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Lab 02: Decision Tree

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1. Introduction

A Decision Tree is a type of supervised machine learning algorithm. It works by splitting the data into subsets, selecting the feature that most significantly impacts the outcome at each node, and then creating new branches for other features if possible.

The data used to train and test the model is very important, as it determines the accuracy of the model.

In this project, we will use 529 data samples from the Breast Cancer Wisconsin (Diagnostic) dataset to train a model that predicts whether a tumor is benign or malignant.

2. Preparing the data sets

We use the dataset provided in Python as instructed in Lab 02, which comes from the ucimlrepo library.

From this dataset, we divide it into feature and label sets, where the features are the characteristic values that influence the label – the final result in each case.

To facilitate visualization in the next step, we convert the values in the label set to 0 and 1, corresponding to benign and malignant tumors, respectively.

As required by the task, we need to split the dataset into two parts for training and testing. To ensure the model's accuracy, we choose multiple ratios to split these two sets, specifically 40/60, 60/40, 80/20, and 90/10.

However, we only need to specify one value in each pair (e.g., train_size or test_size), as the train_test_split function will automatically calculate the remaining value. Therefore, we create the splitSize array with the following values:

Here, splitSize will hold the proportions for the train set sizes, allowing the train_test_split function to handle the splitting appropriately based on these values.

For the actual splitting, we can use the train_test_split function available in the sklearn library. This function will split the dataset according to the parameter conditions we specify.

X_train, X_test, y_train, y_test = train_test_split(features, labels, train_size=size/100, random_state=1, shuffle=True, stratify=labels)

In this context, features are the input characteristics, and labels are the target set. The train_size parameter represents the size of the training set for each proportion, while the size of the test set does not need to be specified, as it will automatically be the remainder of the corresponding feature and label sets.

To shuffle the data, we set the shuffle parameter to True. However, to make the results easier to observe, we set the random_state parameter to a specific number, ensuring that the data remains consistent across different shuffling runs.

Additionally, to maintain the distribution of labels corresponding to their features, we use the stratify = labels parameter. This tells the function to ensure that each label value is properly paired with its corresponding features and that the label distribution is preserved during the shuffle.

After splitting, we have 4 subsets, we store the new training_feature, training_label, test_feature, test_label into an array and continue the process until all proportions have been handled, then we have 16 subsets. We have an array named "listData" after the loop.

* Visualizing all data sets

Since we have previously encoded the labels, they now only contain values of 0 (benign) or 1 (malignant). We count the number of occurrences of 0 and 1 in the original dataset using the bincount function from NumPy and save this information.

```
originalSet_labelCounts = list(np.bincount(labels))
```

We then iterate through the training and test sets stored in the listData array. For each set, we count the occurrences of 0 and 1 in the label column.

There might be cases where the train/test split results in one of the sets not containing all label values. To handle this, we use the minlength parameter in bincount to automatically pad with 0 for any missing label values.

```
trainingSet_labelCounts = list(np.bincount(y_train, minlength=len(listLabels)))
testingSet_labelCounts = list(np.bincount(y_test, minlength=len(listLabels)))
```

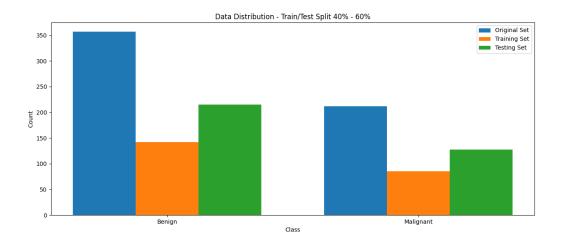
After obtaining the counts, we adjust the size of the plot and the position and size of each bar accordingly. We use Matplotlib to create bar charts to visualize the data after the split, ensuring that the data was split correctly.

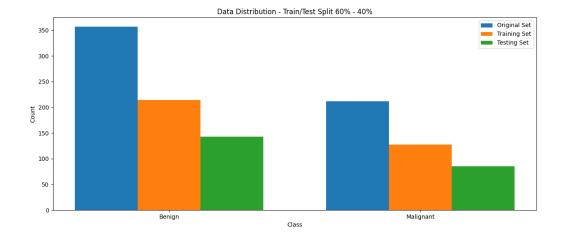
```
plt.bar(x - width, originalSet_labelCounts, width, label="Original Set")
plt.bar(x, trainingSet_labelCounts, width, label="Training Set")
plt.bar(x + width, testingSet_labelCounts, width, label="Testing Set")
```

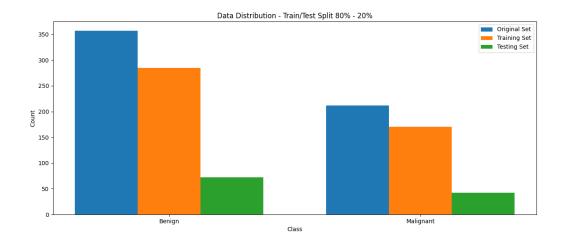
Because each list has two elements, is amount of 0 and 1 values, so we will have two group of bar chart, '0' group for Benign and '1' for Malignant.

