart-disease.csv")
8 X, y = df.drop("target", axis=1), df["target"]
10 # Define cross-validation strategy
folds = StratifiedKFold(n_splits=5, shuffle=True, random_state=0)
13 # Initialize classifiers
14 knn_predictor = KNeighborsClassifier(n_neighbors=5)
15 nb_predictor = GaussianNB()
# Evaluate classifiers
18 knn_accs = cross_val_score(knn_predictor, X, y, cv=folds, scoring="accuracy")
nb_accs = cross_val_score(nb_predictor, X, y, cv=folds, scoring="accuracy")
21 # Plot boxplots
22 plt.figure(figsize=(7, 5))
23 b_plot = plt.boxplot(
[knn_accs, nb_accs], patch_artist=True, labels=["kNN", "Naive Bayes"]
```

```
25 )
26
27 colors = ["#1f77b4", "#E40071"]
28 for patch, color in zip(b_plot["boxes"], colors):
29    patch.set_facecolor(color)
30 for median in b_plot["medians"]:
31    median.set_color("black")
32
33 plt.ylabel("Accuracy")
34 plt.grid(axis="y")
35 plt.show()
```

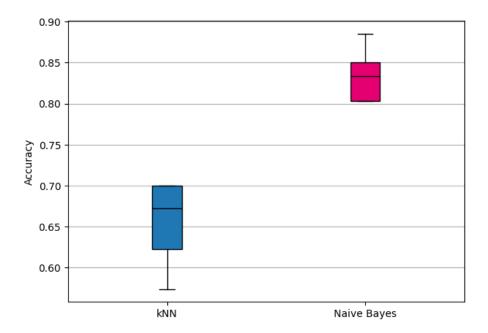


Figure 1: Boxplot of the fold accuracies for each classifier

b. Report the accuracy of both models, this time scaling the data with a Min-Max scaler before training the models. Explain the impact that this preprocessing step has on the performance of each model, providing an explanation for the results.

```
import matplotlib.pyplot as plt, pandas as pd
from sklearn.model_selection import StratifiedKFold, cross_val_score
from sklearn.neighbors import KNeighborsClassifier
from sklearn.naive_bayes import GaussianNB
from sklearn.preprocessing import MinMaxScaler
from sklearn.pipeline import Pipeline

# Read the ARFF file and prepare data
df = pd.read_csv("./heart-disease.csv")
X, y = df.drop("target", axis=1), df["target"]

# Define cross-validation strategy
folds = StratifiedKFold(n_splits=5, shuffle=True, random_state=0)
```

```
15 # Create pipelines for scaling
16 knn_pipeline = Pipeline([("scaler", MinMaxScaler()), ("knn",
     KNeighborsClassifier(n_neighbors=5))])
17 nb_pipeline = Pipeline([("scaler", MinMaxScaler()), ("nb", GaussianNB())])
# Evaluate classifiers
20 knn_accs = cross_val_score(knn_pipeline, X, y, cv=folds, scoring="accuracy")
21 nb_accs = cross_val_score(nb_pipeline, X, y, cv=folds, scoring="accuracy")
23 # Plot boxplots
24 plt.figure(figsize=(7, 5))
25 b_plot = plt.boxplot(
      [knn_accs, nb_accs], patch_artist=True, labels=["kNN", "Naive Bayes"]
29 colors = ["#1f77b4", "#E40071"]
30 for patch, color in zip(b_plot["boxes"], colors):
      patch.set_facecolor(color)
32 for median in b_plot["medians"]:
      median.set_color("black")
35 plt.ylabel("Accuracy")
36 plt.grid(axis="y")
37 plt.show()
```

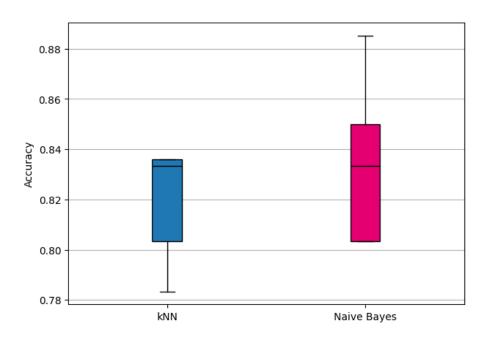


Figure 2: Accuracy of both models with Min-Max scaling

- c. Using scipy, test the hypothesis "the kNN model is statistically superior to naive Bayes regarding accuracy", asserting whether it is true.
  - (2) a 80-20 train-test split, vary the number of neighbors of a kNN classifier using

 $k = \{1, 5, 10, 20, 30\}$ . Additionally, for each k, train one classifier using uniform weights and distance weights.

a. Plot the train and test accuracy for each model

