Hands On Exercise 3: Decision Trees

Chapter 6 – Decision Trees

File name convention: For group 42 and memebers Richard Stallman and Linus Torvalds it would be "03_Goup42_Stallman_Torvalds.pdf".

Submission via blackboard (UA).

Feel free to answer free text questions in text cells using markdown and possibly $\LaTeX$ if you want to.

You don't have to understand every line of code here and it is not intended for you to try to understand every line of code.
Big blocks of code are usually meant to just be clicked through.

Setup

In [ ]:
```
# Python ≥3.5 is required
import sys
assert sys.version_info >= (3, 5)

# Scikit-Learn ≥0.20 is required
import sklearn
assert sklearn.__version__ >= "0.20"

# Common imports
import numpy as np
import os

# to make this notebook's output stable across runs
np.random.seed(42)

# To plot pretty figures
%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
```

```
mpl.rc('axes', labelsize=14)
mpl.rc('xtick', labelsize=12)
mpl.rc('ytick', labelsize=12)
```

Loading the data

You might remember the Iris Flower Data Set from last lecture. If you're curious about the data set, feel free to check out the wikipedia article in the hotlink listed here. Basically, it contains information about several species of iris flowers along with a classification of which species of iris they are.

In [ ]:
```
from sklearn.datasets import load_iris

iris = load_iris()
X = iris.data[:, 2:] # petal length and width
y = iris.target
```

In [ ]:
```
X.shape  # 150 instances, 2 features per instance (petal length and width)
```

Out[ ]:
```
(150, 2)
```

In [ ]:
```
y.shape
```

Out[ ]:
```
(150,)
```

Now that we have the data we can fit a model to it.

Decision Trees for Classification

At their core, **decision trees are branching networks** that take data and pose a series of rules-based questions at each branching point in the tree. **A branch might look like the following: if the number is greater two, take the left branch. Otherwise, take the right branch**. The idea is to **construct a network of these rules-based conditions that**, when imposed on your input data, **get you to a desired output**.

Task 1

Build a simple decision tree classifier with `max_depth` of 2 and `random_state` of 42. Fit to the data `X`, `y`.

In [ ]:
```
from sklearn.tree import DecisionTreeClassifier
```

↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓ your code goes below

In [ ]:
```
# tree_clf
```

In [ ]:
```
tree_clf= DecisionTreeClassifier(max_depth=2, random_state=42)
tree_clf.fit(X,y)
```

Out[ ]:
```
▾ DecisionTreeClassifier
DecisionTreeClassifier(max_depth=2, random_state=42)
```

↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑ your code goes above this

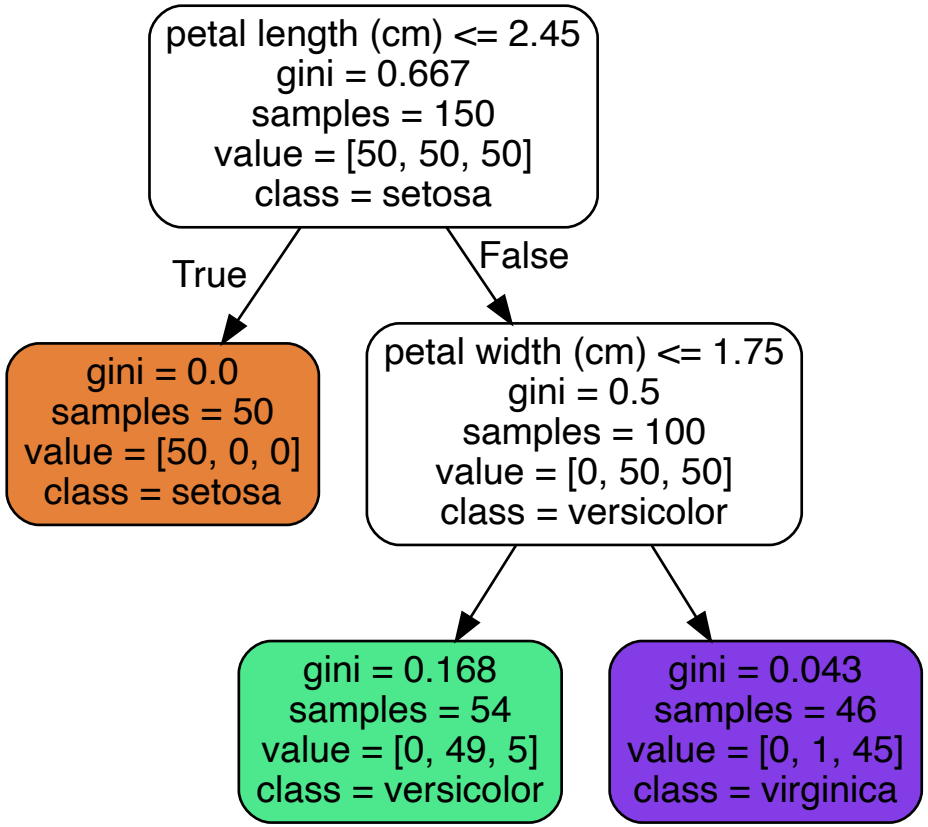
Visualization of the Decision Tree

In the following, we use the `graphviz` package to visualize decision trees in the form of flowcharts.