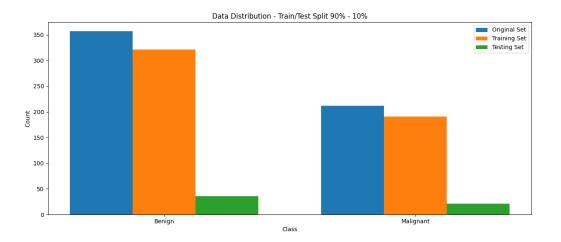
After creating the bar charts, save them to the "Output" folder for easy viewing and reporting.

These are the charts:









We can see that the splitting is quite good through these charts. The ratio between the train and test splits is as expected, and the number of elements in each group within the splits is also fairly balanced

3. Building the decision tree classifiers

To build a Decision Tree with the train and test sets after splitting according to the ratio, we use the DecisionTreeClassifier class and its functions from the sklearn library.

clf = DecisionTreeClassifier(criterion='entropy', random_state=2)

The criterion parameter specifies the function used to measure the quality of a split in the decision tree; in this case, we use the entropy index.

The random_state parameter can be any number. Setting this ensures that we get consistent results if we don't change the input values.

We can easily build a Decision Tree by using the fit function of the DecisionTreeClassifier class to find the optimal parameters based on the data, thus creating the best prediction model.

```
clf.fit(X_train, y_train)
```

To visualize the trees after building them, we use functions available in the Matplotlib library, specifically the plot tree function.

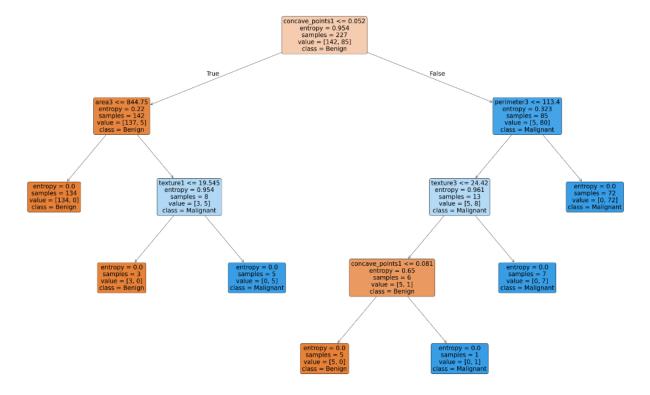
This function takes as input an object of the DecisionTreeClassifier class, which contains the Decision Tree model after it has been built. Additionally, we need to provide information about the names of the feature sets, target sets, cell sizes, etc.

To avoid overlapping branches in the decision tree visualizations, we should adjust the font size for each tree.

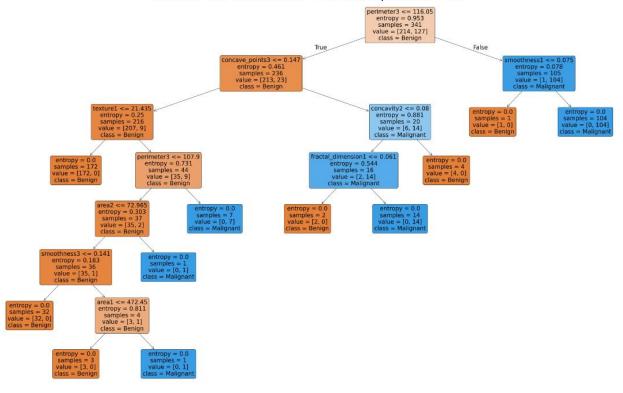
We should save these models to a list, so we don't need to train model again in other steps, we can named this is listTree

We save the results of each model into the "Output" folder for easy checking and reporting.

