Homework 2 - Group 076

Aprendizagem 2021/2022

1 Pen and Paper

1) Applying the linear basis function $\phi(\mathbf{x}) = (1, \|\mathbf{x}\|_2, \|\mathbf{x}\|_2^2, \|\mathbf{x}\|_2^3)$ (with $\|\mathbf{x}\|_2 = \sqrt{x_1^2 + x_2^2 + x_3^2}$) to each instance $\mathbf{x}^{(i)}$ $(i = 1, ..., 8)$ in the training set, we get a new design matrix:

$$\mathbf{\Phi} = \begin{bmatrix} — & (\phi(\mathbf{x}^{(1)}))^T & — \\ — & (\phi(\mathbf{x}^{(2)}))^T & — \\ & \vdots & \\ — & (\phi(\mathbf{x}^{(8)}))^T & — \end{bmatrix} = \begin{bmatrix} 1.0 & 1.4142 & 2.0 & 2.8284 \\ 1.0 & 5.1962 & 27.0 & 140.2961 \\ 1.0 & 4.4721 & 20.0 & 89.4427 \\ 1.0 & 3.7417 & 14.0 & 52.3832 \\ 1.0 & 7.2801 & 53.0 & 385.8458 \\ 1.0 & 1.7321 & 3.0 & 5.1962 \\ 1.0 & 2.8284 & 8.0 & 22.6274 \\ 1.0 & 9.2195 & 85.0 & 783.6613 \end{bmatrix}$$

To learn the regression model, we must compute the weight vector $\mathbf{w}$ that minimizes the Sum of Squares error between the outputs $\mathbf{z} = \begin{bmatrix} 1 & 3 & 2 & 0 & 6 & 4 & 5 & 7 \end{bmatrix}^T$ and predictions $\hat{\mathbf{z}} = \mathbf{\Phi w}$ (i.e., $\mathbf{w} = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{z}$):

$$\mathbf{\Phi}^T\mathbf{\Phi} = \begin{bmatrix} 8.0 & 35.8843 & 212.0 & 1482.2811 \\ 35.8843 & 212.0 & 1482.2811 & 11436.0 \\ 212.0 & 1482.2811 & 11436.0 & 93573.5164 \\ 1482.2811 & 11436.0 & 93573.5164 & 793976.0 \end{bmatrix}$$

$$(\mathbf{\Phi}^T\mathbf{\Phi})^{-1} = \begin{bmatrix} 8.1955 & -6.2313 & 1.3049 & -0.0793 \\ -6.2313 & 5.0781 & -1.1044 & 0.0686 \\ 1.3049 & -1.1044 & 0.2472 & -0.0157 \\ -0.0793 & 0.0686 & -0.0157 & 0.001 \end{bmatrix}$$

$$(\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T = \begin{bmatrix} 1.7686 & -0.0811 & -0.6694 & -1.0069 & 1.3794 & 0.9051 & -0.785 & -0.5107 \\ -1.0644 & -0.0319 & 0.5312 & 0.904 & -1.307 & -0.3922 & 0.8501 & 0.5101 \\ 0.1933 & 0.0436 & -0.0907 & -0.1868 & 0.3232 & 0.0524 & -0.1954 & -0.1395 \\ -0.0107 & -0.0043 & 0.0044 & 0.0109 & -0.0214 & -0.0022 & 0.0123 & 0.011 \end{bmatrix}$$

$$\mathbf{w} = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{z} = \begin{bmatrix} 4.5835 & -1.6872 & 0.3377 & -0.0133 \end{bmatrix}^T$$

2) Similarly to the previous question, we compute the image of each instance $\mathbf{x}^{(i)}$ $(i \in \{1, 2\})$ from the testing set and place the image $\phi(\mathbf{x}^{(i)})$ in each row of the matrix $\mathbf{\Phi}$. Using the obtained weight vector $\mathbf{w}$, we have the following estimates vector:

$$\hat{\mathbf{z}} = \mathbf{\Phi w} = \begin{bmatrix} 1.0 & 2.0 & 4.0 & 8.0 \\ 1.0 & 2.4495 & 6.0 & 14.6969 \end{bmatrix} \begin{bmatrix} 4.5835 \\ -1.6872 \\ 0.3377 \\ -0.0133 \end{bmatrix} = \begin{bmatrix} 2.4536 \\ 2.2816 \end{bmatrix}$$

Computing the root mean square error, we have:

$$\text{RMSE}(\hat{\mathbf{z}}, \mathbf{z}) = \sqrt{\frac{1}{2}\sum_{i=1}^{2}(\hat{z}_i - z_i)^2} = 1.2567$$

