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Homework II – Group 28

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Part I: Pen and Paper

Consider the following dataset (y_3 - y_5 are all categorical variables and the domain of y_2 is $[0, 1]$):

D	y_1	y_2	y_3	y_4	y_5	y_6
$\mathbf{x}_1$	0.24	0.36	1	1	0	A
$\mathbf{x}_2$	0.16	0.48	1	0	1	A
$\mathbf{x}_3$	0.32	0.72	0	1	2	A
$\mathbf{x}_4$	0.54	0.11	0	0	1	B
$\mathbf{x}_5$	0.66	0.39	0	0	0	B
$\mathbf{x}_6$	0.76	0.28	1	0	2	B
$\mathbf{x}_7$	0.41	0.53	0	1	1	B
$\mathbf{x}_8$	0.38	0.52	0	1	0	A
$\mathbf{x}_9$	0.42	0.59	0	1	1	B

1. **Consider x_1 - x_7 to be training observations, x_8 - x_9 to be testing observations, y_1 - y_5 to be input variables and y_6 to be the target variable.**
   ***Hint*: you can use `scipy.stats.multivariate_normal` for multivariate distribution calculus**

   (a) **Learn a Bayesian classifier assuming: i) $\{y_1, y_2\}$, $\{y_3, y_4\}$ and $\{y_5\}$ sets of independent variables (e.g., $y_1 \perp\!\!\!\perp y_3$ yet $y_1 \not\perp\!\!\!\perp y_2$), and ii) $y_1 \times y_2 \in \mathbb{R}^2$ is normally distributed. Show all parameters (distributions and priors for subsequent testing).**

   As stated by the question prompt, variable sets $\{y_1, y_2\}$, $\{y_3, y_4\}$ and $\{y_5\}$ are independent. Since we have seven training observations, we'll use those to train a Bayesian classifier.

   We'll refer to the outcome, which can be A or B, as class.

   To estimate $P(\text{class}|y_1, y_2, y_3, y_4, y_5)$, we can use Bayes' theorem:

$$P(\text{class}|y_1, y_2, y_3, y_4, y_5) = \frac{P(y_1, y_2, y_3, y_4, y_5|\text{class}) \times P(\text{class})}{P(y_1, y_2, y_3, y_4, y_5)} \tag{1}$$

   Since we know $\{y_1, y_2\}$, $\{y_3, y_4\}$ and $\{y_5\}$ are independent, we can rewrite $P(y_1, y_2, y_3, y_4, y_5)$ as $P(y_1, y_2) \cdot P(y_3, y_4) \cdot P(y_5)$. Rewriting (1) with this, results in:

$$P(\text{class}|y_1, y_2, y_3, y_4, y_5) = \frac{P(y_1, y_2|\text{class})P(y_3, y_4|\text{class})P(y_5|\text{class}) \times P(\text{class})}{P(y_1, y_2)P(y_3, y_4)P(y_5)} \tag{2}$$

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

$$
\begin{aligned}
\hat{z} &= \underset{c\in\{A,B\}}{\arg\max}\ \{P(\mathrm{c}|O)\} \\
&= \underset{c\in\{A,B\}}{\arg\max}\ \left\{\frac{P(y_1,y_2|c)P(y_3,y_4|c)P(y_5|c)\times P(c)}{P(y_1,y_2)P(y_3,y_4)P(y_5)}\right\} \\
&= \underset{c\in\{A,B\}}{\arg\max}\ \{P(y_1,y_2|c)P(y_3,y_4|c)P(y_5|c)\times P(c)\} \qquad \text{(we can remove parameters that don't depend on } c\text{)}
\end{aligned} \tag{3}
$$

We can therefore start calculating all these parameters.

Note: Even though $P(y_1, y_2)$, $P(y_3, y_4)$ and $P(y_5)$ are not necessary to apply the model, we'll still calculate them for the sake of showing all parameters.

Calculating $P(\mathrm{A})$, $P(\mathrm{B})$ and all parameters involving y_1 through y_5 is straightforward, since they can be infered from the table.