In [ ]:
```
from graphviz import Source
from sklearn.tree import export_graphviz

IMAGES_PATH = os.path.join(".", "images")
os.makedirs(IMAGES_PATH, exist_ok=True)

export_graphviz(
        tree_clf,
        out_file=os.path.join(IMAGES_PATH, "iris_tree.dot"),
        feature_names=iris.feature_names[2:],
        class_names=iris.target_names,
        rounded=True,
        filled=True
    )
```

```
Source.from_file(os.path.join(IMAGES_PATH, "iris_tree.dot"))
```

Out[ ]:

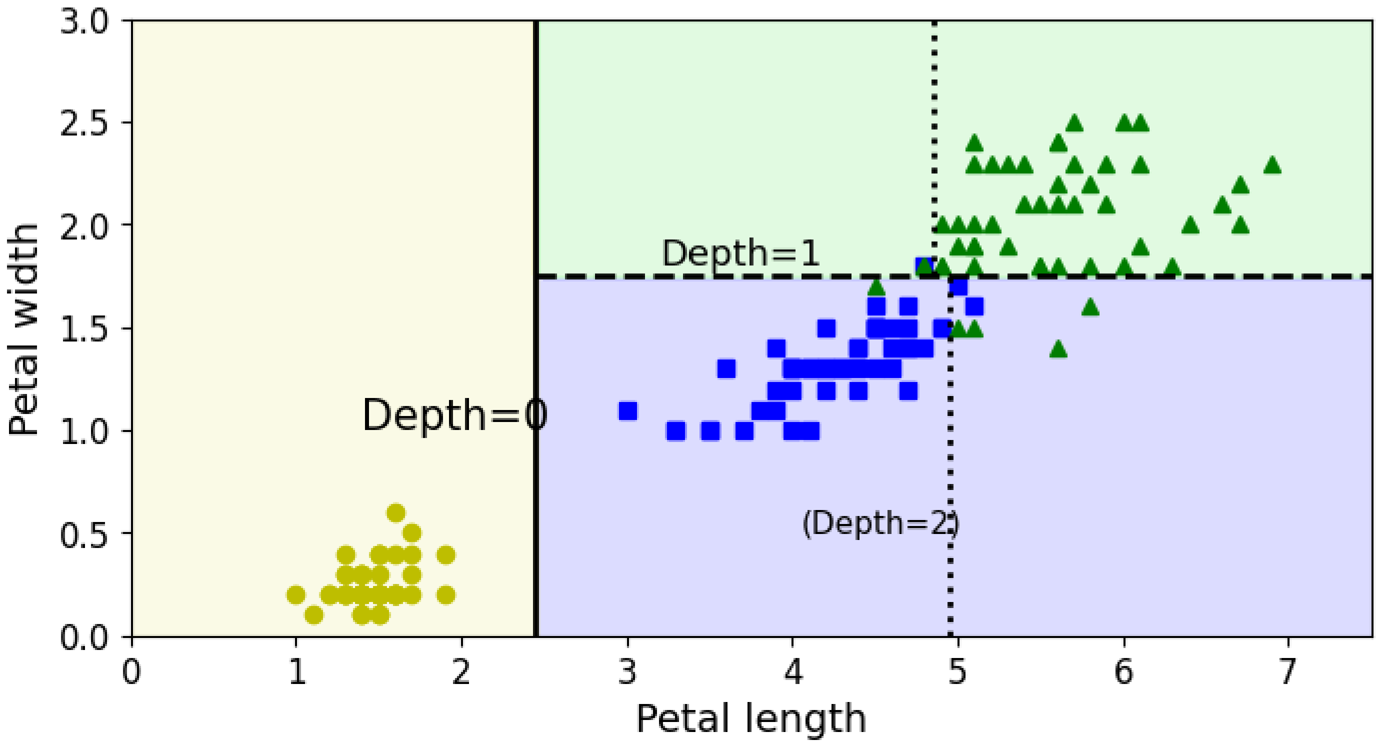


Don't worry about understanding the following code but do try to understand the plot itself. This isn't the first time we've looked at plots of decision boundaries before. Reminder, a decision boundary is some cutoff point we determine within the data that separates one classification from another.

In [ ]:

```
from matplotlib.colors import ListedColormap

def plot_decision_boundary(clf, X, y, axes=[0, 7.5, 0, 3], iris=True, legend=False, plot_training=True):
    x1s = np.linspace(axes[0], axes[1], 100)
    x2s = np.linspace(axes[2], axes[3], 100)
    x1, x2 = np.meshgrid(x1s, x2s)
    X_new = np.c_[x1.ravel(), x2.ravel()]
    y_pred = clf.predict(X_new).reshape(x1.shape)
    custom_cmap = ListedColormap(['#fafab0','#9898ff','#a0faa0'])
    plt.contourf(x1, x2, y_pred, alpha=0.3, cmap=custom_cmap)
```

```
    if not iris:
        custom_cmap2 = ListedColormap(['#7d7d58','#4c4c7f','#507d50'])
        plt.contour(x1, x2, y_pred, cmap=custom_cmap2, alpha=0.8)
    if plot_training:
        plt.plot(X[:, 0][y==0], X[:, 1][y==0], "yo", label="Iris setosa")
        plt.plot(X[:, 0][y==1], X[:, 1][y==1], "bs", label="Iris versicolor")
        plt.plot(X[:, 0][y==2], X[:, 1][y==2], "g^", label="Iris virginica")
        plt.axis(axes)
    if iris:
        plt.xlabel("Petal length", fontsize=14)
        plt.ylabel("Petal width", fontsize=14)
    else:
        plt.xlabel(r"$x_1$", fontsize=18)
        plt.ylabel(r"$x_2$", fontsize=18, rotation=0)
    if legend:
        plt.legend(loc="lower right", fontsize=14)

plt.figure(figsize=(8, 4))
plot_decision_boundary(tree_clf, X, y)
plt.plot([2.45, 2.45], [0, 3], "k-", linewidth=2)
plt.plot([2.45, 7.5], [1.75, 1.75], "k--", linewidth=2)
plt.plot([4.95, 4.95], [0, 1.75], "k:", linewidth=2)
plt.plot([4.85, 4.85], [1.75, 3], "k:", linewidth=2)
plt.text(1.40, 1.0, "Depth=0", fontsize=15)
plt.text(3.2, 1.80, "Depth=1", fontsize=13)
plt.text(4.05, 0.5, "(Depth=2)", fontsize=11)

plt.show()
```



