Lab 7: Classification with Scikit-Learn

The objective of this notebook is to learn about the **Scikit-Learn** library (official documentation) and **classification models**.

Firstly, run the next cell to import useful libraries to complete this lab.

In [1]:
```
import pandas as pd
import numpy as np
from sklearn.datasets import load_iris
from sklearn.svm import SVC
from sklearn.inspection import DecisionBoundaryDisplay
from sklearn import tree, neighbors
from sklearn.model_selection import train_test_split
from sklearn.metrics import confusion_matrix, classification_report, accuracy_score
from sklearn.ensemble import RandomForestClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import f1_score

import matplotlib.pyplot as plt
import warnings
warnings.filterwarnings("ignore")
```

1. Load dataset

We will use the **Iris** dataset as our first classification problem. *Iris* is a genus of flowering plants that contains several species, including **Iris setosa**, **Iris versicolor**, and **Iris virginica**.

The dataset consists of:

- 150 samples
- 3 labels: species of Iris (*Iris setosa*, *Iris versicolor*, and *Iris virginica*)
- 4 features: *Sepal length*, *Sepal width*, *Petal length*, and *Petal width* in centimeters

Your objective is to build a **multiclass classifier** that can predict the target class (i.e., the species of Iris) given the feature values (i.e., Sepal length, Sepal width, Petal length, and Petal width).

You can find an **exploratory analysis of the dataset** here.

Scikit-Learn comes with built-in datasets for the **Iris** classification problem. The next cell loads the iris dataset from Scikit-Learn and stores it in a Pandas DataFrame.

In [2]:
```
iris = load_iris() # Load Data

df = pd.DataFrame(iris.data, columns = iris.feature_names) # Create a dataframe
df['target'] = iris.target
df['target name'] = df['target'].apply(lambda x: 'sentosa' if x == 0 else ('versicolor' if x == 1 else 'virginica'))
```

In [3]:
```
df
```

Out[3]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target	target name
0	5.1	3.5	1.4	0.2	0	sentosa
1	4.9	3.0	1.4	0.2	0	sentosa
2	4.7	3.2	1.3	0.2	0	sentosa
3	4.6	3.1	1.5	0.2	0	sentosa
4	5.0	3.6	1.4	0.2	0	sentosa
...	...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	2	virginica
146	6.3	2.5	5.0	1.9	2	virginica
147	6.5	3.0	5.2	2.0	2	virginica
148	6.2	3.4	5.4	2.3	2	virginica
149	5.9	3.0	5.1	1.8	2	virginica

150 rows × 6 columns

In [4]:
```
n_labels = len(set(df['target']))
print(f'Number of labels: {n_labels}')
print(f"labels: {set(df['target name'])}")
```

```
Number of labels: 3
labels: {'versicolor', 'virginica', 'sentosa'}
```

In [5]:
```
labels = ["sentosa", "versicolor", "virginica"]
label2id = {"sentosa":0, "versicolor":1, "virginica":2}
```

The following cell describes the dataset by computing the *mean*, *std*, *min*, *max*, and *quantiles* of each column.

In [6]:
```
df.describe()
```

Out[6]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
count	150.000000	150.000000	150.000000	150.000000	150.000000
mean	5.843333	3.057333	3.758000	1.199333	1.000000
std	0.828066	0.435866	1.765298	0.762238	0.819232
min	4.300000	2.000000	1.000000	0.100000	0.000000
25%	5.100000	2.800000	1.600000	0.300000	0.000000
50%	5.800000	3.000000	4.350000	1.300000	1.000000
75%	6.400000	3.300000	5.100000	1.800000	2.000000
max	7.900000	4.400000	6.900000	2.500000	2.000000

The following cell counts the number of *null* values in each column.

In [7]:
```
nan_count = df.isna().sum()
print(nan_count )
```

```
sepal length (cm)    0
sepal width (cm)     0
petal length (cm)    0
petal width (cm)     0
target               0
target name          0
dtype: int64
```

As you can see, there are no *null* values (i.e., **missing values**) in the dataset.

The next cell **counts the number of examples for each class label**.

In [8]:
```
df.value_counts("target")
```

Out[8]:
```
target
0    50
1    50
2    50
dtype: int64
```

As you can see, the labels are **equally represented** in the dataset. Therefore, it is a **balanced** dataset.

2. Classification with 2D input features

Now, you will perform the classification task (i.e., predict the species of Iris) using the first **two input features** of the dataset (i.e., *sepal length* and *sepal width*).

