lab3

December 4, 2018

1 COMP3222/6246 Machine Learning Technologies (2018/19)

1.1 Week 6 – Decision Trees, Random Forests, Ensemble Learning

Follow each code block at your own pace, you can have a look at the book or ask questions to demonstrators if you find something confusing.

2 Chapter 6 - Decision Trees

"*Decision Trees* are versatile Machine Learning algorithms that can perform both classification and regression tasks, and even multioutput tasks." [Geron2017]

```
In [2]: %matplotlib inline


        import numpy as np

        np.random.seed(42) # to ensure our results exactly like the book
```

2.1 6.1 Training and Visualizing a Decision Tree

First, let's load the iris dataset from sci-kit learn library.

```
In [3]: from sklearn.datasets import load_iris
        from sklearn.tree import DecisionTreeClassifier

        iris = load_iris()
```

2.1.1 6.1.1 Determine Targets

Let's determine which columns will be in our interest and print them.

```
In [4]: X = iris.data[:, 2:] # only focus on petal length and width
        Y = iris.target
        feature_names = iris.feature_names[2:]
        print("given:",feature_names,
              "\npredict whether:", iris.target_names)
```

```
given: ['petal length (cm)', 'petal width (cm)']
predict whether: ['setosa' 'versicolor' 'virginica']
```

2.1.2 Exercise 6.1.1: Plot the data set

Plot the data set and have a look at the two features that are selected.

```
In [5]: # use matplotlib as you did on previous labs
```

2.1.3 6.1.2 Train the dataset

Without separating the dataset as we did in previous labs, let's use all the data set and train the decision tree.

```
In [6]: tree_clf = DecisionTreeClassifier(max_depth=2)
        tree_clf.fit(X,Y)

Out[6]: DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=2,
                    max_features=None, max_leaf_nodes=None,
                    min_impurity_decrease=0.0, min_impurity_split=None,
                    min_samples_leaf=1, min_samples_split=2,
                    min_weight_fraction_leaf=0.0, presort=False, random_state=None,
                    splitter='best')
```

There are many hyperparameters that a decision tree classifier has. You can see from the ouput above the parameters that will be used for predictions. Two criterions that you can use with decision trees in sci-kit learn. These metrics are calculated in each node of decision tree. * **Gini impurity** `criterion='gini'` is a measure of how often a randomly chosen element from a set would be incorrectly labeled. Formally it is computed by:

$$I_G(p) = \sum_{i=1}^{J} p_i \sum_{k \neq i} p_k$$

where J denotes classes and p_i is the fraction of items which are labeled with class i. For a concrete example have a look: https://stats.stackexchange.com/a/339514 * **Information Gain** `criterion='entropy'` is a mesaure of entropy, which is used in thermodynamics as a measure of molecular disorder. Entropy=0 means the molecules are well ordered.

$$H(T) = I_E(p) = -\sum_{i=1}^{J} p_i \log_2 p_i$$

$p_1, p_2, ...$ as in gini impurity are the fractions that add up to 1.

These two metrics are used for deciding the splits while training a decision tree.

2.1.4 Exercise 6.1.2: Gini or Entropy

- Should you use Gini impurity or entropy?
- Which one is faster to compute and why?
- Visualize the tree that you trained above in 6.1.2.

- Why does *gini impurity* metric decrease in deeper nodes?
- Which cases do you see that the metric is zero?

Your answer here

2.1.5 6.1.2 Visualization

You can export the decision tree as a `dot` file from sci-kit learn. You can convert `dot` to `png` image by installing `graphviz`.