Predicting classes and class probabilities

Task 2

Next, predict the probabilities and the class for the following values: `X=[[5, 1.5]]` for petal length and petal width.

You will need the functions `tree_clf.predict_proba()` and `tree_clf.predict()`. You do not need to import these as these are functions already included with your decision tree classifier.

↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓ your code goes below

In [ ]:
```
# pred_prob =
# pred_prob
pred_prob = tree_clf.predict_proba([[5,1.5]])
pred_prob
```

Out[ ]:
```
array([[0.        , 0.90740741, 0.09259259]])
```

In [ ]:
```
# y_pred =
# y_pred
y_pred = tree_clf.predict([[5,1.5]])
y_pred
```

Out[ ]:
```
array([1])
```

↑↑ your code goes above this

You can also check in the plot above what class you would put the instance `X=[[5, 1.5]]` into. In the plot, yellow corresponds to class 0 (Iris setosa), blue corresponds to class 1 (Iris versicolor), and green corresponds to class 2 (Iris virginica).

Sensitivity to training set details

Task 3

Next, we want to explore the sensitivity to the training set details. We will train the same decision tree model, but with slightly different training data.

Task 3a (bonus): The statements in the next two cells are the same. For bonus points you can explain why that's the case.

Hint: refer to the dataset description and think about the slicing of the array below. Which values are selected and which data do they show? It helps to evaluate parts of the expression separately and try to understand them.

In [ ]:
```
X[(X[:, 1]==X[:, 1][y==1].max()) & (y==1)]
```

Out[ ]:
```
array([[4.8, 1.8]])
```

In [ ]:
```
X[(X[:, 1]==[1.8]) & (y==1)]
```

Out[ ]:
```
array([[4.8, 1.8]])
```

↓↓ your answer goes below

Task 3a (bonus) answer:

These two lines of codes have the same function. the result of the first line x[:,1][y==1].max() searched is 1.8, so that it is equal to the second one [1.8]. Therefore, these two statements are logically equivalent.

↑↑ your answer goes above this

Task 3b: Now, what if we select the values that are NOT
1.8. Which data would the dataset represent?

↓↓ your answer goes below

Task 3b answer:

If the values that are NOT 1.8, then it will remove all the values equal 1.8. Since 1.8 is the maximum petal width in the Iris Versicolor category, the remaining dataset will only include values less than 1.8. The remaining data still represents the Iris Versicolor category, but due to the missing data, the model's learning ability may be negatively affected, leading to a decrease in prediction accuracy.

↑↑ your answer goes above this

In [ ]:
```
not_1_8 = (X[:, 1]!=1.8) | (y==2)
X_tweaked = X[not_1_8]
y_tweaked = y[not_1_8]
```

Task 3c: Fit a new Decision Tree Classifier to these values
(`X_tweaked` , `y_tweaked`) with the initial parameter values
`max_depth = 2` and `random_state = 40` .

↓↓ your code goes below

In [ ]:
```
# tree_clf_tweaked
tree_clf_tweaked = DecisionTreeClassifier(max_depth=2, random_state=40)
tree_clf_tweaked.fit(X_tweaked,y_tweaked)
```

Out[ ]:

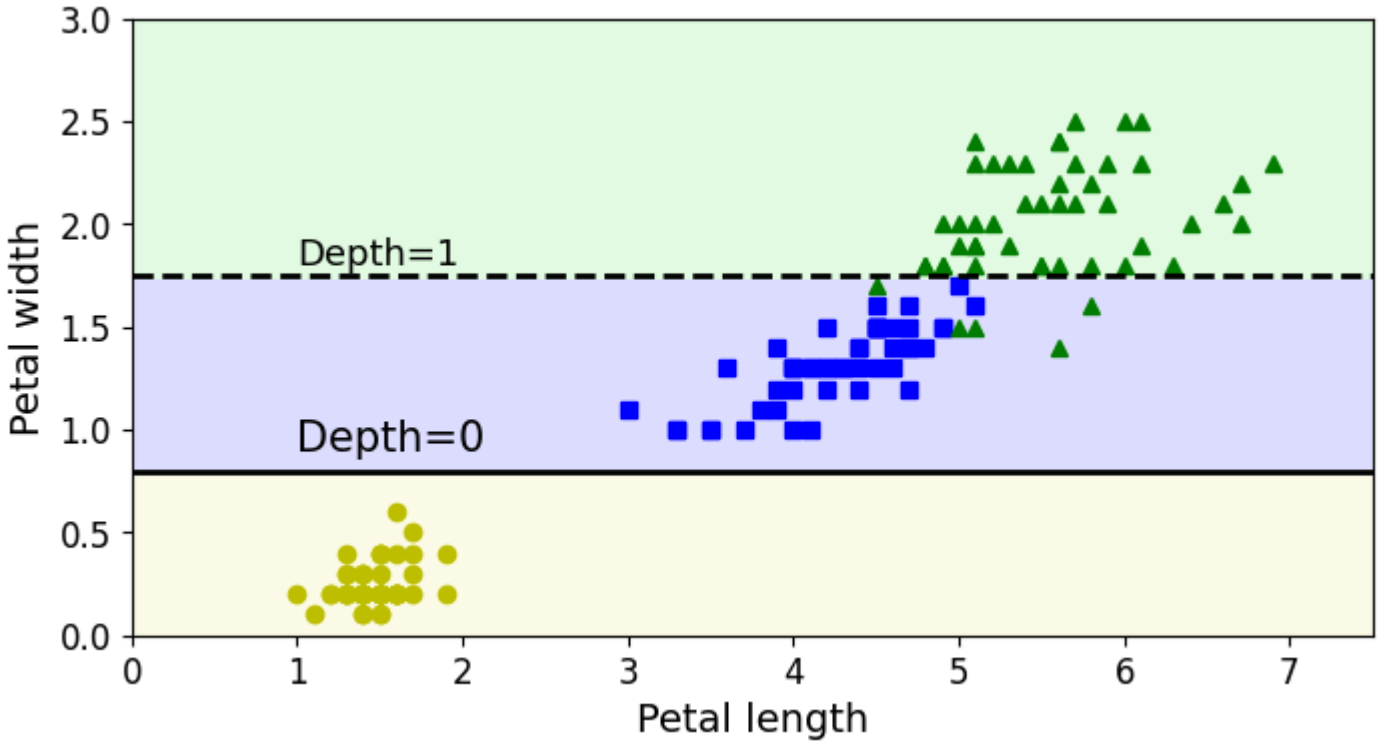
```
DecisionTreeClassifier(max_depth=2, random_state=40)
```

↑↑ your code goes above this

So now we have trained a new decision tree `tree_clf_tweaked` that has slightly different training data **(actually only *one* element less)**.
Let's visualize the new decision tree.

In [ ]:

```
plt.figure(figsize=(8, 4))
plot_decision_boundary(tree_clf_tweaked, X_tweaked, y_tweaked, legend=False)
plt.plot([0, 7.5], [0.8, 0.8], "k-", linewidth=2)
plt.plot([0, 7.5], [1.75, 1.75], "k--", linewidth=2)
plt.text(1.0, 0.9, "Depth=0", fontsize=15)
plt.text(1.0, 1.80, "Depth=1", fontsize=13)

plt.show()
```



Task 3d: Describe how the new decision tree is different from the one before.

↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓ your answer goes below

Task 3d answer: The new decision tree removed the samples with petal width = 1.8 from the Iris Versicolor category, but the two datasets remained unchanged in terms of the number of classes. The overall decision boundary has changed—the previous model was significantly influenced by both petal length and petal width, while the new model is primarily influenced by petal width. It demonstrates that decision trees are highly sensitive to changes in the dataset.

↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑ your answer goes above this

Regression Trees

In this subsection, we will be working with a regression task.
Notice that the dataset below is different. Here we are using a **training set generated by a quadratic function with the addition of some random noise**.

In [ ]:
```
np.random.seed(42)
m = 200
X = np.random.rand(m, 1)
y = 4 * (X - 0.5) ** 2
y = y + np.random.randn(m, 1) / 10
```

Task 4

Similar to what you've done above, create a decision tree regressor with the following hyperparameters:

- `max_depth=2`
- `random_state=42`

Fit it to `X`, `y`.

In [ ]:
```
from sklearn.tree import DecisionTreeRegressor
```

↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓ your code goes below

In [ ]:
```
# tree_reg =
```

In [ ]:
```
tree_reg = DecisionTreeRegressor(max_depth=2, random_state=42)
tree_reg.fit(X,y)
```

Out[ ]:
```
DecisionTreeRegressor
DecisionTreeRegressor(max_depth=2, random_state=42)
```

