Hands-On #4

Chapter 7 – Ensemble Learning and Random Forests

File name convention: For group 42 and memebers Richard Stallman and Linus Torvalds it would be "04_Random_Forests_Stallman_Torvalds.pdf".

Submission via blackboard (UA).

Feel free to answer free text questions in text cells using markdown and possibly $L\!\!\!/ T_F X$ 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

```
import sys
import sklearn
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
from matplotlib.colors import ListedColormap

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

You don't need to understand the next 3 code blocks

Let's create some functions we'll need for the following tasks. plot_digit plots a 28x28 image as if it were a heatmap. plot_decision_boundary plots a decision boundary as we saw last week. plot_predictions plots predictions made by one regressor or the sum of multiple regressors on a single plot.

```
In [ ]: def plot digit(data):
            image = data.reshape(28, 28)
            plt.imshow(image, cmap = mpl.cm.hot,
                       interpolation="nearest")
            plt.axis("off")
In []: def plot decision boundary(clf, X, y, axes=[-1.5, 2.45, -1, 1.5],
                                    alpha=0.5, contour=True):
            x1s = np.linspace(axes[0], axes[1], 100)
            x2s = np.linspace(axes[2], axes[3], 100)
            x1, x2 = np.meshgrid(x1s, x2s)
            X \text{ new} = \text{np.c } [x1.ravel(), x2.ravel()]
            v 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 contour:
                custom cmap2 = ListedColormap(['#7d7d58','#4c4c7f','#507d50'])
                plt.contour(x1, x2, y_pred, cmap=custom_cmap2, alpha=0.8)
            plt.plot(X[:, 0][y==0], X[:, 1][y==0], "yo", alpha=alpha)
            plt.plot(X[:, 0][y==1], X[:, 1][y==1], "bs", alpha=alpha)
            plt.axis(axes)
            plt.xlabel(r"$x 1$", fontsize=18)
            plt.ylabel(r"$x 2$", fontsize=18, rotation=0)
In [ ]: def plot_predictions(regressors, X, y, axes, label=None, style="r-",
                              data_style="b.", data_label=None):
            x1 = np.linspace(axes[0], axes[1], 500)
            y_pred = sum(regressor.predict(x1.reshape(-1, 1))  for regressor in regressors)
            plt.plot(X[:, 0], y, data_style, label=data_label)
            plt.plot(x1, y_pred, style, linewidth=2, label=label)
            if label or data label:
                plt.legend(loc="upper center", fontsize=16)
            plt.axis(axes)
```

Task 1

Task 1a)

As we did in the last assignment, load the moon dataset with 500

```
train_test_split on it. Use the default split value of 25% test.
In [ ]: from sklearn.model selection import train test split
         from sklearn.datasets import make moons
         In []: X, y = make moons(n samples=500, noise=0.3, random state=42)
        X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)
         \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow your code goes above this
         Now, we are going to build a voting classifier with the following estimators:

    logistic regression (solver="lbfgs", random_state=42)