We have 3 observations of A and 4 observations of B, out of a total of 7 training observations. Therefore,

$$P(\mathrm{A}) = \tfrac{3}{7} \quad P(\mathrm{B}) = \tfrac{4}{7}$$

In a similiar manner we can obtain the probabilities for y_5,

$$P(y_5 = 0) = \tfrac{2}{7} \quad P(y_5 = 1) = \tfrac{3}{7} \quad P(y_5 = 2) = \tfrac{2}{7}$$

Now for the conditional probabilities of y_5,

$$
\begin{aligned}
P(y_5 = 0\,|\mathrm{A}) = \tfrac{1}{3}, \quad P(y_5 = 1\,|\mathrm{A}) = \tfrac{1}{3}, \quad P(y_5 = 2\,|\mathrm{A}) = \tfrac{1}{3} \\
P(y_5 = 0\,|\mathrm{B}) = \tfrac{1}{4}, \quad P(y_5 = 1\,|\mathrm{B}) = \tfrac{2}{4}, \quad P(y_5 = 2\,|\mathrm{B}) = \tfrac{1}{4}
\end{aligned}
$$

For the four possible combinations of y_3 and y_4 we can follow the same logic as above,

$$
\begin{aligned}
P(y_3 = 0,\ y_4 = 0) = \tfrac{2}{7}, \quad P(y_3 = 0,\ y_4 = 1) = \tfrac{2}{7} \\
P(y_3 = 1,\ y_4 = 0) = \tfrac{2}{7}, \quad P(y_3 = 1,\ y_4 = 1) = \tfrac{1}{7}
\end{aligned}
$$

Finally, considering each class and the four possible combinations of y_3 and y_4, we can use the table to calculate the following:

$$
\begin{aligned}
P(y_3 = 0,\ y_4 = 0\,|\mathrm{A}) = \tfrac{0}{3}, \quad P(y_3 = 0,\ y_4 = 1\,|\mathrm{A}) = \tfrac{1}{3} \\
P(y_3 = 1,\ y_4 = 0\,|\mathrm{A}) = \tfrac{1}{3}, \quad P(y_3 = 1,\ y_4 = 1\,|\mathrm{A}) = \tfrac{1}{3} \\
P(y_3 = 0,\ y_4 = 0\,|\mathrm{B}) = \tfrac{2}{4}, \quad P(y_3 = 0,\ y_4 = 1\,|\mathrm{B}) = \tfrac{1}{4} \\
P(y_3 = 1,\ y_4 = 0\,|\mathrm{B}) = \tfrac{1}{4}, \quad P(y_3 = 1,\ y_4 = 1\,|\mathrm{B}) = \tfrac{0}{4}
\end{aligned}
$$

Calculating now the parameters related to the variable set $\{y_1, y_2\}$. We know that (y_1, y_2) follows a Multivariate Gaussian Distribution. Therefore,

$$P\left((y_1, y_2)|\boldsymbol{\mu}, \Sigma\right) = \mathcal{N}\left((y_1, y_2)|\boldsymbol{\mu}, \Sigma\right) \tag{4}$$

We can use the observations we have to approximate a value for the 2-dimensional mean vector ($\boldsymbol{\mu}$) and the covariance matrix (Σ).

$$\boldsymbol{\mu} = \frac{1}{7}\sum_{i=1}^{7}\begin{bmatrix} y_{1,i} \\ y_{2,i} \end{bmatrix} = \frac{1}{7}\left(\begin{bmatrix} 0.24 \\ 0.36 \end{bmatrix} + \begin{bmatrix} 0.16 \\ 0.48 \end{bmatrix} + \begin{bmatrix} 0.32 \\ 0.72 \end{bmatrix} + \begin{bmatrix} 0.54 \\ 0.11 \end{bmatrix} + \begin{bmatrix} 0.66 \\ 0.39 \end{bmatrix} + \begin{bmatrix} 0.76 \\ 0.28 \end{bmatrix} + \begin{bmatrix} 0.41 \\ 0.53 \end{bmatrix}\right)$$
$$= \begin{bmatrix} 0.4414 \\ 0.41 \end{bmatrix}$$

$$\Sigma_{00} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{1,i} - \mu_1)^2 = \frac{1}{7-1}\left[(0.24 - 0.4414)^2 + \cdots + (0.41 - 0.4414)^2\right] \approx 0.0491$$

$$\Sigma_{11} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{2,i} - \mu_2)^2 = \frac{1}{7-1}\left[(0.36 - 0.41)^2 + \cdots + (0.53 - 0.41)^2\right] \approx 0.0375$$

$$\Sigma_{01} = \Sigma_{10} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{1,i} - \mu_1)(y_{2,i} - \mu_2)$$
$$= \frac{1}{7-1}\left[(0.24 - 0.4414)(0.36 - 0.41) + \cdots + (0.41 - 0.4414)(0.53 - 0.41)\right]$$
$$\approx -0.0211$$

$$\Sigma = \begin{bmatrix} \Sigma_{00} & \Sigma_{10} \\ \Sigma_{01} & \Sigma_{11} \end{bmatrix} = \begin{bmatrix} 0.0491 & -0.0211 \\ -0.0211 & 0.0375 \end{bmatrix}$$