3) To make an equal depth binarization of y_3, we compute the median of the values of y_3 of all the instances in the dataset:

$$\text{median}(\{y_3^{(i)}\}_{i=1}^{10}) = 2.5$$

and make the following transformation to y_3:

$$y_3 := \begin{cases} 0, & \text{if } y_3 < \text{median} \\ 1, & \text{otherwise} \end{cases}$$

Considering the given class targets, we have the following data table:

y_1	y_2	y_3	t
1	1	0	N
1	1	1	N
0	2	1	N
1	2	1	N
2	0	1	P
1	1	0	P
2	0	0	P
0	2	1	P

- Starting entropy:

$$H(t) = -\sum_{i=0}^{1} \frac{\#\{k|t^{(k)} = i\}}{8} \log_2\left(\frac{\#\{k|t^{(k)} = i\}}{8}\right) = -\left(\frac{1}{2}\log_2\left(\frac{1}{2}\right) + \frac{1}{2}\log_2\left(\frac{1}{2}\right)\right) = 1\;bit$$

- Variable conditional entropies and corresponding information gains ($\text{IG}(y_i) = H(t) - H(t|y_i)$):

$$\begin{aligned} H(t|y_1) &= \sum_{i=0}^{2} \frac{\#\{k|y_1^{(k)} = i\}}{8} H(t|y_1 = i) \\ &= -\sum_{i=0}^{2} \frac{\#\{k|y_1^{(k)} = i\}}{8} \sum_{j=0}^{1} \frac{\#\{k|y_1^{(k)} = i, t^{(k)} = j\}}{\#\{k|t^{(k)} = j\}} \log_2\left(\frac{\#\{k|y_1^{(k)} = i, t^{(k)} = j\}}{\#\{k|t^{(k)} = j\}}\right) \\ &= -\frac{1}{4}\left(\frac{1}{2}\log_2\left(\frac{1}{2}\right) + \frac{1}{2}\log_2\left(\frac{1}{2}\right)\right) - \frac{1}{2}\left(\frac{3}{4}\log_2\left(\frac{3}{4}\right) + \frac{1}{4}\log_2\left(\frac{1}{4}\right)\right) - \frac{1}{2}\left(0\log_2(0) + 1\log_2(1)\right) \\ &= 0.6556\;bit \\ H(t|y_2) &= -\frac{1}{4}\left(0\log_2(0) + 1\log_2(1)\right) - \frac{3}{8}\left(\frac{2}{3}\log_2\left(\frac{2}{3}\right) + \frac{1}{3}\log_2\left(\frac{1}{3}\right)\right) - \frac{3}{8}\left(\frac{2}{3}\log_2\left(\frac{2}{3}\right) + \frac{1}{3}\log_2\left(\frac{1}{3}\right)\right) \\ &= 0.68872\;bit \\ H(t|y_3) &= -\frac{3}{8}\left(\frac{1}{3}\log_2\left(\frac{1}{3}\right) + \frac{2}{3}\log_2\left(\frac{2}{3}\right)\right) - \frac{5}{8}\left(\frac{3}{5}\log_2\left(\frac{3}{5}\right) + \frac{2}{5}\log_2\left(\frac{2}{5}\right)\right) = 0.95121\;bit \end{aligned}$$

$$\text{IG}(y_1) = 1 - 0.6556 = 0.34436\;bit \quad \text{IG}(y_2) = 0.31128\;bit \quad \text{IG}(y_3) = 0.04879\;bit$$

Since y_1 yields the biggest information gain, it will take part in the first node in the decision tree and the following division in the dataset is obtained:

$y_1 = 0$			$y_1 = 1$			$y_1 = 2$		
y_2	y_3	t	y_2	y_3	t	y_2	y_3	t
2	1	N	1	0	N	0	1	P
2	1	P	1	1	N	0	0	P
			2	1	N			
			1	0	P			

Partition $(y_1 = 2)$ has no uncertainty and we cannot reduce uncertainty in partition $(y_1 = 0)$ (note that there is only one value of y_2 (resp. y_3), so $H(t|y_2, y_1 = 1) = H(t|y_1 = 1)$ (resp., $H(t|y_3, y_1 = 1)$), and there is no possible information gain). We thus proceed to divide partition $(y_1 = 1)$ even further in an analogous way as before:

- Starting entropy:

$$H(t|y_1 = 1) = -\sum_{i=0}^{1} \frac{\#\{k|t^{(k)} = i \wedge y_1^{(k)} = 1\}}{\#\{k|y_1^{(k)} = 1\}} \log_2 \left(\frac{\#\{k|t^{(k)} = i \wedge y_1^{k} = 1\}}{\#\{k|y_1^{(k)} = 1\}} \right)$$
$$= -\left(\frac{3}{5} \log_2 \left(\frac{3}{4} \right) + \frac{1}{4} \log_2 \left(\frac{1}{4} \right) \right) = 0.81127\, bit$$