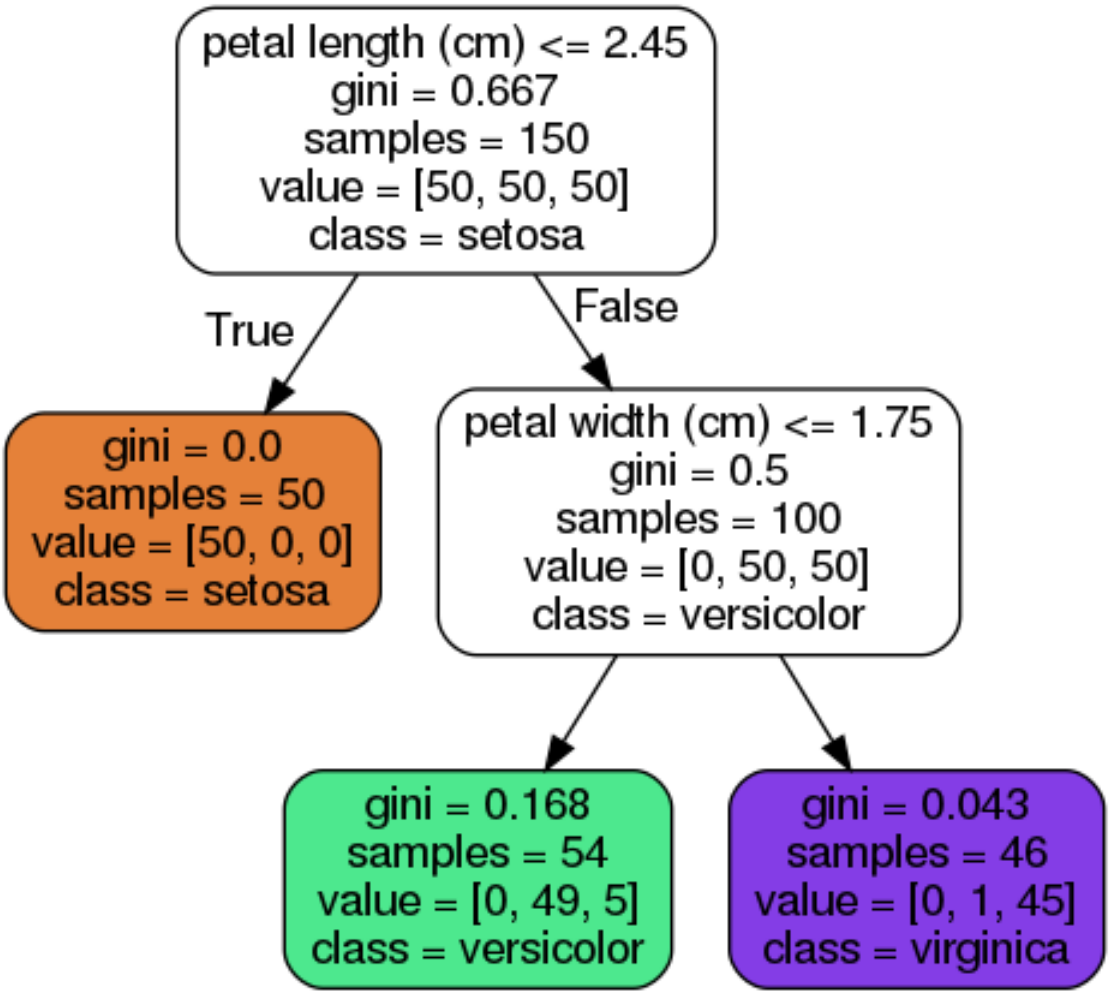
```
In [7]: from sklearn.tree import export_graphviz
        export_graphviz(tree_clf,
                        out_file="iris_tree.dot",
                        feature_names=feature_names,
                        class_names=iris.target_names,
                        rounded=True,
                        filled=True
                       )
```

```
In [8]: # Make sure you installed graphviz (exclamation mark is for shell commands)
        !apt install graphviz

        # Convert dot file to png file.
        !dot -Tpng iris_tree.dot -o iris_tree.png
```

```
E: Could not open lock file /var/lib/dpkg/lock - open (13: Permission denied)
E: Unable to lock the administration directory (/var/lib/dpkg/), are you root?
```

```
In [9]: from IPython.display import Image
        Image(filename='iris_tree.png')
```

```
Out[9]:
```



To see a better visualization example of decision trees, have a look at this page.