Therefore, $P(y_1, y_2) \sim \mathcal{N}\left((y_1, y_2)|\boldsymbol{\mu} = \begin{bmatrix} 0.4414 \\ 0.41 \end{bmatrix}, \Sigma = \begin{bmatrix} 0.0491 & -0.0211 \\ -0.0211 & 0.0375 \end{bmatrix}\right)$.
We can repeat the process for both classes (A and B).
Starting with A:

$$\boldsymbol{\mu} = \frac{1}{3}\sum_{i=1}^{3}\begin{bmatrix} y_{1,i}|\mathrm{A} \\ y_{2,i}|\mathrm{A} \end{bmatrix} = \frac{1}{3}\left(\begin{bmatrix} 0.24 \\ 0.36 \end{bmatrix} + \begin{bmatrix} 0.16 \\ 0.48 \end{bmatrix} + \begin{bmatrix} 0.32 \\ 0.72 \end{bmatrix}\right) = \begin{bmatrix} 0.24 \\ 0.52 \end{bmatrix}$$

$$\Sigma_{00} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{1,i}|\mathrm{A} - \mu_1)^2 = \frac{1}{3-1}\left[(0.24 - 0.24)^2 + \cdots + (0.32 - 0.24)^2\right] \approx 0.0064$$

$$\Sigma_{11} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{2,i}|\mathrm{A} - \mu_2)^2 = \frac{1}{3-1}\left[(0.36 - 0.52)^2 + \cdots + (0.72 - 0.52)^2\right] \approx 0.0336$$

$$\Sigma_{01} = \Sigma_{10} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{1,i}|\mathrm{A} - \mu_1)(y_{2,i}|\mathrm{A} - \mu_2)$$
$$= \frac{1}{3-1}\left[(0.24 - 0.24)(0.36 - 0.52) + \cdots + (0.32 - 0.24)(0.72 - 0.52)\right] \approx 0.0096$$

$$\Sigma = \begin{bmatrix} \Sigma_{00} & \Sigma_{10} \\ \Sigma_{01} & \Sigma_{11} \end{bmatrix} = \begin{bmatrix} 0.0064 & 0.0096 \\ 0.0096 & 0.0336 \end{bmatrix}$$

Therefore, $P(y_1, y_2|\mathrm{A}) \sim \mathcal{N}\left((y_1, y_2)|\boldsymbol{\mu} = \begin{bmatrix} 0.24 \\ 0.52 \end{bmatrix}, \Sigma = \begin{bmatrix} 0.0064 & 0.0096 \\ 0.0096 & 0.0336 \end{bmatrix}\right)$.
And now the B:

$$\boldsymbol{\mu} = \frac{1}{4}\sum_{i=1}^{4}\begin{bmatrix} y_{1,i}|\mathrm{B} \\ y_{2,i}|\mathrm{B} \end{bmatrix} = \frac{1}{4}\left(\begin{bmatrix} 0.54 \\ 0.11 \end{bmatrix} + \begin{bmatrix} 0.66 \\ 0.39 \end{bmatrix} + \begin{bmatrix} 0.76 \\ 0.28 \end{bmatrix} + \begin{bmatrix} 0.41 \\ 0.53 \end{bmatrix}\right) = \begin{bmatrix} 0.5925 \\ 0.3275 \end{bmatrix}$$

$$\Sigma_{00} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{1,i}|\mathrm{B} - \mu_1)^2 = \frac{1}{4-1}\left[(0.54 - 0.5925)^2 + \cdots + (0.41 - 0.5925)^2\right] \approx 0.0229$$

$$\Sigma_{11} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{2,i}|\mathrm{B} - \mu_2)^2 = \frac{1}{4-1}\left[(0.11 - 0.3275)^2 + \cdots + (0.53 - 0.3275)^2\right] \approx 0.0315$$

$$\Sigma_{01} = \Sigma_{10} = \frac{1}{N-1}\sum_{i=1}^{N}(y_{1,i}|\mathrm{B} - \mu_1)(y_{2,i}|\mathrm{B} - \mu_2)$$

$$= \frac{1}{4-1}\left[(0.54 - 0.5925)(0.11 - 0.3275) + \cdots + (0.41 - 0.5925)(0.53 - 0.3275)\right] \approx -0.0098$$

$$\Sigma = \begin{bmatrix} \Sigma_{00} & \Sigma_{10} \\ \Sigma_{01} & \Sigma_{11} \end{bmatrix} = \begin{bmatrix} 0.0229 & -0.0098 \\ -0.0098 & 0.0315 \end{bmatrix}$$