- Variable conditional entropies and corresponding information gains (where $\text{IG}(y_i|y_1 = 1) = H(t|y_1 = 1) - H(t|y_i, y_1 = 1)$; also note that $\#\{k|y_2^{(k)} = 0 \wedge y_1^{(k)} = 1\} = 0$, so $H(t|y_2 = 0, y_1 = 1)$ is not defined and we discard that term from the first sum):

$$H(t|y_2, y_1 = 1) = \sum_{i=1}^{2} \frac{\#\{k|y_2^{(k)} = i \wedge y_1^{(k)} = 1\}}{\#\{k|y_1^{(k)} = 1)\}} H(t|y_2 = i, y_1 = 1)$$
$$= -\sum_{i=1}^{2} \frac{\#\{k|y_2^{(k)} = i \wedge y_1^{(k)} = 1)\}}{\#\{k|y_1^{(k)} = 1\}} \sum_{j=0}^{1} \frac{\#\{k|t^{(k)} = j \wedge y_2^{(k)} = i \wedge y_1^{(k)} = 1)\}}{\#\{k|y_2^{(k)} = i \wedge y_1^{(k)} = 1\}} \log_2 \left(\frac{\#\{k|t^{(k)} = j \wedge y_2^{(k)} = i \wedge y_1^{(k)} = 1)\}}{\#\{k|y_2^{(k)} = i \wedge y_1^{(k)} = 1\}} \right)$$
$$= -\frac{3}{4} \left(\frac{2}{3} \log_2 \left(\frac{2}{3} \right) + \frac{1}{3} \log_2 \left(\frac{1}{3} \right) \right) - \frac{1}{4} \left(1 \log_2(1) + 0 \log_2(0) \right) = 0.688721\, bit$$
$$H(t|y_3, y_1 = 1) = -\frac{1}{2} \left(\frac{1}{2} \log_2 \left(\frac{1}{2} \right) + \frac{1}{2} \log_2 \left(\frac{1}{2} \right) \right) = 0.5\, bit$$

$$\text{IG}(y_2|y_1 = 1) = 0.81127 - 0.688721 = 0.1225979\, bit \quad \text{IG}(y_3|y_1 = 1) = 0.81127 - 0.5 = 0.31127\, bit$$

As y_3 provides the biggest information gain, it will divide the partition $(y_1 = 1)$. The resulting dataset cannot be further partitioned ($(y_1 = 1, y_3 = 1)$ has no uncertainty and we can't obtain information gain from dividing $(y_1 = 1, y_3 = 0)$ for the same argument as the one applied to $(y_1 = 0)$):

$y_1 = 0$			$y_1 = 1$				$y_1 = 2$		
y_2	y_3	t	$y_3 = 0$		$y_3 = 1$		y_2	y_3	t
2	1	N	y_2	t	y_2	t	0	1	P
2	1	P	1	N	1	N	0	0	P
			1	P	2	N			

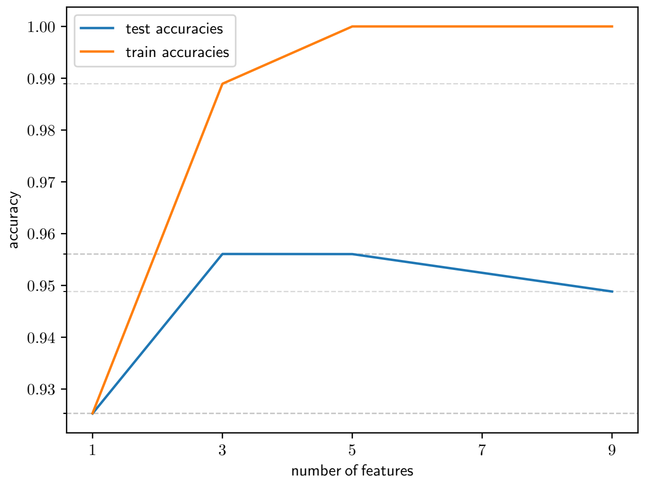
Thus, we have the desired decision tree:

$$\begin{tikzcd}
y_1 = 0 \arrow[d] & & y_1 = 1 \arrow[d] & & y_1 = 2 \arrow[d] \\
\text{N/P} & y_3 = 0 \arrow[d] & {} & y_3 = 1 \arrow[d] & \text{P} \\
& \text{N/P} & & \text{N} &
\end{tikzcd}$$