Exercise 2.1

Select the **first two columns** of the dataset and store them in a variable `X_2d`.

In [9]:
```
y = df.target
y_names = df["target name"]

#### START CODE HERE (~1 line) ####
X_2d = df.iloc[:, :2]
#### END CODE HERE ####
```

In [10]:
```
X_2d.head()
```

Out[10]:

	sepal length (cm)	sepal width (cm)
0	5.1	3.5
1	4.9	3.0
2	4.7	3.2
3	4.6	3.1
4	5.0	3.6

Expected output

```
sepal length (cm)  sepal width (cm)
0                5.1                3.5
1                4.9                      3.0
2                4.7                      3.2
```

3	4.6	3.1
4	5.0	3.6

In [11]:
```
y
```

Out[11]:
```
0      0
1      0
2      0
3      0
4      0
      ..
145    2
146    2
147    2
148    2
149    2
Name: target, Length: 150, dtype: int64
```

In [12]:
```
y_names
```

Out[12]:
```
0         sentosa
1         sentosa
2         sentosa
3         sentosa
4         sentosa
          ...
145    virginica
146    virginica
147    virginica
148    virginica
149    virginica
Name: target name, Length: 150, dtype: object
```

Exercise 2.2

Split the dataset `X_2d` into **training** and **test** sets using the train_test_split function provided by the Scikit-Learn library. Store the features of the training set in `X_train_2d`, the features of the test `X_test_2d`, the labels of the training set in `y_train`, and the labels of the test set in `y_test`. Split the dataset with 80% of samples for training and 20% of samples for testing. **Shuffle** the data and set the **random state** to 42.

In [13]:
```
#### START CODE HERE (~1 line) ####
X_train_2d, X_test_2d, y_train, y_test = train_test_split(X_2d, y, test_size=0.2, shuffle=True, random_state=42)
#### END CODE HERE ####
```

In [14]:
```
print(f"{len(X_train_2d)} training examples")
print(f"{len(X_test_2d)} test examples")
```

```
120 training examples
30 test examples
```

Expected output

`120 training examples`

`30 test examples`

The following cell **plots** the examples of the **training set** in the **plane**, with a different color based on the target label.