Therefore, $P(y_1, y_2|\mathrm{B}) \sim \mathcal{N}\left((y_1, y_2)|\boldsymbol{\mu} = \begin{bmatrix} 0.5925 \\ 0.3275 \end{bmatrix}, \Sigma = \begin{bmatrix} 0.0229 & -0.0098 \\ -0.0098 & 0.0315 \end{bmatrix}\right)$.

We now have all the parameters necessary to apply the Bayesian classifier to new observations.

(b) **Under a MAP assumption, classify each testing observation showing all of your calculus.**

Since we will need the (y_1, y_2) pdf values for the following exercises, let's calculate them using `scipy.multivariate_normal`, just like it was suggested in the hint:

```
from scipy.stats import multivariate_normal

x8 = multivariate_normal.pdf([0.38, 0.52], mean=[0.4414, 0.41],
                             cov=[[0.0491, -0.0211], [-0.0211, 0.0375]])
x9 = multivariate_normal.pdf([0.42, 0.59], mean=[0.4414, 0.41],
                             cov=[[0.0491, -0.0211], [-0.0211, 0.0375]])

x8_A = multivariate_normal.pdf([0.38, 0.52], mean=[0.24, 0.52],
                               cov=[[0.0064, 0.0096], [0.0096, 0.0336]])
x8_B = multivariate_normal.pdf([0.38, 0.52], mean=[0.5925, 0.3275],
                               cov=[[0.0229, -0.0098], [-0.0098, 0.03149]])
x9_A = multivariate_normal.pdf([0.42, 0.59], mean=[0.24, 0.52],
                               cov=[[0.0064, 0.0096], [0.0096, 0.0336]])
x9_B = multivariate_normal.pdf([0.42, 0.59], mean=[0.5925, 0.3275],
                               cov=[[0.0229, -0.0098], [-0.0098, 0.03149]])
```

From the code above we get the following:

$$P(y_1 = 0.38, y_2 = 0.52) \approx 3.6225, \quad P(y_1 = 0.42, y_2 = 0.59) \approx 2.5387$$

$$P(y_1 = 0.38, y_2 = 0.52|A) \approx 0.9847, \quad P(y_1 = 0.38, y_2 = 0.52|B) \approx 1.9623$$
$$P(y_1 = 0.42, y_2 = 0.59|A) \approx 0.4031, \quad P(y_1 = 0.42, y_2 = 0.59|B) \approx 1.7285$$

Since we are under a Maximum a Posteriori assumption, we can just use the expression at (3) and replace the values for each of the testing observations (x_8 and x_9).

Starting with x_8:

$$P(y_1 = 0.38, y_2 = 0.52|A)P(y_3 = 0, y_4 = 1|A)P(y_5 = 0|A) \times P(A) = 0.9847 \times \frac{1}{3} \times \frac{1}{3} \times \frac{3}{7} \approx 0.04689$$

$$P(y_1 = 0.38, y_2 = 0.52|B)P(y_3 = 0, y_4 = 1|B)P(y_5 = 0|B) \times P(B) = 1.9623 \times \frac{1}{4} \times \frac{1}{4} \times \frac{4}{7} \approx 0.07008$$

$$\begin{aligned}\hat{z}_{x_8} &= \underset{c\in\{A,B\}}{\arg\max}\ \{P(y_1 = 0.38, y_2 = 0.52|c)P(y_3 = 0, y_4 = 1|c)P(y_5 = 0|c) \times P(c)\} \\ &= \arg\max\ \{P(y_1, y_2|A)P(y_3, y_4|A)P(y_5|A) \times P(A); P(y_1, y_2|B)P(y_3, y_4|B)P(y_5|B) \times P(B)\} \\ &= B\end{aligned}$$