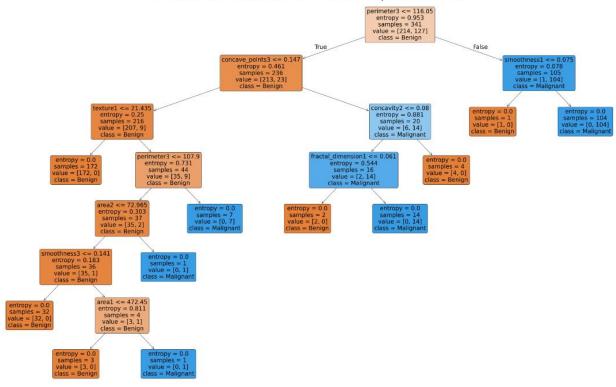
Decision Tree Visualization - Train/Test Split 40% - 60%



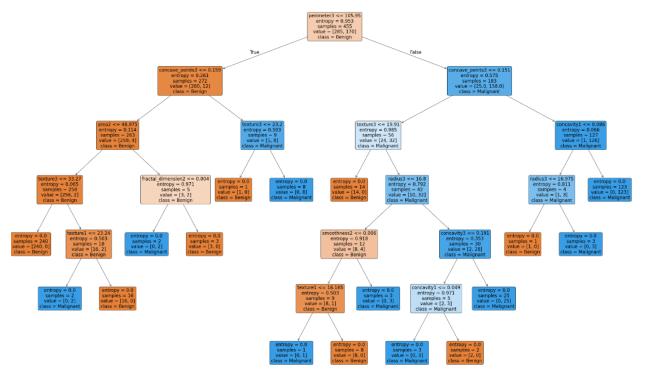
Decision Tree Visualization - Train/Test Split 60% - 40%



Decision Tree Visualization - Train/Test Split 60% - 40%



Decision Tree Visualization - Train/Test Split 80% - 20%



Decision Tree Visualization - Train/Test Split 90% - 10%

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4. Evaluating the decision tree classifiers

Iterating through listTree and listData, for each tree model and test data in data list (ignore train set, because we have the model before, so we don't need them), we replace the feature values in the test set to obtain the predicted y values. Combining these predicted values with the actual y values (taken from the label column of the test file), we pass them into the classification_report function to generate a classification report.

However, instead of saving the data as a CSV file, we want to save it as an image. To do this, we use functions available in Matplotlib, convert the data from CSV format into a table, and then save it as an image.

To create the confusion matrix, we pass the predicted y values obtained earlier, along with the actual y values from the label column in the test set, into the confusion_matrix() function. To visualize the confusion matrix, we use the Seaborn library and the heatmap function. We adjust information such as the chart title, column names, etc., to be appropriate before saving it into the "Output" folder.

Differences Between Classification Report and Confusion Matrix:

- Confusion Matrix: It is a table that represents the prediction results against the actual results based on True Positive and True Negative values. It simply shows the number of people with Benign and Malignant tumors in reality versus the model's predictions, giving an overview of the model's accuracy.
- Classification Report: It is also built on the differences between predicted and actual values, but it focuses on metrics calculated from those differences. The most important metrics are:
 - o **Precision**: The proportion of people who actually have Malignant tumors compared to those predicted to have Malignant tumors.
 - Recall: The proportion of people who actually have Malignant tumors that are predicted correctly, and vice versa for Benign tumors.
 - Other: Support (number of sample), F1-score (is the harmonic mean of Precision and Recall, used to balance these two metrics), macro avg (mean without number of sample), weighted avg (mean with number of sample)

User **accuracy**, which is derived from the factors mentioned above, to assess the overall accuracy of the model.

If not for the support from the built-in confusion_matrix() function in Python, calculating these metrics would have to be done based on the Confusion Matrix values. For details, see [1].

Based on these two metrics, we can assess the accuracy of a model. Additionally, the discrepancy between these two values can indicate issues the model is facing, providing a basis for further development and improvement.

Classification Report Visualization:

Classification Report - Train/Test Split 40% - 60%

	precision	recall	f1-score	support
Benign	0.95	0.96	0.95	215.00
Malignant	0.93	0.91	0.92	127.00
accuracy			0.94	0.94
macro avg	0.94	0.93	0.94	342.00
weighted avg	0.94	0.94	0.94	342.00

Classification Report - Train/Test Split 60% - 40%

Classification report - fram, lest spit 00% - 40%				
	precision	recall	f1-score	support
Benign	0.93	0.96	0.94	143.00
Malignant	0.92	0.87	0.90	85.00
accuracy			0.93	0.93
macro avg	0.93	0.91	0.92	228.00
weighted avg	0.93	0.93	0.92	228.00