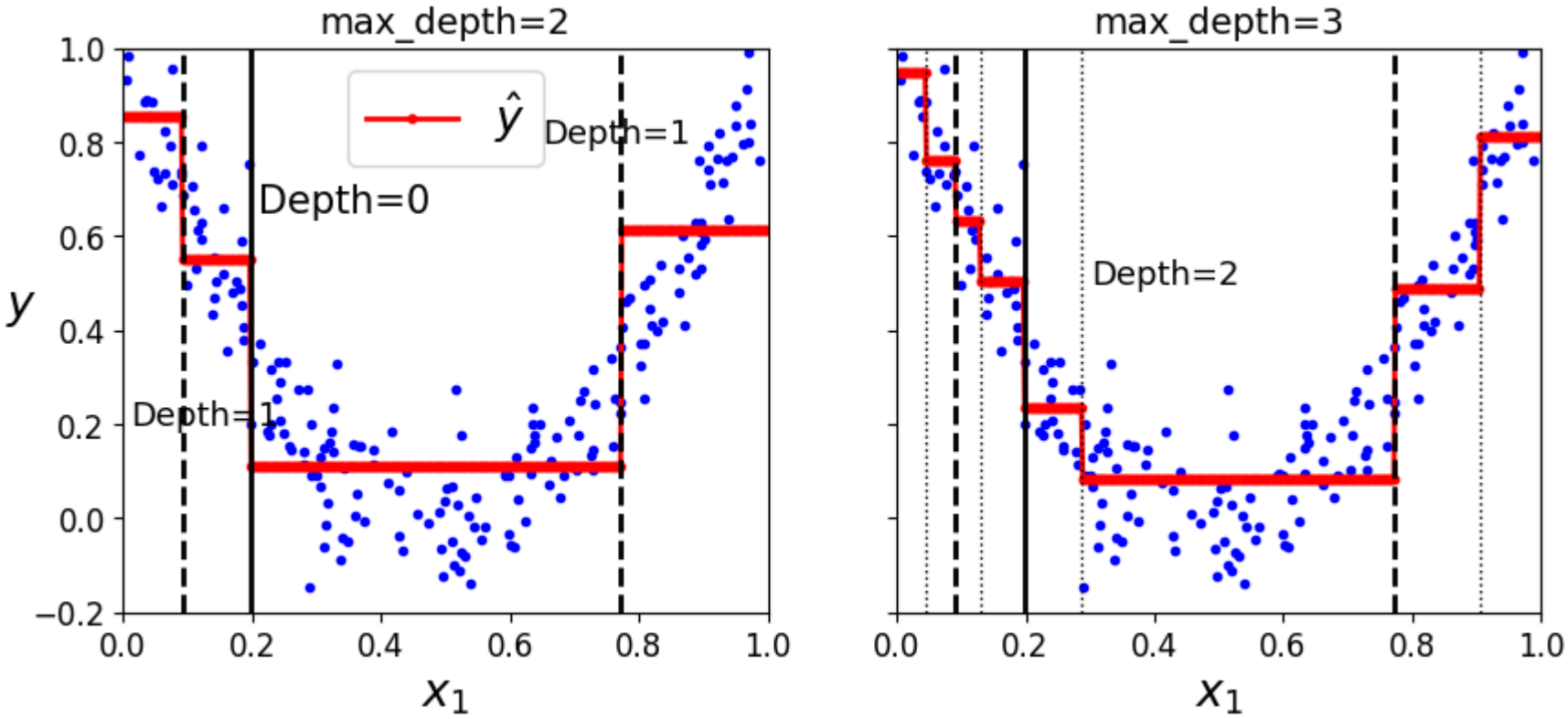
↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑ your code goes above this

Below, you'll see the difference in the prediction for an increased value of the `max_depth` parameter. What can you say about the results?

Again, the important thing is to understand the plots but not necessarilly all of the code

In [ ]:
```
from sklearn.tree import DecisionTreeRegressor

tree_reg1 = DecisionTreeRegressor(random_state=42, max_depth=2)
tree_reg2 = DecisionTreeRegressor(random_state=42, max_depth=3)
tree_reg1.fit(X, y)
tree_reg2.fit(X, y)

def plot_regression_predictions(tree_reg, X, y, axes=[0, 1, -0.2, 1], ylabel="$y$"):
    x1 = np.linspace(axes[0], axes[1], 500).reshape(-1, 1)
    y_pred = tree_reg.predict(x1)
    plt.axis(axes)
    plt.xlabel("$x_1$", fontsize=18)
    if ylabel:
        plt.ylabel(ylabel, fontsize=18, rotation=0)
    plt.plot(X, y, "b.")
    plt.plot(x1, y_pred, "r.-", linewidth=2, label=r"$\hat{y}$")

fig, axes = plt.subplots(ncols=2, figsize=(10, 4), sharey=True)
plt.sca(axes[0])
plot_regression_predictions(tree_reg1, X, y)
for split, style in ((0.1973, "k-"), (0.0917, "k--"), (0.7718, "k--")):
    plt.plot([split, split], [-0.2, 1], style, linewidth=2)
```