And now with x_9:

$$P(y_1 = 0.42, y_2 = 0.59|A)P(y_3 = 0, y_4 = 1|A)P(y_5 = 1|A) \times P(A) = 0.4031 \times \frac{1}{3} \times \frac{1}{3} \times \frac{3}{7} \approx 0.0192$$

$$P(y_1 = 0.42, y_2 = 0.59|B)P(y_3 = 0, y_4 = 1|B)P(y_5 = 1|B) \times P(B) = 1.7285 \times \frac{1}{4} \times \frac{2}{4} \times \frac{4}{7} \approx 0.1235$$

$$\begin{aligned}\hat{z}_{x_9} &= \underset{c\in\{A,B\}}{\arg\max}\ \{P(y_1 = 0.42, y_2 = 0.59|c)P(y_3 = 0, y_4 = 1|c)P(y_5 = 1|c) \times P(c)\} \\ &= \arg\max\ \{P(y_1, y_2|A)P(y_3, y_4|A)P(y_5|A) \times P(A); P(y_1, y_2|B)P(y_3, y_4|B)P(y_5|B) \times P(B)\} \\ &= B\end{aligned}$$

Therefore, we conclude that under a MAP assumption, observations x_8 and x_9 will be classified with B and B, respectively.

(c) **Consider that the default decision threshold of $\theta = 0.5$ can be adjusted according to**

$$f(\mathbf{x}|\theta) = \begin{cases} A, & P(A|\mathbf{x}) > \theta \\ B, & \text{otherwise} \end{cases}$$

Under a maximum likelihood assumption, what thresholds optimize testing accuracy?

On question 1.b) we calculated the following values:

$$P(A) = \frac{3}{7}$$

$$P(B) = \frac{4}{7}$$

$$P(x_8|A) * P(A) \approx 0.04689$$

$$P(x_8|B) * P(B) \approx 0.07008$$

$$P(x_9|A) * P(A) \approx 0.0192$$

$$P(x_9|B) * P(B) \approx 0.1235$$

So, to discover the maximum likelihood ($P(x_x|class)$), we have to split them by $P(class)$. Here are the results:

$$P(x_8|A) = 0.10941$$

$$P(x_8|B) = 0.12264$$

$$P(x_9|A) = 0.0448$$

$$P(x_9|B) \approx 0.2161$$

According to the *FAQ*, we can use the values we calculated as a **rough proxy for posteriors**. The next step is **normalizing** them so we can ensure their sum is 1 and get the maximum a posteriori:

$$P(A|x_8) = \frac{0.10941}{0.10941 + 0.12264} \approx 0.4715$$

$$P(B|x_8) = \frac{0.12264}{0.10941 + 0.12264} \approx 0.5285$$

$$P(A|x_9) = \frac{0.0448}{0.0448 + 0.2161} \approx 0.1717$$

$$P(B|x_9) = \frac{0.216125}{0.0448 + 0.2161} \approx 0.8283$$

Therefore, we can conclude that the threshold of values for θ is $[0.1717, 0.4715]$.

2. **Let y_1 be the target numeric variable, y_2 - y_6 be the input variables where y_2 is binarized under an equal-width (equal-range) discretization. For the evaluation of regressors, consider a 3-fold cross-validation over the full dataset (x_1 - x_9) without shuffling the observations.**

   (a) **Identify the observations and features per data fold after the binarization procedure.**

   To do the **binarization procedure** with an **equal-width discretization**, we need to divide y_2 into two intervals. Which are:

$$\text{interval}_1 = [0, 0.5]$$

$$\text{interval}_2 = [0.5, 1]$$

   Here is the binarization of y_2 based on those intervals:

D	y_1	y_2	y_3	y_4	y_5	y_6
x_1	0.24	0	1	1	0	A
x_2	0.16	0	1	0	1	A
x_3	0.32	1	0	1	2	A
x_4	0.54	0	0	0	1	B
x_5	0.66	0	0	0	0	B
x_6	0.76	0	1	0	2	B
x_7	0.41	1	0	1	1	B
x_8	0.38	1	0	1	0	A
x_9	0.42	1	0	1	1	B

The next step is identifying our folds, which will be:

$$\text{Fold 1} = x_1\ x_2\ x_3$$
$$\text{Fold 2} = x_4\ x_5\ x_6$$
$$\text{Fold 3} = x_7\ x_8\ x_9$$

So our datasets will be:

Fold 1

D	y_1	y_2	y_3	y_4	y_5	y_6
x_1	0.24	0	1	1	0	A
x_2	0.16	0	1	0	1	A
x_3	0.32	1	0	1	2	A