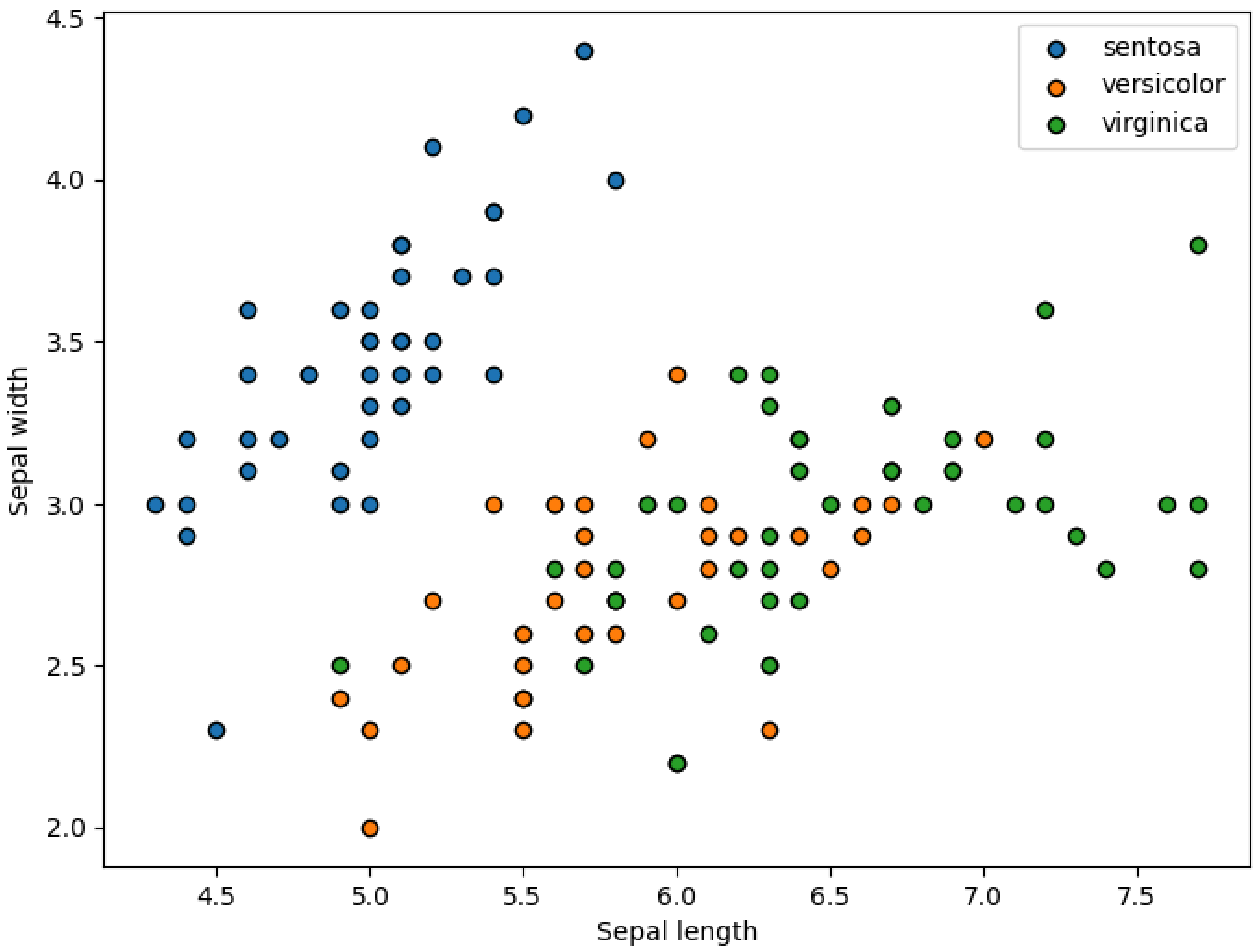
In [15]:
```
plt.figure(2, figsize=(8, 6))
plt.clf()

for label_id, label in enumerate(labels):
    X_temp = X_train_2d.loc[y_train == label_id]
    plt.scatter(X_temp.iloc[:, 0], X_temp.iloc[:, 1], cmap=plt.cm.Set1, edgecolor="k", label=label)

plt.xlabel("Sepal length")
plt.ylabel("Sepal width")

plt.xticks()
plt.yticks()
plt.legend()
```

Out[15]:
```
<matplotlib.legend.Legend at 0x7fca6352fa30>
```



Train a Support Vector Machine SVM classifier

Here, you will train a **Support Vector Machine SVM** Classifier using the *Scikit-Learn* library. You can learn more about **Support Vector Machines** here. You can find the official Scikit-Learn documentation for **SVM** for classification here. For this exercise, you can use the **SVC** implementation here.

Exercise 2.3

Create an **SVC object** with the following parameters `gamma=0.1`, `kernel="rbf"`, `probability=True` in a variable `svm_model`.

Feel free to change the parameters and see how it affects the results.

In [16]:
```
#### START CODE HERE (~1 line) ####
svm_model = SVC(gamma=0.1, kernel="rbf", probability=True)
#### END CODE HERE ####
```

Exercise 2.4

Fit (i.e., train) the `svm_model` with the training data. You should pass the input features and the targets of the training set. Please refer to the documentation for the parameters of the **fit()** method.

In [17]:
```
#### START CODE HERE (~1 line) ####
svm_model.fit(X_train_2d, y_train)
#### END CODE HERE ####
```

Out[17]:
```
▾ SVC
SVC(gamma=0.1, probability=True)
```

Exercise 2.5

Predict the labels for the **test dataset** and store them in a variable `y_test_pred_svm`. You should pass the input features of the test data. Please refer to the documentation for the parameters of the **predict()** method.

In [18]:
```
#### START CODE HERE (~1 line) ####
y_test_pred_svm = svm_model.predict(X_test_2d)
#### END CODE HERE ####
```

Confusion Matrix

Exercise 2.6

Compute the **confusion matrix** for the predictions on the test set in a variable `cm`. You should pass the **real labels** (i.e., ground-truth labels) and the **predicted labels** by the classifier. Use the `confusion_matrix` function of the Scikit-Learn library. You can find the documentation here.

You can learn how to interpret a **confusion matrix** here.