2.1.6 Extra: Another way to visualize decision trees

There is a brand new visualization library from creators of ANTLR (parser generator) for decision trees called `dtreeviz`. You can find some other examples from their repository for better visualization. Follow the steps below:

```
In [10]: # install the package
         !pip install dtreeviz
         # (optional)
         !apt-get install msttcorefonts -qq
```

```
Requirement already satisfied: dtreeviz in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/p
Requirement already satisfied: pandas in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/pyt
Requirement already satisfied: matplotlib in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib
Requirement already satisfied: scikit-learn in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/l
Requirement already satisfied: graphviz>=0.9 in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/
```

```
Requirement already satisfied: numpy in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/pytl
Requirement already satisfied: python-dateutil>=2.5.0 in /home/tdgunes/Projects/COMP6246-2018Fa
Requirement already satisfied: pytz>=2011k in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/li
Requirement already satisfied: pyparsing!=2.0.4,!=2.1.2,!=2.1.6,>=2.0.1 in /home/tdgunes/Projec
Requirement already satisfied: kiwisolver>=1.0.1 in /home/tdgunes/Projects/COMP6246-2018Fall/.v
Requirement already satisfied: cycler>=0.10 in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/l
Requirement already satisfied: scipy>=0.13.3 in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/
Requirement already satisfied: six>=1.5 in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/p
Requirement already satisfied: setuptools in /home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib
E: Could not open lock file /var/lib/dpkg/lock - open (13: Permission denied)
E: Unable to lock the administration directory (/var/lib/dpkg/), are you root?
```

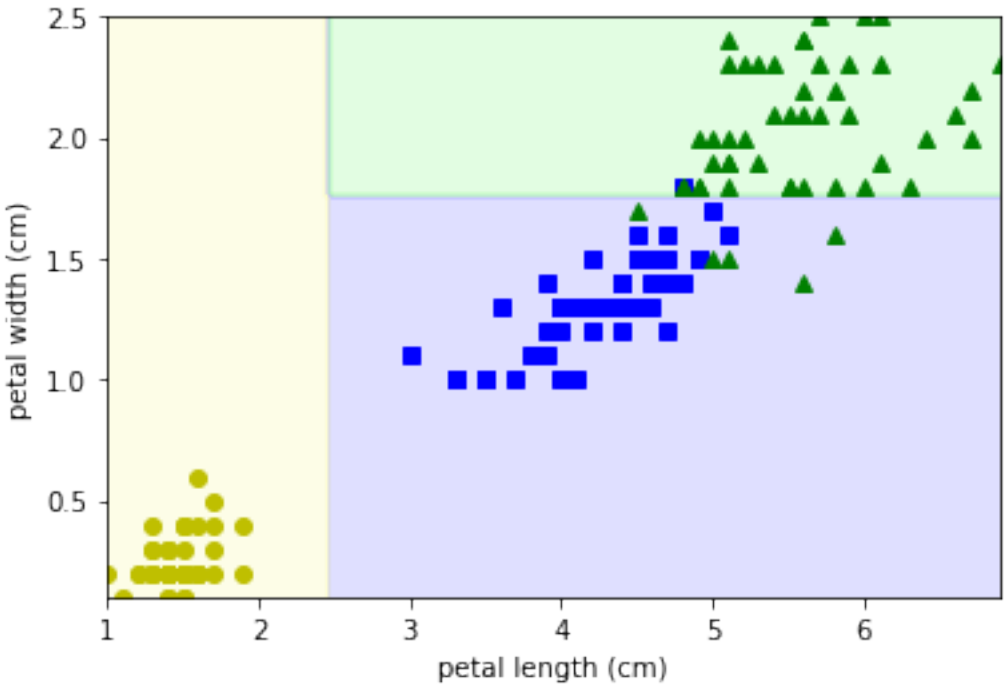
```
In [11]: from dtreeviz.trees import dtreeviz
         import matplotlib as mpl

         mpl.rcParams['axes.facecolor'] = 'white'
         viz = dtreeviz(tree_clf,
                        X,
                        Y,
                        target_name='flower type',
                        feature_names=feature_names,
                        class_names=list(iris.target_names),
                        fancy=True,
                        orientation ='TD')

         # uncomment this
         # viz
```

```
/home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/python3.6/site-packages/matplotlib/font_mana
  (prop.get_family(), self.defaultFamily[fontext]))
```