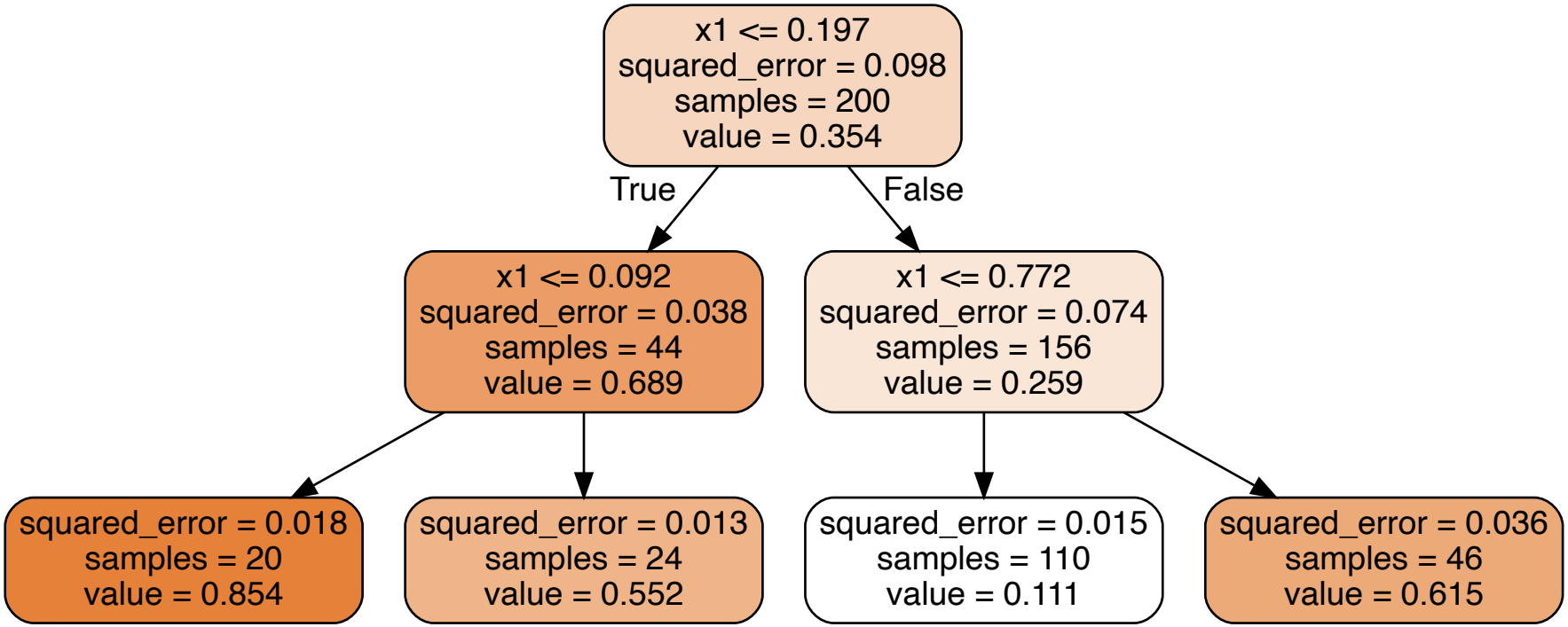
```
plt.text(0.21, 0.65, "Depth=0", fontsize=15)
plt.text(0.01, 0.2, "Depth=1", fontsize=13)
plt.text(0.65, 0.8, "Depth=1", fontsize=13)
plt.legend(loc="upper center", fontsize=18)
plt.title("max_depth=2", fontsize=14)

plt.sca(axes[1])
plot_regression_predictions(tree_reg2, X, y, ylabel=None)
for split, style in ((0.1973, "k-"), (0.0917, "k--"), (0.7718, "k--")):
    plt.plot([split, split], [-0.2, 1], style, linewidth=2)
for split in (0.0458, 0.1298, 0.2873, 0.9040):
    plt.plot([split, split], [-0.2, 1], "k:", linewidth=1)
plt.text(0.3, 0.5, "Depth=2", fontsize=13)
plt.title("max_depth=3", fontsize=14)

plt.show()
```



In [ ]:
```
export_graphviz(
        tree_reg1,
        out_file=os.path.join(IMAGES_PATH, "regression_tree.dot"),
        feature_names=["x1"],
```

```
        rounded=True,
        filled=True
    )
Source.from_file(os.path.join(IMAGES_PATH, "regression_tree.dot"))
```

Out[ ]:



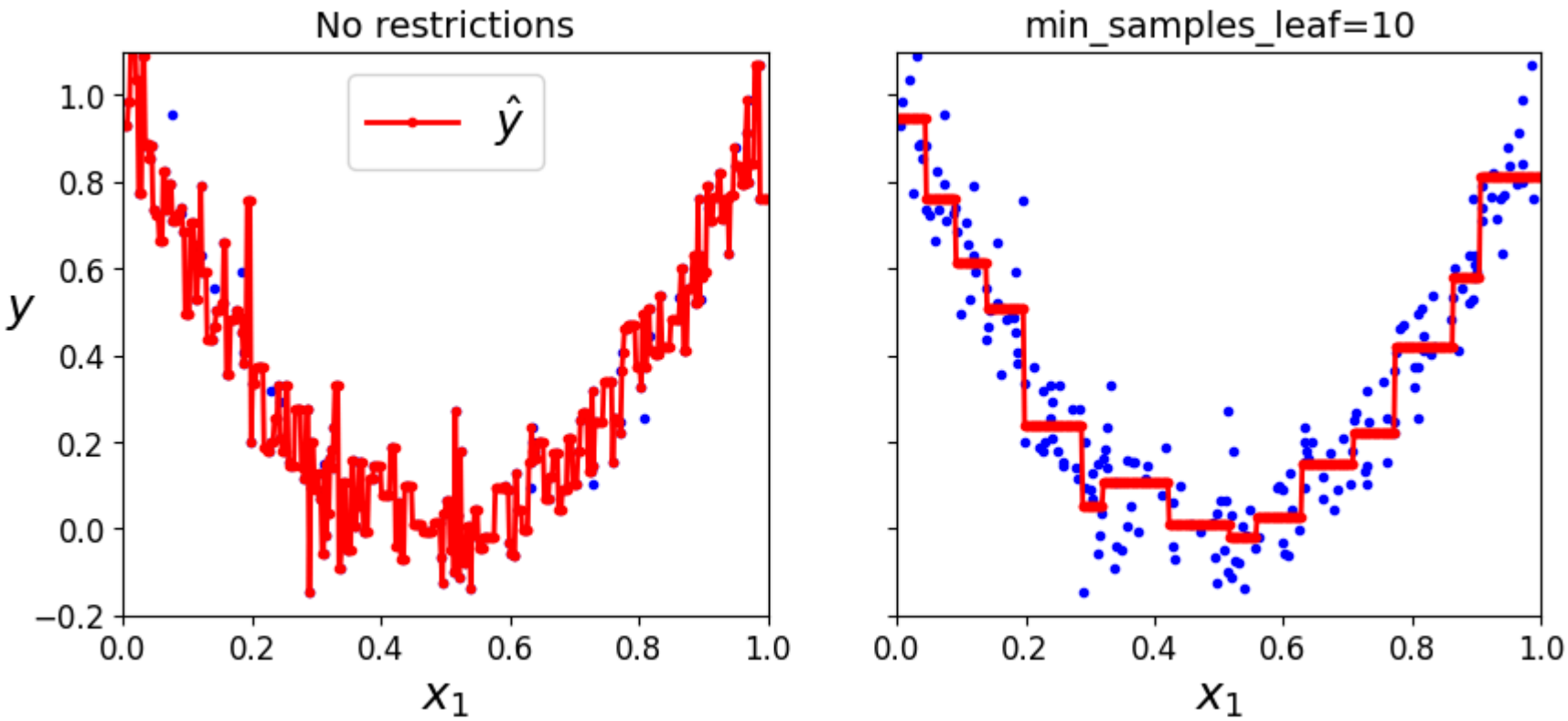
Restricting the Tree with `min_samples_leaf`