Fold 2

D	y_1	y_2	y_3	y_4	y_5	y_6
x_4	0.54	0	0	0	1	B
x_5	0.66	0	0	0	0	B
x_6	0.76	0	1	0	2	B

Fold 3

D	y_1	y_2	y_3	y_4	y_5	y_6
x_7	0.41	1	0	1	1	B
x_8	0.38	1	0	1	0	A
x_9	0.42	1	0	1	1	B

(b) **Consider a distance-weighted *k*NN with k = 3, Hamming distance (*d*), and 1 / *d* weighting. Compute the MAE of this *k*NN regressor for the 1^{st} iteration of the cross-validation (i.e. train observations have the lower indices).**

The formula for **weighted average**, considering that k=3, is the following:

$$\text{Weighted Average} = \frac{\frac{1}{d_1} \cdot y_1 + \frac{1}{d_2} \cdot y_2 + \frac{1}{d_3} \cdot y_3}{\frac{1}{d_1} + \frac{1}{d_2} + \frac{1}{d_3}} \tag{5}$$

And the equation for the **mean absolute error** is given by:

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i| \tag{6}$$

As stated in the prompt, we will use Folds 1 and 2 for training, reserving Fold 3 for testing. Let's start by computing the **Hamming distances**, for x_7 first:

	x_1	x_2	x_3	x_4	x_5	x_6
$H(x_7, x_j)$	4	4	2	2	3	4

Now, for x_8:

	x_1	x_2	x_3	x_4	x_5	x_6
$H(x_8, x_j)$	2	4	1	4	3	5

Finally, for x_9:

	x_1	x_2	x_3	x_4	x_5	x_6
$H(x_9, x_j)$	4	4	2	2	3	4

Now let's determine the **three closest neighbors** to each test observation:

- For x_7 it is x_3, x_4 and x_5
- For x_8 it is x_1, x_3 and x_5
- For x_9 it is x_3, x_4 and x_5

The next step is calculating their **weighted average**. By replacing the formula on (5), we get the following values:

$$\text{Weighted average for } x_7 = 0.4875$$
$$\text{Weighted average for } x_8 = 0.36$$
$$\text{Weighted average for } x_9 = 0.4875$$

Finally, let's compute the mean absolute error by using the equation on (6):

$$MAE = 0.055$$

Part II: Programming and critical analysis

Considering the `column_diagnosis.arff` dataset available at the course webpage's homework tab. Using `sklearn`, apply a 10-fold stratified cross-validation with shuffling (`random_state=0`) for the assessment of predictive models along this section.

1. **Compare the performance of *k*NN with k = 5 and Naïve Bayes with Gaussian assumption (consider all remaining parameters for each classifier as `sklearn`'s default):**

   (a) **Plot two boxplots with the fold accuracies for each classifier.**

```python
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 scipy.io.arff import loadarff

# Read the ARFF file and prepare data
data = loadarff("./data/column_diagnosis.arff")
```

```
df = pd.DataFrame(data[0])
df["class"] = df["class"].str.decode("utf-8")
X, y = df.drop("class", axis=1), df["class"]

# Define cross-validation strategy
folds = StratifiedKFold(n_splits=10, shuffle=True, random_state=0)

# Initialize classifiers
knn_predictor = KNeighborsClassifier(n_neighbors=5)
nb_predictor = GaussianNB()

# Evaluate classifiers
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")

# Plot boxplots
plt.figure(figsize=(7, 5))
b_plot = plt.boxplot(
    [knn_accs, nb_accs], patch_artist=True, labels=["kNN", "Naive Bayes"]
)

colors = ["#f8766d", "#00bfc4"]
for patch, color in zip(b_plot["boxes"], colors):
    patch.set_facecolor(color)
for median in b_plot["medians"]:
    median.set_color("black")

plt.ylabel("Accuracy")
plt.grid(axis="y")
plt.show()
```