2.1.7 6.1.3 Plot training data set

```
In [12]: import matplotlib.pyplot as plt
         from matplotlib.colors import ListedColormap
         CUSTOM_CMAP = ListedColormap(['#fafab0','#9898ff','#a0faa0'])

         # helper function to plot the boundaries
         def plot_decision_boundary(clf, x, y):
             color_map = ["yo", "bs", "g^"]
             for target_index, target_name in enumerate(iris.target_names):
                 plt.plot(x[:, 0][y==target_index], # petal length on X axis (the ones that eq
                          x[:, 1][y==target_index], # petal width on Y axis (the ones that equ
                          color_map[target_index],
                          label=target_name)
```

```
    x1s = np.linspace(np.min(x[:, 0]), np.max(x[:, 0]), 100)
    x2s = np.linspace(np.min(x[:, 1]), np.max(x[:, 1]), 100)
    x1, x2 = np.meshgrid(x1s, x2s)
    x_test = np.c_[x1.ravel(), x2.ravel()]
    y_pred = clf.predict(x_test).reshape(x1.shape)
    plt.contourf(x1, x2, y_pred, alpha=0.3, cmap=CUSTOM_CMAP)

plot_decision_boundary(tree_clf, X, Y)

plt.xlabel(feature_names[0]) # petal length (cm)
plt.ylabel(feature_names[1]) # petal width (cm)
plt.show()
```



2.1.8 Exercise 6.1: Plot decision boundaries

1. Write down which colour correspond to which node in the decision tree.
2. Try to increase/decrease `max_depth` of decision tree classifier and observe the changes in the decision boundaries. What would you set `max_depth`?
3. If the helper function (`plot_decision_boundary`) was not available to you, how would you visualize the decision boundaries? Tip: try to create X's that ranges from $[1, 0]$ to $[7, 2.5]$ where. You can use:

```
In [13]: # check np.mgrid[minX1:maxX1:increment, minX2:maxX2:increment]
         X = np.mgrid[0:10:1, -5:0:1].reshape(2,-1).T
         X
```

```
Out[13]: array([[ 0, -5],
                [ 0, -4],
                [ 0, -3],
                [ 0, -2],
                [ 0, -1],
                [ 1, -5],
                [ 1, -4],
                [ 1, -3],
                [ 1, -2],
                [ 1, -1],
                [ 2, -5],
                [ 2, -4],
                [ 2, -3],
                [ 2, -2],
                [ 2, -1],
                [ 3, -5],
                [ 3, -4],
                [ 3, -3],
                [ 3, -2],
                [ 3, -1],
                [ 4, -5],
                [ 4, -4],
                [ 4, -3],
                [ 4, -2],
                [ 4, -1],
                [ 5, -5],
                [ 5, -4],
                [ 5, -3],
                [ 5, -2],
                [ 5, -1],
                [ 6, -5],
                [ 6, -4],
                [ 6, -3],
                [ 6, -2],
                [ 6, -1],
                [ 7, -5],
                [ 7, -4],
                [ 7, -3],
                [ 7, -2],
                [ 7, -1],
                [ 8, -5],
                [ 8, -4],
                [ 8, -3],
                [ 8, -2],
                [ 8, -1],
                [ 9, -5],
                [ 9, -4],
                [ 9, -3],
```

```
                [ 9, -2],
                [ 9, -1]])
```

2.1.9 Exercise 6.1a: Solution

```
In [14]: # Tip: try each point in the space
```

2.1.10 6.1.4 Estimating Class Probabilities

To estimate the probability of an instance belongs to a class, you can use `predict_proba`, to determine the class that an instance will be assigned to use `predict`.

```
In [15]: tree_clf.predict_proba([[5, 1.5]])
```

```
Out[15]: array([[0.        , 0.90740741, 0.09259259]])
```

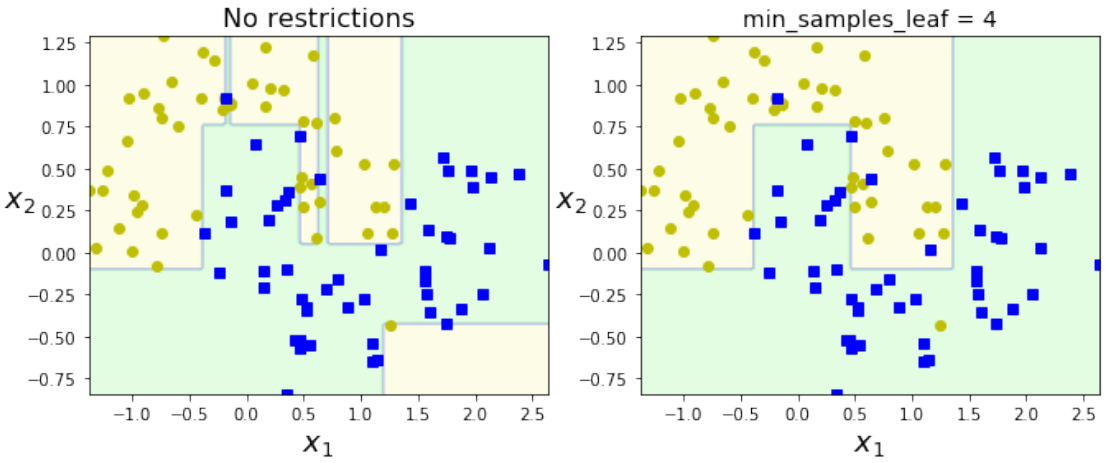
```
In [16]: tree_clf.predict([[5, 1.5]])
```

```
Out[16]: array([1])
```