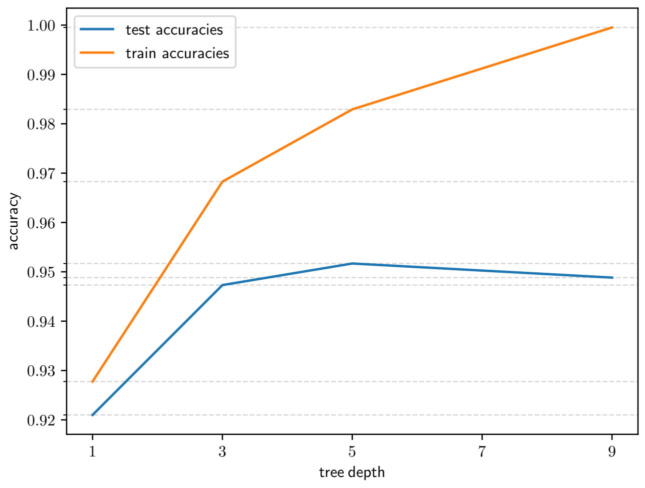
4) Considering the computed decision tree, for $\mathbf{x}^{(9)} = \begin{bmatrix} 2 & 0 & 0 \end{bmatrix}^T$ we have that $\hat{\mathbf{t}}(\mathbf{x}^{(9)}) = \text{P}$, and, for $\mathbf{x}^{(10)} = \begin{bmatrix} 1 & 2 & 1 \end{bmatrix}^T$, we have that $\hat{\mathbf{t}}(\mathbf{x}^{(10)}) = \text{N}$. Since $\mathbf{t}(\mathbf{x}^{(9)}) = \text{N}$ and $\mathbf{t}(\mathbf{x}^{(10)}) = \text{P}$, there are no true positives and no true negatives in the classification of these instances. Hence, accuracy on the testing data is 0 according to the formula Accuracy $= \frac{TP+TN}{P+N}$.

2 Programming and critical analysis

5) (i)



(ii)



6) With the increase of tree size (by number of relevant features or depth), test accuracy grows but training accuracy starts to fall after a certain point, thus revealing a tendency of overfitting to the training data. These behaviours can be explained by the following reasons:

- considering features that are not very relevant to classification (according to mutual information) can originate rules that are too specific to regularities of the training data, making it harder for the tree to generalize to unseen data;
- loosening the tree depth threshold can cause an excessive split granularity (and thus the formation of meaningless rules).

7) According to the plot in question 5) (ii), the most suitable tree depth is 5, since it is the one that maximizes mean testing accuracy across train/test folds. Consequently, it is the one that is less expected to overfit, following the last argument in the previous question.

3 Appendix

```python
import numpy as np
import pandas as pd
from scipy.io import arff
from sklearn import feature_selection, model_selection, tree
import matplotlib.pyplot as plt
plt.rcParams["text.usetex"] = True

def load_data(filename):
    dataset = arff.loadarff(filename)
    dataset = pd.DataFrame(dataset[0])
    dataset[dataset.columns[-1]] = dataset[dataset.columns[-1]].str.decode('utf8')
    dataset = dataset.dropna()
    return dataset

def compare_accuracy(inputs, outputs, folds, mode):
    test_accuracies = []
    train_accuracies = []
    for param in (1, 3, 5 ,9):
        if mode == "features":
            inputs_new = feature_selection.SelectKBest(feature_selection.mutual_info_classif, \
                                                        k = param).fit_transform(inputs, outputs)
            estimator = tree.DecisionTreeClassifier(criterion = "entropy", random_state = 76)
            label = "number\:of\:features"
        elif mode == "tree_depths":
            inputs_new = inputs
            estimator = tree.DecisionTreeClassifier(criterion = "entropy", \
                                                    max_depth = param, random_state = 76)
            label = "tree\:depth"
        results = model_selection.cross_validate(estimator = estimator, \
                                                 X = inputs_new, y = outputs, \
                                                 scoring = "accuracy", cv = folds, \
                                                 return_train_score = True)
        test_accuracies.append(np.mean(results["test_score"]))
        train_accuracies.append(np.mean(results["train_score"]))
    fig, ax = plt.subplots()
    ax.plot([1, 3, 5, 9], test_accuracies, label = "test accuracies")
    ax.plot([1, 3, 5, 9], train_accuracies, label = "train accuracies")
    ax.set_yticks(test_accuracies + train_accuracies, minor=True)
    ax.set_xticks([1,3,5,7,9])
    ax.yaxis.grid(True, which='minor', alpha = 0.5, linestyle = "dashed")
    ax.legend(loc = "best")
    ax.set_xlabel(label)
    ax.set_ylabel("accuracy")
    plt.savefig(f"output/accuracy_n_{mode}.pdf")

dataset = load_data("../data/breast.w.arff")
inputs = dataset.iloc[:, :-1].to_numpy()
outputs = dataset.iloc[:, [-1]].to_numpy().T.flatten()
kf = model_selection.KFold(n_splits = 10, shuffle = True, random_state = 76)
compare_accuracy(inputs, outputs, kf, "features")
compare_accuracy(inputs, outputs, kf, "tree_depths")
```