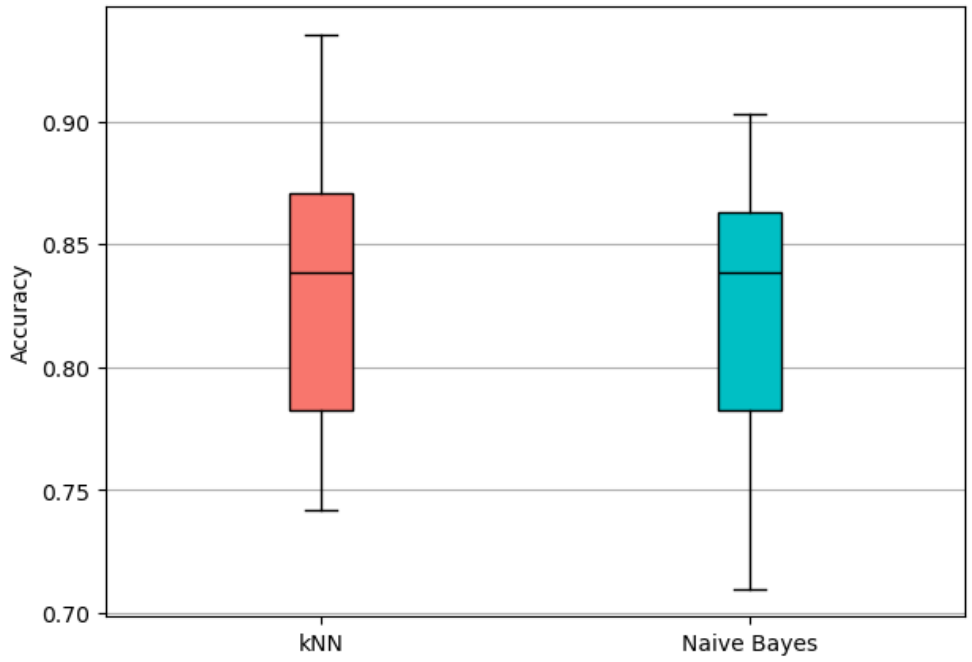

Figure 1: Boxplots with the fold accuracies of *k*NN (k = 5) and Naïve Bayes

(b) **Using `scipy`, test the hypothesis "*k*NN is statistically superior to Naïve Bayes regarding accuracy", asserting whether is true.**

We'll consider the null hypothesis and alternate hypothesis below and perform a single-tailed test using the accuracies obtained in the previous answer,

$$H_0: \quad \text{accuracy}_{k\text{NN}} = \text{accuracy}_{\text{Naïve Bayes}}$$
$$H_1: \quad \text{accuracy}_{k\text{NN}} > \text{accuracy}_{\text{Naïve Bayes}}$$

```python
from scipy.stats import ttest_rel

# Is knn better than naive bayes?
res = ttest_rel(knn_accs, nb_accs, alternative="greater")
print("Is knn > naive bayes? pval =", res.pvalue)
```

Using `scipy` we get a p-value of, approximately, 0.190428 = 19.0428 %.

This means we cannot reject the hypothesis H_0 at common significance levels (1%, 5% and 10%).

Therefore, we cannot assert that *k*NN is statistically superior to Naïve Bayes. We also cannot state that the hypothesis on the statement is outright false without checking other statistical tests.

2. **Consider two *k*NN predictors with k = 1 and k = 5 (uniform weights, Euclidean distance, all remaining parameters as default). Plot the differences between the two cumulative confusion matrices of the predictors. Comment.**

```python
import numpy as np, matplotlib.pyplot as plt, pandas as pd, seaborn as sns
from sklearn.model_selection import StratifiedKFold
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import confusion_matrix
from scipy.io.arff import loadarff

# Read the ARFF file and prepare data
data = loadarff("./data/column_diagnosis.arff")
df = pd.DataFrame(data[0])
df["class"] = df["class"].str.decode("utf-8")
X, y = df.drop("class", axis=1), df["class"]

# Initialize StratifiedKFold with 10 folds and shuffling
folds = StratifiedKFold(n_splits=10, shuffle=True, random_state=0)

# Create kNN classifiers with k=1 and k=5
knn_1 = KNeighborsClassifier(n_neighbors=1)
knn_5 = KNeighborsClassifier(n_neighbors=5)

labels = ["Hernia", "Normal", "Spondylolisthesis"]
cm_1, cm_5 = np.zeros((3, 3)), np.zeros((3, 3))
for train_k, test_k in folds.split(X, y):
    X_train, X_test = X.iloc[train_k], X.iloc[test_k]
    y_train, y_test = y.iloc[train_k], y.iloc[test_k]

    # Fit kNN classifiers and assess
    knn_1.fit(X_train, y_train)
    knn_5.fit(X_train, y_train)
    knn_1_pred, knn_5_pred = knn_1.predict(X_test), knn_5.predict(X_test)
```

```
    cm_1 += np.array(confusion_matrix(y_test, knn_1_pred, labels=labels))
    cm_5 += np.array(confusion_matrix(y_test, knn_5_pred, labels=labels))

# Calculate cumulative confusion matrices
cm_diff = cm_1 - cm_5
cm_diff_df = pd.DataFrame(cm_diff, index=labels, columns=labels)

# Plot the differences
plt.figure(figsize=(9, 7))
sns.heatmap(
    cm_diff_df, cmap="Purples", annot=True, annot_kws={"fontsize": 14}, fmt="g"
)
plt.xlabel("Predicted")
plt.ylabel("Real")
plt.show()
```