2.1.11 6.1.5 Regularization Hyperparameters

"Constraining a model to make it simpler and reduce the risk of overfitting is called _regularization" [Geron2017, page 27] To avoid overfitting, you can limit the generation of a node by `min_samples_leaf` (the minimum samples that a node must have to able to be splitted.).

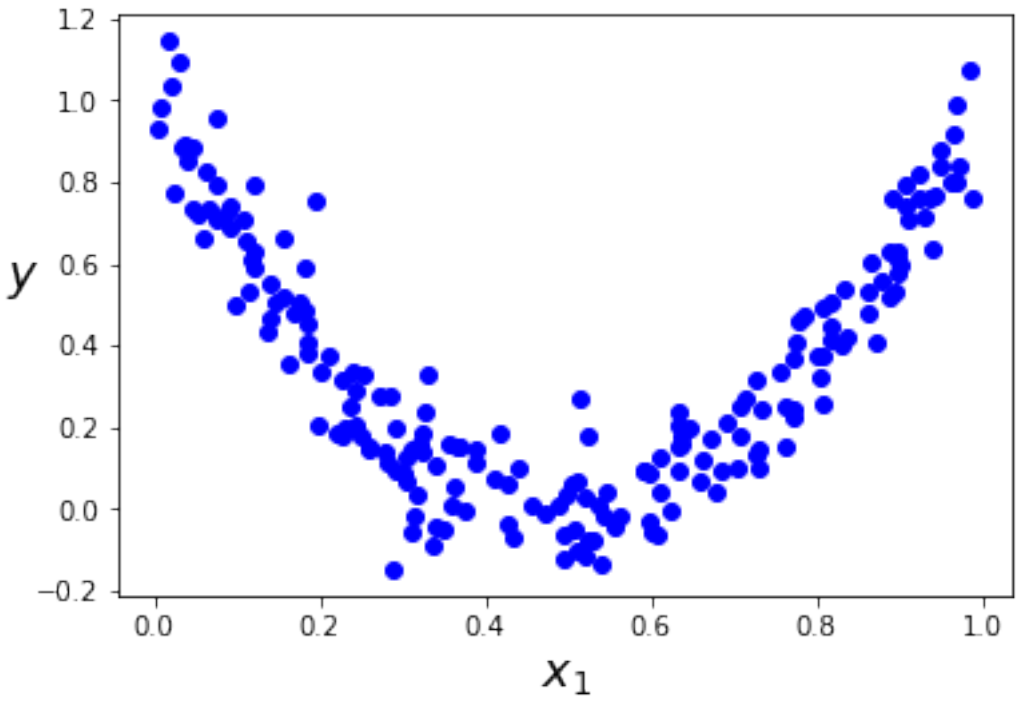
```
In [17]: from sklearn.datasets import make_moons
         Xm, ym = make_moons(n_samples=100, noise=0.25, random_state=53)

         deep_tree_clf1 = DecisionTreeClassifier(random_state=42)
         deep_tree_clf2 = DecisionTreeClassifier(min_samples_leaf=4, random_state=42)
         deep_tree_clf1.fit(Xm, ym)
         deep_tree_clf2.fit(Xm, ym)

         plt.figure(figsize=(11, 4))
         plt.subplot(121)

         plt.xlabel(r"$x_1$", fontsize=18)
         plt.ylabel(r"$x_2$", fontsize=18, rotation=0)
         plot_decision_boundary(deep_tree_clf1, Xm, ym)
         plt.title("No restrictions", fontsize=16)
         plt.subplot(122)

         plt.xlabel(r"$x_1$", fontsize=18)
         plt.ylabel(r"$x_2$", fontsize=18, rotation=0)
         plot_decision_boundary(deep_tree_clf2, Xm, ym)
         plt.title("min_samples_leaf = {}".format(deep_tree_clf2.min_samples_leaf), fontsize=1


         plt.show()
```