Here we are restricting the tree to `min_samples_leaf=10`. You can read about it in the documentation but basically it is adding the requirement that, before we end a branch, we need **10 data points** that fit **each side** of the final decision boundary.

In [ ]:

```
tree_reg1 = DecisionTreeRegressor(random_state=42)
tree_reg2 = DecisionTreeRegressor(random_state=42, min_samples_leaf=10)
tree_reg1.fit(X, y)
tree_reg2.fit(X, y)

x1 = np.linspace(0, 1, 500).reshape(-1, 1)
y_pred1 = tree_reg1.predict(x1)
y_pred2 = tree_reg2.predict(x1)
```

```
fig, axes = plt.subplots(ncols=2, figsize=(10, 4), sharey=True)

plt.sca(axes[0])
plt.plot(X, y, "b.")
plt.plot(x1, y_pred1, "r.-", linewidth=2, label=r"$\hat{y}$")
plt.axis([0, 1, -0.2, 1.1])
plt.xlabel("$x_1$", fontsize=18)
plt.ylabel("$y$", fontsize=18, rotation=0)
plt.legend(loc="upper center", fontsize=18)
plt.title("No restrictions", fontsize=14)

plt.sca(axes[1])
plt.plot(X, y, "b.")
plt.plot(x1, y_pred2, "r.-", linewidth=2, label=r"$\hat{y}$")
plt.axis([0, 1, -0.2, 1.1])
plt.xlabel("$x_1$", fontsize=18)
plt.title("min_samples_leaf={}".format(tree_reg2.min_samples_leaf), fontsize=14)

plt.show()
```



Task 5

Discuss the effect of the restrictions on the regression results.

↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓ your answer goes below

Task 5 answer:

Restrictions can effectively reduce overfitting risk, and improve generalization, which made the regression curve more smoothly and can predict better when the data has noise.

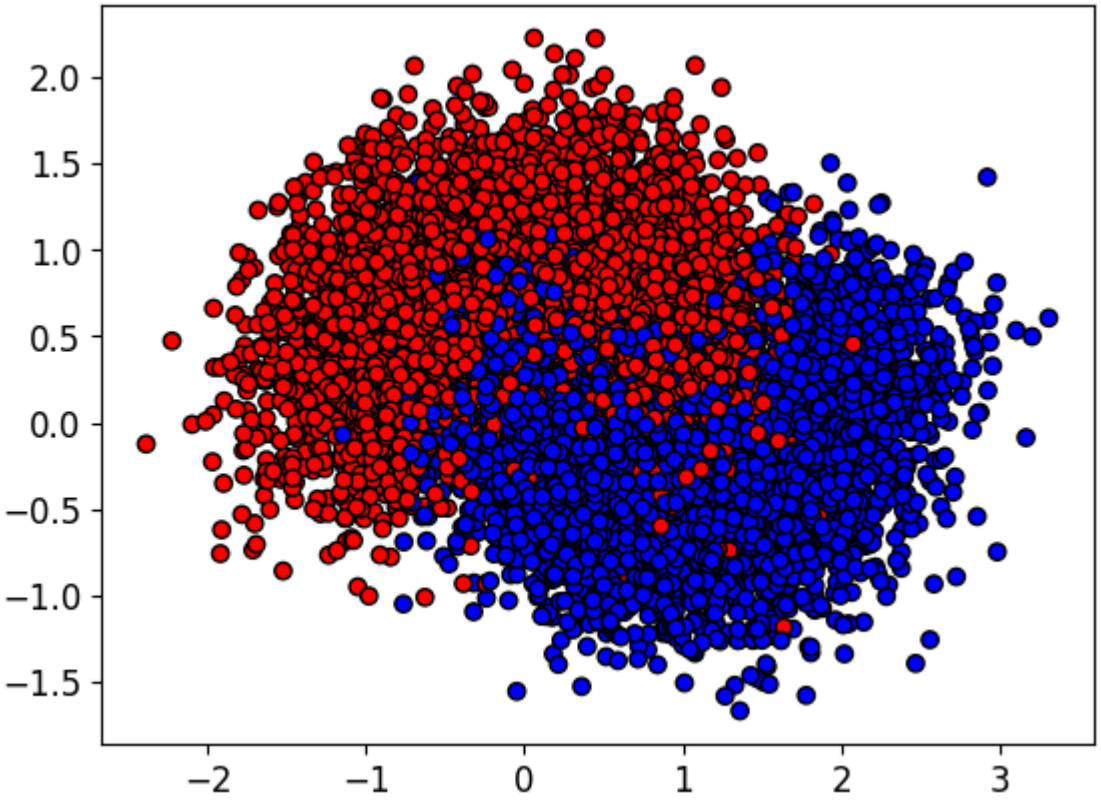
↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑ your answer goes above this