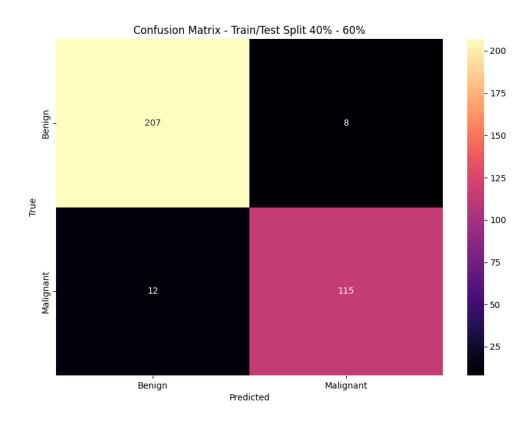
 ${\it Classification \ Report - Train/Test \ Split \ 80\% - 20\%}$

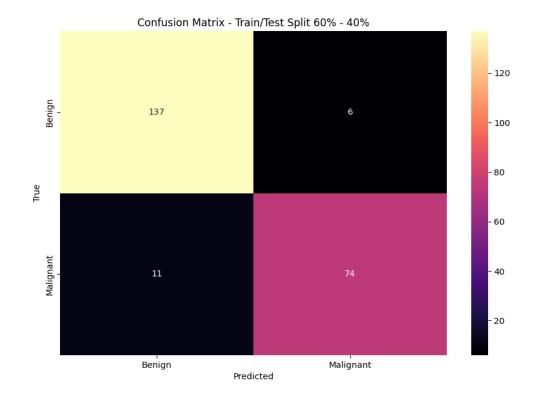
	precision	recall	f1-score	support
Benign	0.95	0.96	0.95	72.00
Malignant	0.93	0.90	0.92	42.00
accuracy			0.94	0.94
macro avg	0.94	0.93	0.93	114.00
weighted avg	0.94	0.94	0.94	114.00

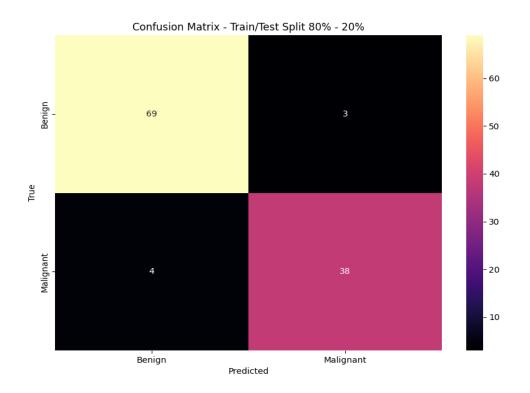
Classification Report - Train/Test Split 90% - 10%

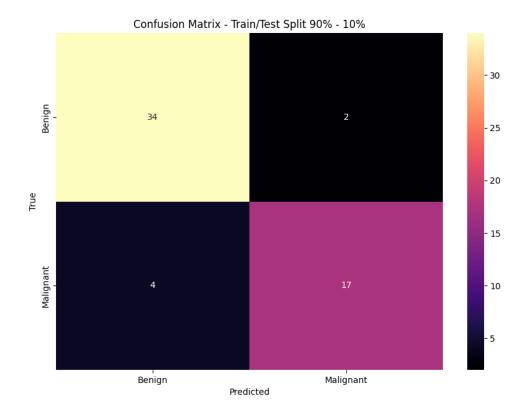
	precision	recall	f1-score	support
Benign	0.89	0.94	0.92	36.00
Malignant	0.89	0.81	0.85	21.00
accuracy			0.89	0.89
macro avg	0.89	0.88	0.88	57.00
weighted avg	0.89	0.89	0.89	57.00

Confusion Matrix Visualization:









5. The depth and accuracy of a decision tree

Adjusting the maximum depth of a Decision Tree has a significant impact on the model's accuracy. Generally, having too many constraints (such as a very small or very large depth) can lead to inaccurate predictions.