2.2 6.2 Regression

Decision trees can be used for regression tasks too. Instead of predicting a class, in regression tasks, the aim is to predict a numberic value (such as the price of a car). Assume that we have this quadratic data set with some noise:

```
In [18]: # Quadratic training set + noise
         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

         plt.plot(X, Y, "bo")
         plt.xlabel("$x_{1}$", fontsize=18)
         plt.ylabel("$y$", fontsize=18, rotation=0)
         plt.show()
```




```
In [19]: from sklearn.tree import DecisionTreeRegressor
         tree_reg = DecisionTreeRegressor(max_depth=2)
         tree_reg.fit(X,Y)
```

```
Out[19]: DecisionTreeRegressor(criterion='mse', max_depth=2, max_features=None,
                    max_leaf_nodes=None, min_impurity_decrease=0.0,
                    min_impurity_split=None, min_samples_leaf=1,
                    min_samples_split=2, min_weight_fraction_leaf=0.0,
                    presort=False, random_state=None, splitter='best')
```

2.2.1 Exercise 6.2: Visualize the regression tree

1. Visualize the regression tree same as before with *graphviz*.
2. Plot this regression tree (Tip: try many values for x (e.g. `np.linspace(min, max, noOfPoints)`)
3. Plot the decision boundaries of `max_depth=2` and `max_depth=3` regression trees (also try `min_samples_leaf=10`)
4. Compare the differences on the difference plots. Notice that the average is taken in the regions which are separated by the decision tree regressor.

```
In [20]: # Tips for 6.2.2:
         Xs = np.linspace(0, 1, 100)
         Xs
         # predict Y values for Xs and plot
```

```
Out[20]: array([0.        , 0.01010101, 0.02020202, 0.03030303, 0.04040404,
                0.05050505, 0.06060606, 0.07070707, 0.08080808, 0.09090909,
                0.1010101 , 0.11111111, 0.12121212, 0.13131313, 0.14141414,
                0.15151515, 0.16161616, 0.17171717, 0.18181818, 0.19191919,
                0.2020202 , 0.21212121, 0.22222222, 0.23232323, 0.24242424,
                0.25252525, 0.26262626, 0.27272727, 0.28282828, 0.29292929,
                0.3030303 , 0.31313131, 0.32323232, 0.33333333, 0.34343434,
                0.35353535, 0.36363636, 0.37373737, 0.38383838, 0.39393939,
                0.4040404 , 0.41414141, 0.42424242, 0.43434343, 0.44444444,
                0.45454545, 0.46464646, 0.47474747, 0.48484848, 0.49494949,
                0.50505051, 0.51515152, 0.52525253, 0.53535354, 0.54545455,
                0.55555556, 0.56565657, 0.57575758, 0.58585859, 0.5959596 ,
                0.60606061, 0.61616162, 0.62626263, 0.63636364, 0.64646465,
                0.65656566, 0.66666667, 0.67676768, 0.68686869, 0.6969697 ,
                0.70707071, 0.71717172, 0.72727273, 0.73737374, 0.74747475,
                0.75757576, 0.76767677, 0.77777778, 0.78787879, 0.7979798 ,
                0.80808081, 0.81818182, 0.82828283, 0.83838384, 0.84848485,
                0.85858586, 0.86868687, 0.87878788, 0.88888889, 0.8989899 ,
                0.90909091, 0.91919192, 0.92929293, 0.93939394, 0.94949495,
                0.95959596, 0.96969697, 0.97979798, 0.98989899, 1.        ])
```

```
In [ ]:
```

3 Chapter 7: Ensemble Learning and Random Forests

Instead of using a single predictor, to improve our predictions we use now use *an ensemble*: **a group of predictors**. It is as if you are asking a number of experts opinion about a problem and you aggregate their answers.