Random Forests

In this exercise you will be using the make_moons dataset. You can see a plot below. Basically, the tool generates fake data of two inter-leaving half-circles or "moons".

In [ ]:
```
from sklearn.datasets import make_moons

X, y = make_moons(n_samples=10000, noise=0.4, random_state=42)
```

In [ ]:
```
cm_bright = ListedColormap(["#FF0000", "#0000FF"])
plt.scatter(X[:,0], X[:,1], c=y, cmap=cm_bright, edgecolors="k");
```



Here we use train_test_split to split our fake data into 20% test and 80% train data.

In [ ]:
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
len(X_train)
```

Out[ ]:
```
8000
```

In [ ]:
```
tree_moons = DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
                        max_features=None, max_leaf_nodes=17,
                        min_impurity_decrease=0.0,
                        min_samples_leaf=1, min_samples_split=2,
                        min_weight_fraction_leaf=0.0,
                        random_state=42, splitter='best')
tree_moons.fit(X_train, y_train)
```

Out[ ]:
```
DecisionTreeClassifier(max_leaf_nodes=17, random_state=42)
```

In [ ]:
```
from sklearn.metrics import accuracy_score

y_pred_moons = tree_moons.predict(X_test)
accuracy_score(y_test, y_pred_moons)
```

Out[ ]:
```
0.8695
```

The decision tree trained with all data has an accuracy as shown above.
Now we will build a forest consisting of trees.

We will be building 100 `DecisionTreeClassifier`s.
First we do a train-test-split to get training and test data.

As you can see, the training data has a size of 8000 instances.
Let's generate 1000 subsets (mini-sets) of `X_train`, each containing 100 instances selected randomly. You may have noticed that that's more than 8000. We'll be reusing multiple datapoints.

Then we will train a separate tree on each of the mini-sets.

Task 6

Grow a forest.
You will have to get the following done, the way you implement it is your choice:

- Split `X_train` into 1000 subsets, each containing 100 instances selected randomly. You can use sklearn's ShuffleSplit for this.
- Train one Decision Tree on each subset. The hyperparameter values below work well:

```
class_weight=None, criterion='gini', max_depth=None,
                       max_features=None, max_leaf_nodes=17,
                       min_samples_leaf=1, min_samples_split=2,
```

```
                        min_weight_fraction_leaf=0.0,
                        random_state=42, splitter='best'
```

You might need `from sklearn.base import clone`. To clone the tree 1000 times.

- Calculate the accuracy on the test data `X_test`, `y_test` for each tree. What is the mean accuracy?
- Build a forest: For each test set instance, generate the predictions of the 1,000 Decision Trees, and keep only the most frequent prediction (you can use SciPy's `scipy.stats.mode()` function for this). This gives you *majority-vote predictions* over the test set. What is the accuracy of your forest? You should get a slightly better accuracy than the one tree trained on all training data.

If you struggle with this task for too long, then you can find the solution here under 8 (bottom of the notebook).

In order you should:

- Attempt to solve this as a group by looking up code documentation
- Raise your hand and ask for help
- Check the official book solutions only for parts of the task you are struggling with
- Look at, understand, and try to replicate the code from the solution

Do NOT directly copy the entire solution into this notebook.

In [ ]:
```
from sklearn.model_selection import ShuffleSplit
from sklearn.base import clone
from scipy.stats import mode


n_trees = 1000
n_instances = 100
mini_sets = []
```

↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓↓ your code goes below

In [ ]:
```
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
```

```python
import numpy as np
shuffle_split = ShuffleSplit(n_splits=n_trees, train_size=n_instances, random_state=42)
for train_idx, _ in shuffle_split.split(X_train):
  X_mini = X_train[train_idx]
  y_mini = y_train[train_idx]
  mini_sets.append((X_mini, y_mini))
tree_clf = DecisionTreeClassifier(
    criterion='gini', max_depth=None,
    max_features=None, max_leaf_nodes=17,min_samples_leaf=1, min_samples_split=2,
    random_state=42
    )
forest = [clone(tree_clf) for _ in range(n_trees)]
for tree,(X_mini, y_mini) in zip(forest, mini_sets):
  tree.fit(X_mini,y_mini)
accuracy_list = [accuracy_score(y_test, tree.predict(X_test)) for tree in forest]
mean_accuracy = np.mean(accuracy_list)
predictions = np.array([tree.predict(X_test) for tree in forest])
final_predictions = mode(predictions, axis=0).mode.flatten()
forest_accuracy = accuracy_score(y_test, final_predictions)
forest_accuracy
```

Out[ ]: 0.872

↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑ your code goes above this