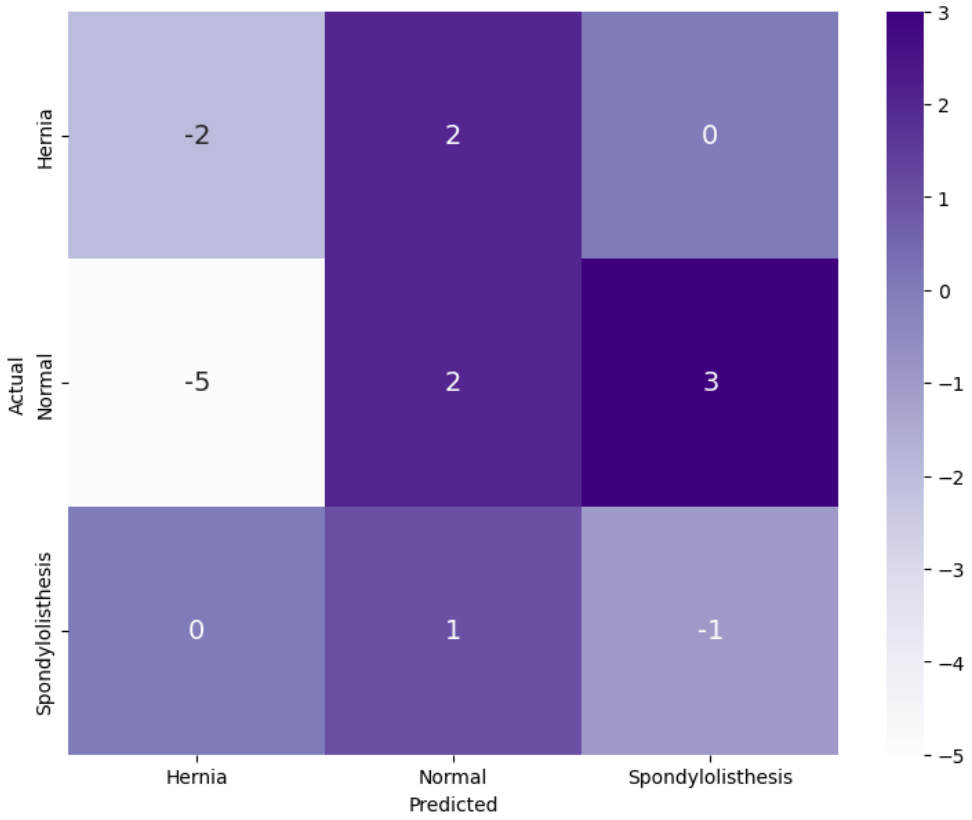

Figure 2: Confusion Matrix Differences Between k=1 and k=5 k-Nearest Neighbors (kNN) Classifiers

Upon examination of the difference matrix derived from the confusion matrices, it is evident that the kNN model with $k = 5$ surpasses the performance of $k = 1$.

For each cell in this matrix, we can determine which model (k=1 or k=5) had the most observations by noting if the cell value is negative or positive. A positive value indicates that $k = 1$ had the most observations, while a negative value indicates the opposite for $k = 5$.

This superiority of the $k = 5$ model is shown by the negative sum of diagonal elements, signifying higher accuracy. Additionally, the fact that the sum of incorrect predictions is positive suggests that $k = 5$ has fewer miss classifications.

Therefore, utilizing $k = 5$ appears to be the preferable choice over $k = 1$ for this task.

3. **Considering the unique properties of `column_diagnosis`, identify three possible difficulties of Naïve Bayes when learning from the given dataset.**

   Here are three possible difficulties of Naïve Bayes when learning from the given dataset, in no particular order:

   - Variable dependencies (inadequacy of independence assumption).
   - Variables not normally distributed (inadequacy of Gaussian assumption). Probability estimates from a limited number of observations (e.g., inadequate estimates, null probabilities).
   - Imbalanced class creating biases in MAP estimates via priors.