3.1 7.1 Voting Classifiers

A brief comparision between `soft` voting and `hard` voting with using three predictors.

```
In [21]: from sklearn.model_selection import train_test_split
         from sklearn.datasets import make_moons

         X, Y = make_moons(n_samples=500, noise=0.30, random_state=42)
         X_train, X_test, Y_train, Y_test = train_test_split(X, Y, random_state=42)
```

Helper function for printing accuracies on test set

```
In [22]: from sklearn.metrics import accuracy_score
         def test_clfs(*clfs): # clf -> classifier
             for clf in clfs:
                 clf.fit(X_train, Y_train) # train the classifier
                 Y_pred = clf.predict(X_test)
                 print(clf.__class__.__name__ + ":", accuracy_score(Y_test, Y_pred))
```

Let's test `hard` voting first.

```
In [23]: from sklearn.ensemble import RandomForestClassifier
         from sklearn.ensemble import VotingClassifier
         from sklearn.linear_model import LogisticRegression
         from sklearn.svm import SVC

         # Don't worry about the warnings,
         # sci-kit community will be fixing it in the next major version 0.20.0

         log_clf = LogisticRegression(random_state=42)
         rnd_clf = RandomForestClassifier(random_state=42)
         svm_clf = SVC(random_state=42, probability=True)

         voting_clf = VotingClassifier(estimators=[('lr', log_clf),
                                                   ('rf', rnd_clf),
                                                   ('svc', svm_clf)],
                                       voting='hard')
         test_clfs(log_clf, rnd_clf, svm_clf, voting_clf)
```

```
LogisticRegression: 0.864
RandomForestClassifier: 0.872
SVC: 0.888
VotingClassifier: 0.896


/home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/python3.6/site-packages/sklearn/linear_model
  FutureWarning)
/home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/python3.6/site-packages/sklearn/ensemble/for
  "10 in version 0.20 to 100 in 0.22.", FutureWarning)
/home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/python3.6/site-packages/sklearn/svm/base.py
  "avoid this warning.", FutureWarning)
/home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/python3.6/site-packages/sklearn/linear_model
  FutureWarning)
/home/tdgunes/Projects/COMP6246-2018Fall/.venv/lib/python3.6/site-packages/sklearn/svm/base.py
  "avoid this warning.", FutureWarning)
```

3.1.1 Exercise 7.1: Which voting to pick?

1. Check the `soft` voting and compare the results. Why do you think it is different?

If you don't know the difference have a look at your book, page 186.
Your answer here:

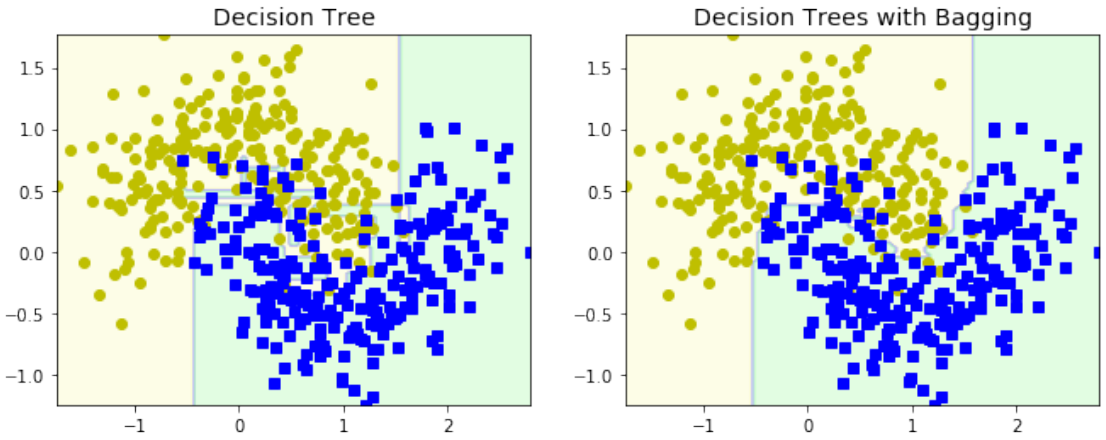
3.2 7.2 Bagging & Pasting

Instead of giving training set to each predictor in our ensemble, another approach to gain more accuracy is to separate the training set and give a different training subset to each predictor. There are two ways: * **Bagging:** (*bootstrapping in statistics*) picking a random subset from training set and not removing this selected set from training set for each predictor, i.e. **sampling with replacement**