          • random forest classifier ( n estimators=100, random state=42 )
          svc (gamma="scale", random_state=42)
         Task 1b)
         Initialize those three objects with the given parameters.
        from sklearn.ensemble import RandomForestClassifier
         from sklearn.linear model import LogisticRegression
         from sklearn.svm import SVC
         In [ ]: log_clf = LogisticRegression(solver="lbfgs", random_state=42)
         rnd_clf = RandomForestClassifier(n_estimators=100, random_state=42)
         svm_clf = SVC(gamma="scale", random_state=42)
         In [ ]: from sklearn.ensemble import VotingClassifier
In [ ]: voting_clf = VotingClassifier(
             estimators=[('lr', log_clf), ('rf', rnd_clf), ('svc', svm_clf)],
             voting='hard')
```

samples, 0.3 for the noise value, and random state to 42. Also, perform

Task 1c)

Explain voting='hard" in the VotingClassifier. What is soft voting?

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Task 1c) answer:

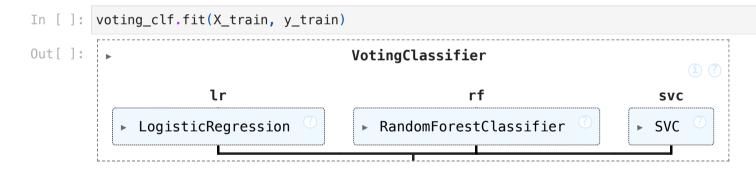
The parameter voting='hard' means that the classifier follows a hard voting strategy. The final prediction is determined by majority voting, meaning the class that gets the most votes from the three individual models is selected.

Soft voting works as follows: each individual classifier outputs class probabilities. The final prediction is based on the average predicted probability across all classifiers. The class with the highest averaged probability is chosen as the final prediction.

 \uparrow your answer goes above this

Task 1d)

Finally, fit the voting classifier to your train dataset.



 \uparrow your code goes above this

Task 2

Now we are going to print out the accuracy scores for each of the classifier above.

Complete the code below as indicated in the comments.

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

for clf in (log_clf, rnd_clf, svm_clf, voting_clf):
        clf.fit(X_train, y_train)
        # predict the y_test with each classifier
        y_pred = clf.predict(X_test)
        # calculate the accuracy score for each
        classifier_accuracy_score = accuracy_score(y_test, y_pred)
        # finally, we will print them out
        print(clf.__class__.__name__, classifier_accuracy_score)
```

LogisticRegression 0.864
RandomForestClassifier 0.896
SVC 0.896
VotingClassifier 0.912

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Task 3: Soft voting

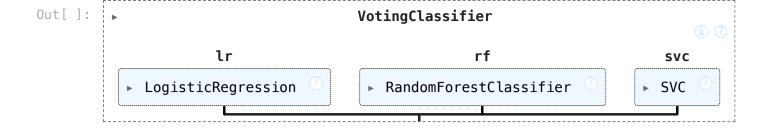
Task 3a)

Now repeat everything in Tasks 1 and 2 but for soft voting. To do that, just change the value in the voting parameter to soft which will implement probability-based voting. You will also need to set probability=True in the SVC model.

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```
In []: log_clf = LogisticRegression(solver="lbfgs", random_state=42)
    rnd_clf = RandomForestClassifier(n_estimators=100, random_state=42)
    svm_clf = SVC(gamma="scale", probability=True, random_state=42)

voting_clf = VotingClassifier(
    estimators=[('lr', log_clf), ('rf', rnd_clf), ('svc', svm_clf)],
    voting='soft')
voting_clf.fit(X_train, y_train)
```



LogisticRegression 0.864 RandomForestClassifier 0.896 SVC 0.896 VotingClassifier 0.92

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Task 3b)

What is the difference in between how the voting is done in the models from 2) and 3a).

Task 3b) answer:

The key difference between hard voting and soft voting in the VotingClassifier lies in how the final prediction is made from the individual model predictions. In the hard voting, each model in the ensemble predicts a discrete class label and the final prediction is determined by majority voting. In the soft voting, each model predicts class probabilities instead of discrete labels. The probabilities from all models are averaged for each class. The class with the highest average probability is chosen as the final prediction.

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Bagging ensembles

In bagging ensembles we essentially **train multiple classifiers on subsets of our total dataset**. The key characteristic about "bagging" is that we **draw**

samples with replacement. That is, we can potentially have multiple different models train on some small amount of overlapping data. The setting for that is bootstrap=True. Below, we'll create a bagginge ensemble of decision trees.

Task 4 Bagging Classifier

Task 4a)

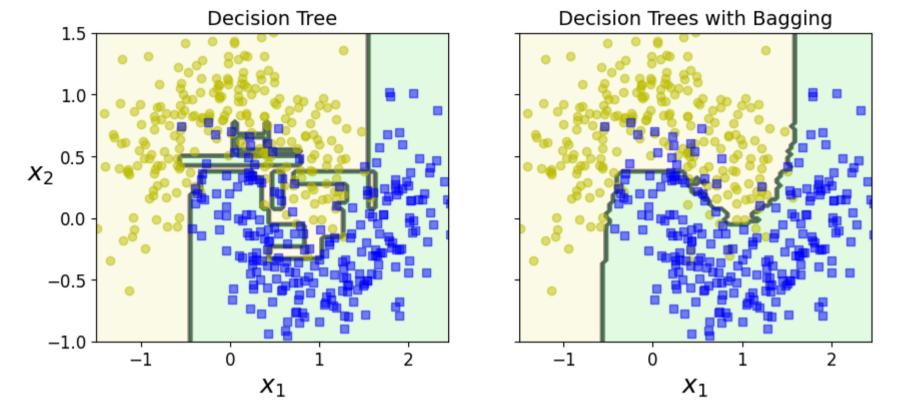
- Initialize a bagging classifier for a decision tree classifier with the following parameters:
 - n_estimators = 500
 - max_samples = 100
 - bootstrap = True
 - random state = 42
- Fit the bagging classifier to the training data and make a prediction.

• Calculate the accuracy score.

Task 4b

Do the same for a Decision Tree Classifier.