In this section, we will use the training and test data from the dataset split at an 80/20 ratio. We will observe the model's predictions compared to the actual results to draw conclusions about the model's accuracy at each specific maximum depth.

clf = DecisionTreeClassifier(max_depth=depth, criterion='entropy', random_state=42)

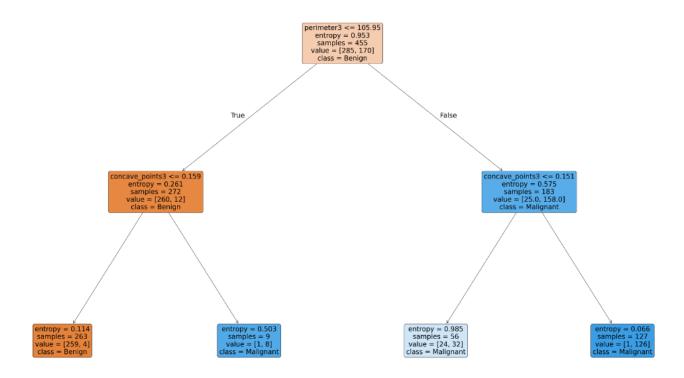
The steps to find optimal parameters and build the tree are similar to those previously described, that we use fit function in DecisionTreeClassifier class, but add parameter 'max_depth'. In this part of the report, I will also cover how to calculate accuracy.

After successfully building the model using the training data (features and target), we use the test data (features) to predict the target values. Then, we use the

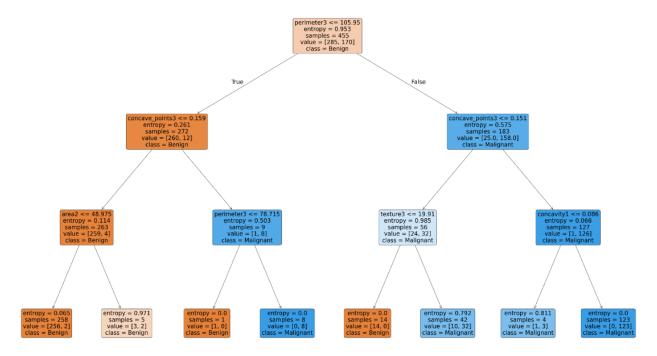
accuracy_score() function to calculate the accuracy by comparing the predicted values with the actual values in the test set.

After building the tree and determining the accuracy, we save the results into the "Output" folder. If the Decision Trees are visualized as plots, the accuracy table will include the name of each column (maximum depth) and the corresponding accuracy values obtained earlier.

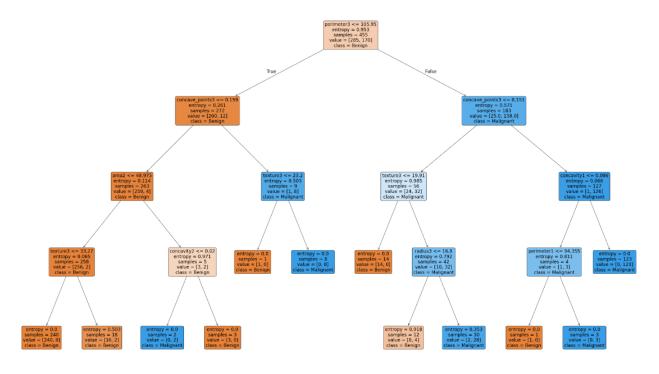
Decision Tree Visualization - max_depth 2



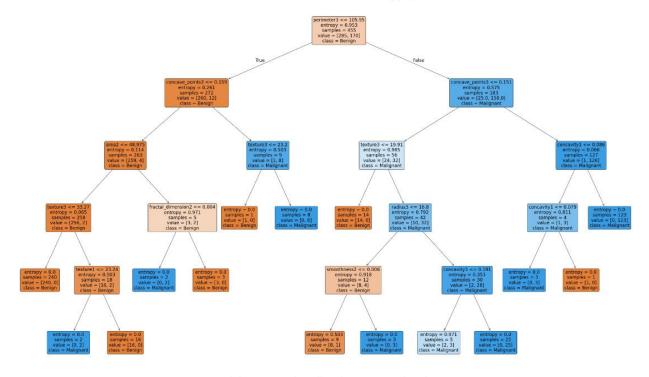
Decision Tree Visualization - max_depth 3



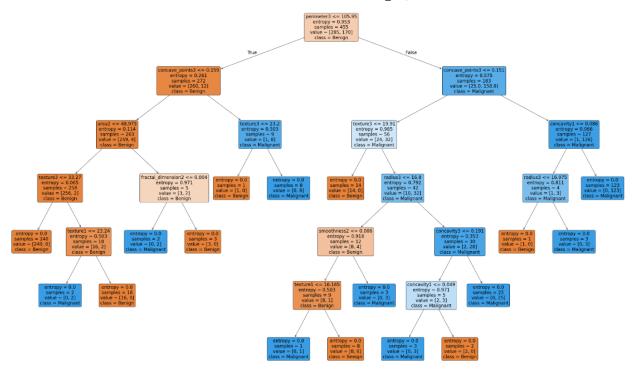
Decision Tree Visualization - max_depth 4