* **Pasting:** picking a random subset from training set and removing this selected set from the training set for each predictor, i.e. **sampling without replacement** If you are still confused, have a look at here.

```
In [24]: from sklearn.ensemble import BaggingClassifier
         from sklearn.tree import DecisionTreeClassifier

         # define our decision tree classifier
         tree_clf = DecisionTreeClassifier(random_state=42)
         # 500 copies of the predictor, which has 100 samples from training set
         # n_jobs=-1 for utilizing all cores
         bag_clf = BaggingClassifier(tree_clf,
                                     n_estimators=500,
                                     max_samples=100,
                                     bootstrap=True,
                                     n_jobs=-1,
                                     random_state=42)

         # fit the bagging classifier
         bag_clf.fit(X_train, Y_train)
         tree_clf.fit(X_train, Y_train)

         Y_pred_bag = bag_clf.predict(X_test)
         Y_pred_tree = tree_clf.predict(X_test)

         from sklearn.metrics import accuracy_score
         print("Bagging Classifier")
         print(accuracy_score(Y_test, Y_pred_bag))
         print("Decision Tree Classifier")
         print(accuracy_score(Y_test, Y_pred_tree))

         plt.figure(figsize=(11,4))
         plt.subplot(121)
         plot_decision_boundary(tree_clf, X, Y)
         plt.title("Decision Tree", fontsize=14)
         plt.subplot(122)
         plot_decision_boundary(bag_clf, X, Y)
         plt.title("Decision Trees with Bagging", fontsize=14)
         plt.show()
```

```
Bagging Classifier
0.904
Decision Tree Classifier
0.856
```



3.2.1 7.2 Exercise: Bagging or Pasting

- What is the difference between these two techniques which select a subset of a training set?
- When do you think it is better to use bagging or pasting?

3.3 7.3 Gradient Boosting

In Gradient Boosting, we start with a single predictor. Sequentially, we add new predictors to *an ensemble* that corrects its predecessor. In detail:

The algorithm is for `3 predictors` in our ensemble: 1. Pick a set of weak predictors (e.g. DecisionTreeRegressor(max_depth=2)) - For this example, it is 3. 2. Train the initial predictor on training set 3. Train the second predictor on residual errors (use only errors, i.e. `y2 = y - predictor1.predict(X)`) 3. Train the third predictor on the residual errors of the second predictor 4. Use all predictors and sum their predictions (if regression)

3.3.1 Exercise 7.3: Implement, Plot and Compare

1. Implement this boosting technique that is explained above with `n` predictors.
    - Use the `quadratic training set` as a regression task.
    - Use `DecisionTreeRegressor(max_depth=2)` as a weak predictor
2. For $n = 3$, plot step by step the evolution of the ensemble predictions
    - First figure with only one predictor
    - Second figure with two predictors
    - Third figure with three predictors
3. Use sci-kit learn's `GradientBoostingRegressor` and compare if your results are similiar.
4. Do you think this boosting technique is scalable in practice?

Tips: - **Plotting**: this is similar as before in Regression section 6.2, as explained earlier. - **GradientBoostingRegressor**: use this code snippet:

```
from sklearn.ensemble import GradientBoostingRegressor
gbrt = GradientBoostingRegressor(max_depth=2, n_estimators=3, learning_rate=1.0)
gbrt.fit(X,Y)
```

```
In [25]: # Your implementation here
```

3.4 Recap

At this point, we demonstrated these concepts:

- training and visualizing various models from Decision Trees and Ensemble Learning
- details about some hyperparameters and how to regularize the models
- different training methods for ensemble learning
- how a boosting technique works and its properties.

Of course, there are some material that we have not be able to cover. In your free time, it can be better to have a look at:

- **Decision Trees**
- How hard is it to find the best split to construct the *optimal tree*?
- Why is CART algorithm called *a greedy algorithm*?
- **Ensemble Learning and Random Forests**
- Difference between Extra-Trees and Random Forests
- How does AdaBoost work?
- Learning Feature Importance with Random Forests
- What is `Stacking`?

```
In [ ]:
```