```
In [ ]: tree_clf = DecisionTreeClassifier(random_state=42)
        # fit
        tree clf.fit(X train, y train)
        # make prediction
        y_pred_tree = tree_clf.predict(X_test)
        pred_tree_accuracy_score = accuracy_score(y_test, y_pred_tree)
        pred_tree_accuracy_score
Out[]: 0.856
        ↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑ your code goes above this
In []: fix, axes = plt.subplots(ncols=2, figsize=(10,4), sharey=True)
        plt.sca(axes[0])
        plot_decision_boundary(tree_clf, X, y)
        plt.title("Decision Tree", fontsize=14)
        plt.sca(axes[1])
        plot_decision_boundary(bag_clf, X, y)
        plt.title("Decision Trees with Bagging", fontsize=14)
        plt.ylabel("")
        plt.show()
```



Task 4cBased only on the decision boundary plots above, which model is more likely to be overfit: bagging ensemble classifier or decision tree classifier.

Task 4c) answer:

The decision tree classifier is more likely to be overfit because its decision boundary is highly complex.

 \uparrow your answer goes above this

Feature importance

Let's use the mnist dataset. It contains 60k handwritten digits for training and 10k for testing. Here we're going to examine what features of a handwritten character a random forest identifies as important.

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

mnist = fetch_openml('mnist_784', version=1)
mnist.target = mnist.target.astype(np.uint8)
```

Task 5: Feature Importance

Task 5a)

Initialize a random forest classifier with 100 estimators.

Fit it to mnist["data"] and mnist["target"]

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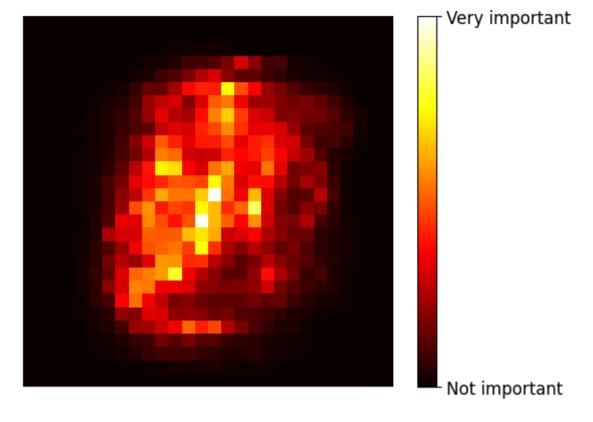
```
In [ ]: rand_forest_clf = RandomForestClassifier(n_estimators=100, random_state=42)
# fit
rand_forest_clf.fit(mnist["data"], mnist["target"])
```

Out[]: RandomForestClassifier

RandomForestClassifier(random_state=42)