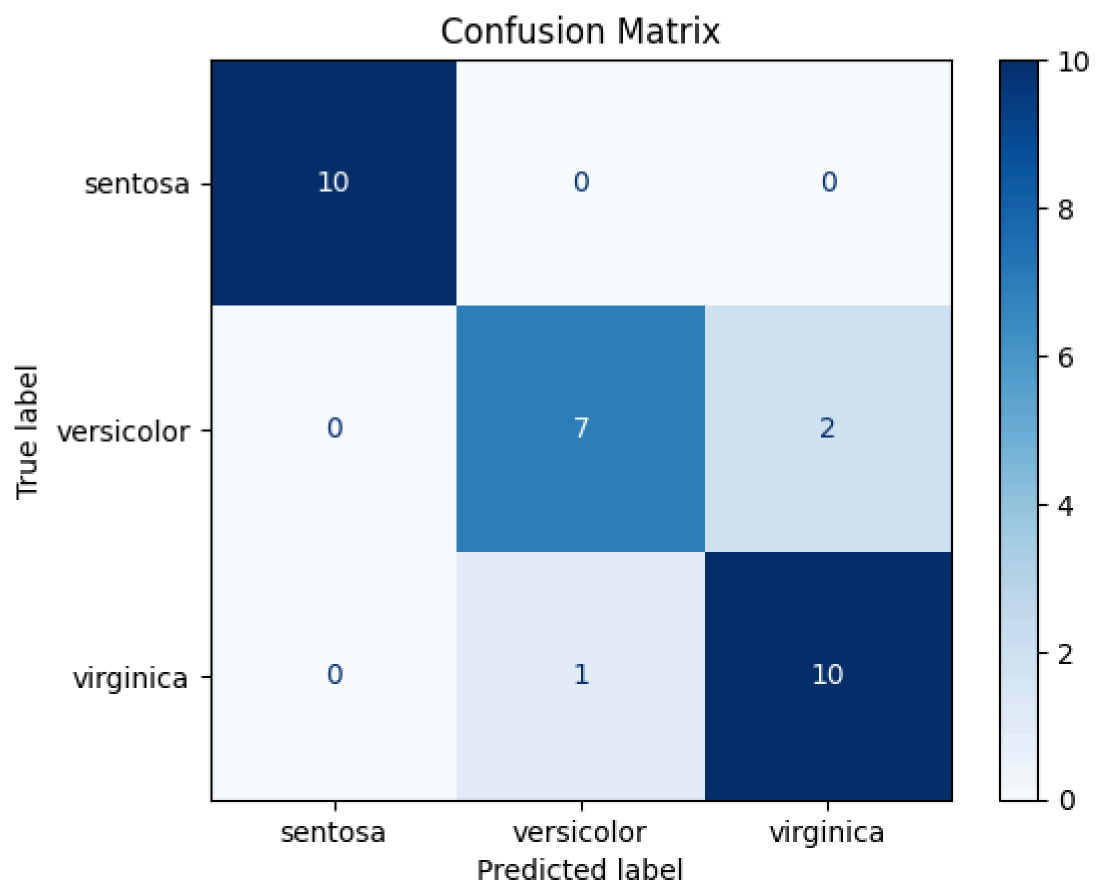
In [19]:
```
#### START CODE HERE (~1 line) ####
cm = confusion_matrix(y_test, y_test_pred_svm)
#### END CODE HERE ####
print(cm)
```

```
[[10  0  0]
 [ 0  7  2]
 [ 0  1 10]]
```

The following cell **plots the confusion matrix**.

In [20]:
```
from sklearn.metrics import ConfusionMatrixDisplay

cmd = ConfusionMatrixDisplay.from_predictions(y_test, y_test_pred_svm, cmap=plt.cm.Blues)
ax = cmd.ax_
ax.set_title('Confusion Matrix')
ax.set_xticklabels(labels)
ax.set_yticklabels(labels)
plt.show()
```



Accuracy and F1 Score

Exercise 2.7

Compute the **accuracy** and the **F1 score** for the predictions on the **test set**, and store the results in the variables `acc_svm` and `f1_svm`, respectively. To compute the **accuracy**, you can use the accuracy_score function of the Scikit-Learn library. Instead, to compute the **F1 score**, you can use the f1_score function of the Scikit-Learn library. For the **F1**, compute the `macro` score (you can specify it in the parameters).

In [21]:
```
#### START CODE HERE (~2 lines) ####
acc_svm = accuracy_score(y_test, y_test_pred_svm)
f1_svm = f1_score(y_test, y_test_pred_svm, average='macro')
#### END CODE HERE ####
```

In [22]:
```
print(f"Accuracy: {acc_svm:.2}")
print(f"F1: {f1_svm:.2}")
```

```
Accuracy: 0.9
F1: 0.9
```

Congratulations. You have trained a very good classifier! It predicts the correct class 9 times out of 10!