```
import matplotlib.pyplot as plt
2 import pandas as pd
3 from sklearn.neighbors import KNeighborsClassifier
4 from sklearn.model_selection import train_test_split
5 from sklearn.preprocessing import StandardScaler
7 # Read the dataset
8 df = pd.read_csv("./heart-disease.csv")
9 X, y = df.drop("target", axis=1), df["target"]
11 # Split the data into training and testing sets
12 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
     random_state=0)
# Standardize the features
scaler = StandardScaler().fit(X_train)
16 X_train_scaled, X_test_scaled = scaler.transform(X_train), scaler.transform(
     X_test)
18 # Define different values of k
19 number_of_neighbors = [1, 5, 10, 20, 30]
21 # Initialize lists to store accuracy results
22 train_acc_uniform, test_acc_uniform = [], []
train_acc_distance, test_acc_distance = [], []
25 # Train and evaluate KNN with 'uniform' weights
26 for k in number_of_neighbors:
      knn_uniform = KNeighborsClassifier(n_neighbors=k, weights="uniform")
      knn_uniform.fit(X_train_scaled, y_train)
      train_acc_uniform.append(knn_uniform.score(X_train_scaled, y_train))
      test_acc_uniform.append(knn_uniform.score(X_test_scaled, y_test))
32 # Train and evaluate KNN with 'distance' weights
33 for k in number_of_neighbors:
      knn_distance = KNeighborsClassifier(n_neighbors=k, weights="distance")
      knn_distance.fit(X_train_scaled, y_train)
      train_acc_distance.append(knn_distance.score(X_train_scaled, y_train))
      test_acc_distance.append(knn_distance.score(X_test_scaled, y_test))
39 # Plot the results
40 plt.figure(figsize=(16, 6))
42 # Plot distance accuracy
43 plt.subplot(1, 2, 1)
44 plt.plot(
      number_of_neighbors,
      test_acc_distance,
      label='Test Accuracy',
  marker='D',
```

```
color='#E40071'
50 )
52 plt.plot(
      number_of_neighbors,
      train_acc_distance,
      label='Train Accuracy',
      marker='o',
      color='#1f77b4')
59 plt.xlabel('Number of neighbors')
60 plt.ylabel('Distance')
61 plt.title('KNN Accuracy with Distance Weights')
62 plt.grid(True)
63 plt.legend()
65 # Plot uniform accuracy
66 plt.subplot(1, 2, 2)
67 plt.plot(
      number_of_neighbors,
      test_acc_uniform,
      label='Test Accuracy',
      marker='D',
      color='#E40071'
73 )
75 plt.plot(
      number_of_neighbors,
      train_acc_uniform,
      label='Train Accuracy',
      marker='o',
      color='#1f77b4'
83 # Add labels and title
84 plt.xlabel('Number of neighbors')
85 plt.ylabel('Uniform')
86 plt.title('KNN Accuracy with Uniform Weights')
87 plt.grid(True)
88 plt.legend()
89 plt.show()
```

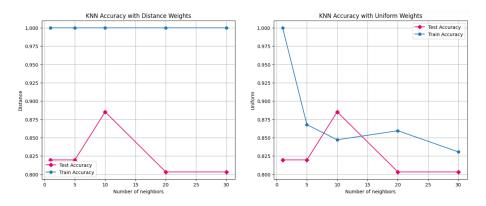


Figure 3: Train and test accuracy for each model

- b. Explain the impact of increasing the neighbors on the generalization ability of the models.
- (3) Considering the unique properties of the heart-disease.csv dataset, identify two possible difficulties of the naïve Bayes model used in the previous exercises when learning from the given dataset.