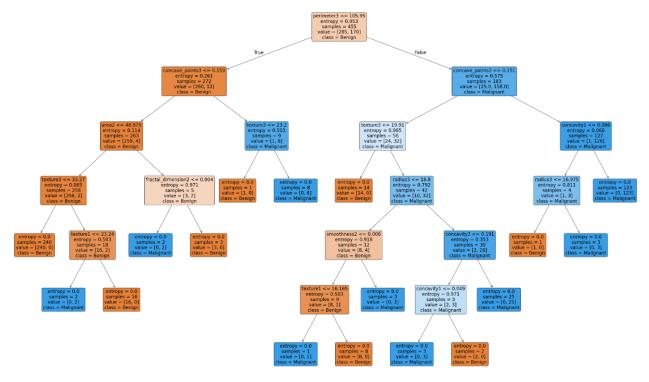
Decision Tree Visualization - max_depth 5



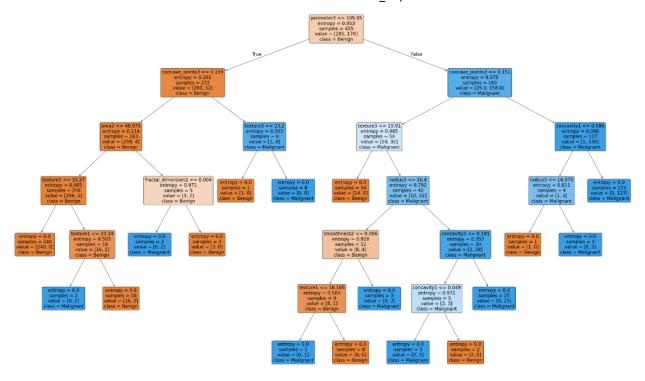
Decision Tree Visualization - max_depth 6



Decision Tree Visualization - max_depth 7



Decision Tree Visualization - max_depth None



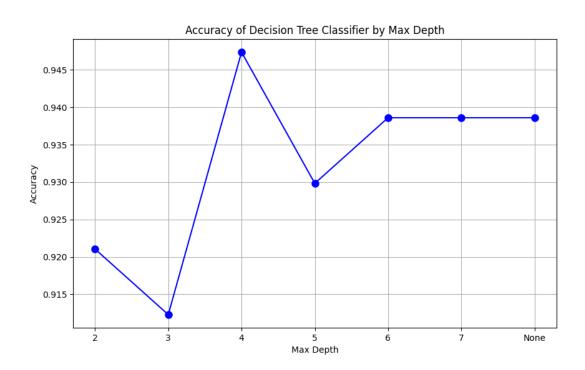
Observation: Since the dataset is relatively small (529 samples), the training data isn't very diverse. As a result, the maximum depth of the tree doesn't change significantly across the levels 6, 7, and None

We calculate the accuracy of each model at different depths, and summarize the results in the following table.

Decision Tree Accuracy by max_depth

max_depth	Accuracy
2	0.92
3	0.91
4	0.95
5	0.93
6	0.94
7	0.94
None	0.94

Or visualize it with a line chart for easier comparison.



Max Depth = 4: The model achieves the highest accuracy. So this is the best model for the data set which split into 80/20 (train/test).

Max Depth = 6, 7, None: The accuracy is the same because the models are similar, as previously noted.

Max Depth = 2, 3: The accuracy is lower due to many constraints leading to early termination of the models.

Max Depth = 5: Although there are fewer constraints, resulting in a decrease in accuracy, it is still higher than at depths 2 and 3.

6. Self Grading

No.	Specifications	Percent
1	Preparing the data sets	100%
2	Building the decision tree classifiers	100%
3	Classification report and confusion	100%
	matrix	
	Comments	100%
4	Trees, tables, and charts	100%
	Comments	100%

7. Reference

[1]: <u>Understanding the Confusion Matrix in Machine Learning - GeeksforGeeks</u> (View at 23/08/2024)

[2]: Matplotlib Tutorial - GeeksforGeeks (View at 22/08/2024)

[3]: <u>Building and Implementing Decision Tree Classifiers with Scikit-Learn: A Comprehensive Guide - GeeksforGeeks</u> (View at 22/08/2024)