Train a Decision Tree Classifier

Here, you will train a **Decision Tree DT** Classifier using the *Scikit-Learn* library. You can learn more about **Decision Trees** here. You can find the official Scikit-Learn documentation for **Decision Tree** here. For this exercise, you should use the **DT Classifier** here.

Exercise 2.6

- Create an `DecisionTreeClassifier` object with the following parameters `max_depth=4` in a variable `dt_model`.
- Fit (i.e., train) the `dt_model` with the training data. You should pass the input features and the targets. Please refer to the documentation.
- Predict the labels for the test dataset and store them in a variable `y_test_pred_dt`. You should pass the input features of the test data.

Feel free to change the parameters and see how it affects the results.

In [23]:
```
#### START CODE HERE (~3 lines) ####
dt_model = DecisionTreeClassifier(max_depth=4)
dt_model.fit(X_train_2d, y_train)
y_test_pred_dt = dt_model.predict(X_test_2d)
#### END CODE HERE ####
```

Train a K-Nearest-Neighbors Classifier

Here, you will train a **K-Nearest-Neighbors** Classifier using the *Scikit-Learn* library. You can learn more about **K-Nearest-Neighbors** here. You can find the official Scikit-Learn documentation for **K-Nearest-Neighbors** here. For this exercise, you should use the **KNeighborsClassifier** here.

Exercise 2.7

- Create an `KNeighborsClassifier` object with the following parameters `n_neighbors=7` in a variable `knn_model`.
- Fit (i.e., train) the `knn_model` with the training data. You should pass the input features and the targets. Please refer to the documentation.
- Predict the labels for the test dataset and store them in a variable `y_test_pred_knn`. You should pass the input features of the test data.

Feel free to change the parameters and see how it affects the results.

In [24]:
```
#### START CODE HERE (~3 lines) ####
knn_model = KNeighborsClassifier(n_neighbors=7)
knn_model.fit(X_train_2d, y_train)
y_test_pred_knn = knn_model.predict(X_test_2d)
#### END CODE HERE ####
```

Train a Random Forest Classifier

Here, you will train a **Random Forest** Classifier using the *Scikit-Learn* library. You can learn more about **Random Forests** here. You can find the official Scikit-Learn documentation for **Random Forest Classifiers** here. For this exercise, you should use the **Random Forest Classifier** here.

Exercise 2.8

- Create an `RandomForestClassifier` object with the following parameters `max_depth=2` in a variable `rf_model`.
- Fit (i.e., train) the `rf_model` with the training data. You should pass the input features and the targets. Please refer to the documentation.
- Predict the labels for the test dataset and store them in a variable `y_test_pred_rf`. You should pass the input features of the test data.

Feel free to change the parameters and see how it affects the results.

In [25]:
```
#### START CODE HERE (~3 lines) ####
rf_model = RandomForestClassifier(max_depth=2)
rf_model.fit(X_train_2d, y_train)
y_test_pred_rf = rf_model.predict(X_test_2d)
#### END CODE HERE ####
```

Plot Decision Boundaries

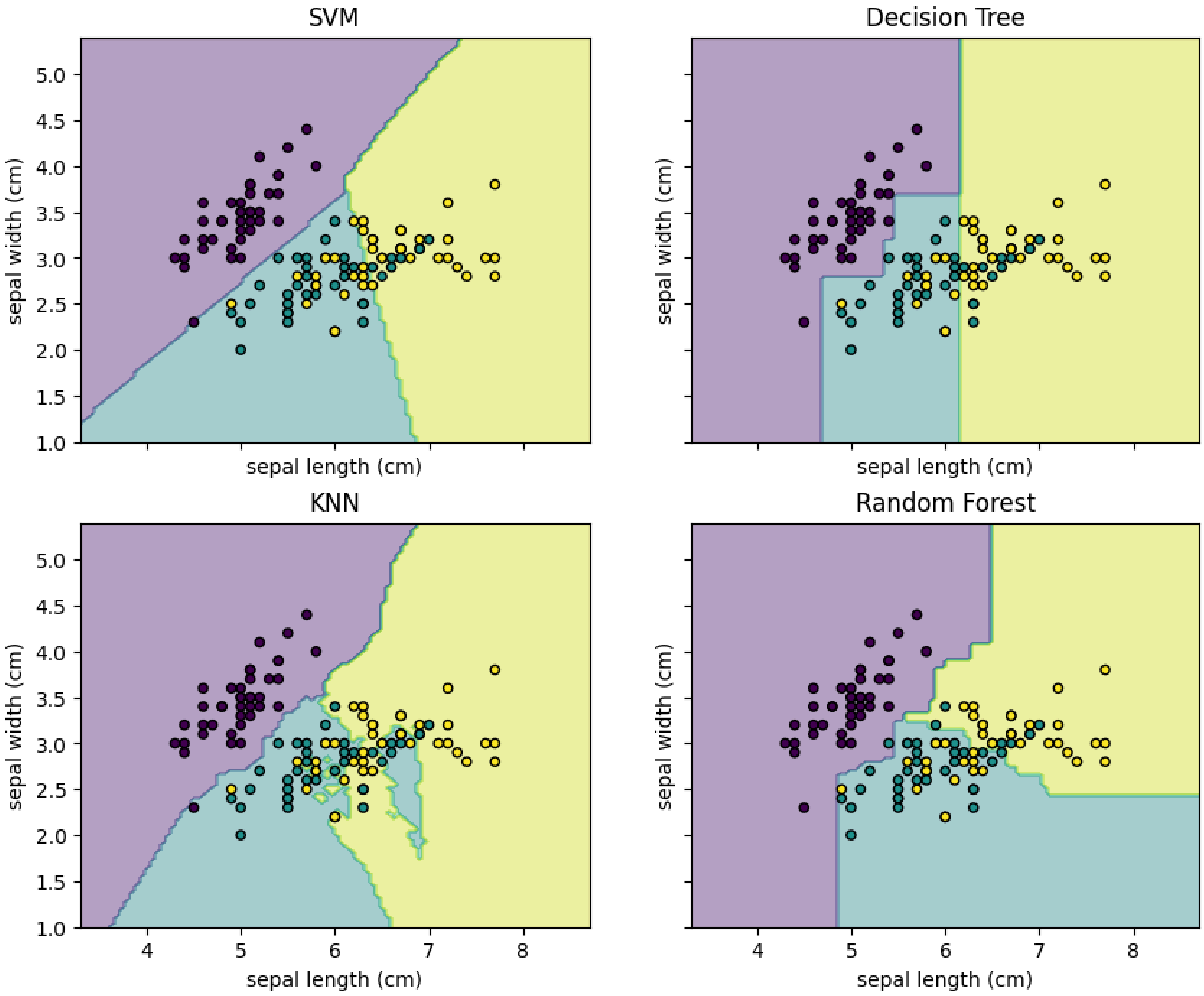
The next cell plots the **decision boundaries** for the SVM, the Decision Tree, the KNN, and the Random Forest. To run this cell, ensure that you correctly named the variables `svm_model`, `dt_model`, `knn_model`, and `rf_model`. You can learn more about **decision boundaries** here.

In [26]:
```
# Plotting decision regions
from itertools import product

f, axarr = plt.subplots(2, 2, sharex="col", sharey="row", figsize=(10, 8))
for idx, clf, tt in zip(product([0, 1], [0, 1]),
```

```
                           [svm_model, dt_model, knn_model, rf_model],
                           ["SVM", "Decision Tree", "KNN", "Random Forest"]):
    DecisionBoundaryDisplay.from_estimator(
        clf, X_train_2d, alpha=0.4, ax=axarr[idx[0], idx[1]], response_method="predict"
    )
    axarr[idx[0], idx[1]].scatter(X_train_2d.iloc[:, 0], X_train_2d.iloc[:, 1], c=y_train, s=20, edgecolor="k")
    axarr[idx[0], idx[1]].set_title(tt)

plt.show()
```



Compare the Classifiers with Quantitative Evaluation Metrics

So far, you have trained 4 different classifiers on the same training data. To assess which performs better, you will calculate **quantitative evaluation** metrics such as **F1**, **Precision**, and **Recall**. Metrics will be calculated either separately for each class or aggregated as a whole.

You can learn more about such quantitative metrics here and here.

Exercise 2.9

Compute the **quantitative metrics** for the **SVM** model in a variable `classification_report_svm`, for the **Decision Tree** in a variable `classification_report_dt`, for the **KNN** in a variable `classification_report_knn`, and for the **Random Forest** in a variable `classification_report_rf`. Use the classification_report function of the Scikit-Learn library. It computes all the metrics for each class and overal at once. Remember that the names of your target labels are stored in the variable `labels`.

In [27]:
```
print(labels)
```

```
['sentosa', 'versicolor', 'virginica']
```

In [28]:
```
#### START CODE HERE (~4 lines) ####
classification_report_svm = classification_report(y_test, y_test_pred_svm, target_names=labels)
classification_report_dt = classification_report(y_test, y_test_pred_dt, target_names=labels)
classification_report_knn = classification_report(y_test, y_test_pred_knn, target_names=labels)
classification_report_rf = classification_report(y_test, y_test_pred_rf, target_names=labels)
#### END CODE HERE ####
```

In [29]:
```
print("SVM")
print(classification_report_svm)

print("\n\nDecision Tree")
print(classification_report_dt)

print("\n\nKNN")
print(classification_report_knn)
```

```
print("\n\nRandom Forest")
print(classification_report_rf)
```

```
SVM
              precision    recall  f1-score   support

      sentosa       1.00      1.00      1.00        10
   versicolor       0.88      0.78      0.82         9
    virginica       0.83      0.91      0.87        11

     accuracy                           0.90        30
    macro avg       0.90      0.90      0.90        30
 weighted avg       0.90      0.90      0.90        30



Decision Tree
              precision    recall  f1-score   support

      sentosa       1.00      0.90      0.95        10
   versicolor       0.75      0.67      0.71         9
    virginica       0.77      0.91      0.83        11

     accuracy                           0.83        30
    macro avg       0.84      0.83      0.83        30
 weighted avg       0.84      0.83      0.83        30



KNN
              precision    recall  f1-score   support

      sentosa       1.00      1.00      1.00        10
   versicolor       0.60      0.67      0.63         9
    virginica       0.70      0.64      0.67        11

     accuracy                           0.77        30
    macro avg       0.77      0.77      0.77        30
 weighted avg       0.77      0.77      0.77        30



Random Forest
              precision    recall  f1-score   support

      sentosa       1.00      1.00      1.00        10
   versicolor       0.64      0.78      0.70         9
    virginica       0.78      0.64      0.70        11

     accuracy                           0.80        30
    macro avg       0.80      0.80      0.80        30
 weighted avg       0.81      0.80      0.80        30
```

What do you think is the best classifier? Why?

3. Classification with all features

Now you will perform the same procedure but using **all the features** in the dataset. Remember that the original dataset contains 4 features but in the previous exercise you used only 2 features.

Exercise 3.1

Select **all the feature columns** of the dataset and store them in a variable `X`. The features are stored in the first 4 columns of the DataFrame `df` (i.e., *sepal length (cm)*, *sepal width (cm)*, *petal length (cm)*, and *petal width (cm)*).

In [30]:
```
y = df.target
y_names = df["target name"]

#### START CODE HERE (~1 line) ####
X = df.iloc[:, :4]
#### END CODE HERE ####
```

In [31]:
```
X.head()
```

Out[31]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)
0	5.1	3.5	1.4	0.2
1	4.9	3.0	1.4	0.2
2	4.7	3.2	1.3	0.2
3	4.6	3.1	1.5	0.2
4	5.0	3.6	1.4	0.2

Expected output

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)
0	5.1	3.5	1.4	0.2
1	4.9	3.0	1.4	0.2
2	4.7	3.2	1.3	0.2
3	4.6	3.1	1.5	0.2
4	5.0	3.6	1.4	0.2

This time the input array have 4 features. Therefore you can't visualize it in the plane.

The following cell **splits the dataset into train and test**.

In [32]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, shuffle=True)
```

In [33]:
```
print(f"Number of training examples {len(X_train)}")
print(f"Number of test examples {len(X_test)}")
```

```
Number of training examples 120
Number of test examples 30
```

Exercise 3.2

Now **train different classifiers using all input features** `X`. You can also use other classifiers in the *Scikit-Learn* library and different hyperparameters. Can you outperform the best model obtained using only 2 input features?

You can find the list of all implemented classification models here.

Remember that the steps are always the same:

1. **Instantiate the model object** you want to use.
2. **Train the model** on the training data using the **fit()** method.
3. **Predict labels for test data** using the **predict()** method.
4. Repeat training and testing **for different models** (and also different hyperparameters of the models).
5. Compute **quantitative evaluation metrics** to identify the best model.

In [ ]:
```

```