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```
In []: plot_digit(rand_forest_clf.feature_importances_)
    cbar = plt.colorbar(ticks=[rand_forest_clf.feature_importances_.min(), rand_forest_clf.feature_importances_.max()])
    cbar.ax.set_yticklabels(['Not important', 'Very important'])
    plt.show()
```



Task 5b)

What can you infer about the model and dataset from the visualization above?

Task 5b) answer:

From the visualization, we can see that the Random Forest classifier has learned to focus on key regions of the image for classification. The feature importance is concentrated in key regions, suggesting that the classifier has identified key patterns. The central region of the image appears to be the most important, which suggests that the dataset contains characters that are centrally aligned. The edges of the image have low feature importance, indicating that background pixels exist and do not contribute much to classification.

 \uparrow your answer goes above this

AdaBoost

AdaBoost is an approach that entails training a classifier on a dataset, evaluating which datapoints it struggles with, then **trains copies of the classifier with the events reweighted** such that data points it struggles with are given higher priority during training. Importantly, **each individual classifier is likely to perform worse** on validation/test data than the original but the **ensemble of the original and copies are likely to perform better**.

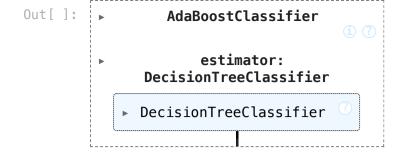
Task 6: AdaBoost

Now, initialize an AdaBoost classifier for a decision tree classifier with the following parameters:

- max_depth = 1 Decision Tree classifier parameter
- n_estimators = 200 Ada Boost classifier parameter
- learning_rate = 0.5 Ada Boost classifier parameter
- algorithm = "SAMME" Ada Boost classifier parameter
- random_state = 42 Ada Boost classifier parameter

Fit it to the training data.

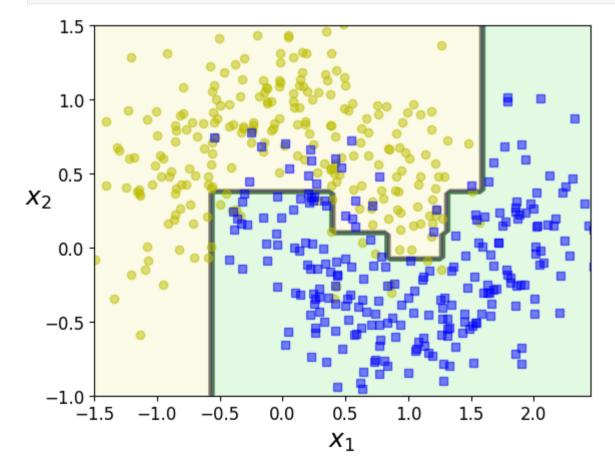
/usr/local/lib/python3.11/dist-packages/sklearn/ensemble/_weight_boosting.py:519: FutureWarning: The parameter 'algorithm' is de precated in 1.6 and has no effect. It will be removed in version 1.8. warnings.warn(



 \uparrow your code goes above this

Plot the decision boundary for ada_clf, X, y

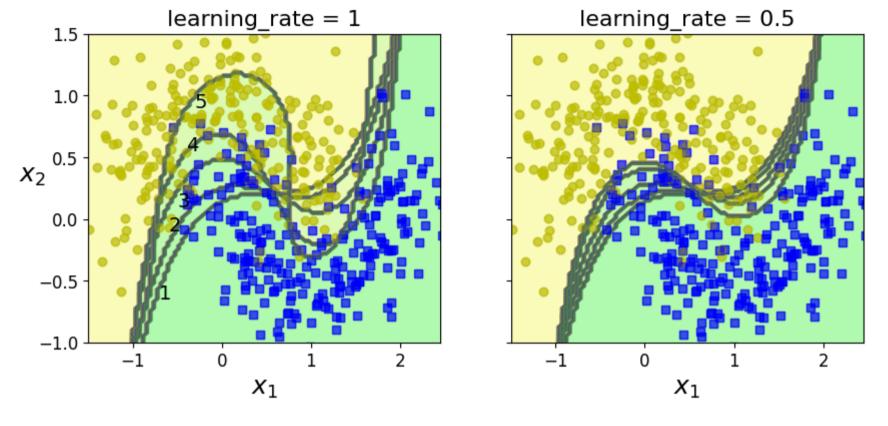
In []: plot_decision_boundary(ada_clf, X, y)



Don't worry about understanding the following code. The important thing is to understand the plots.

The following is essentially implementing the AdaBoost procedure from scratch for a support vector classifier (SVC).

```
In []: m = len(X train)
        fix, axes = plt.subplots(ncols=2, figsize=(10,4), sharey=True)
        for subplot, learning rate in ((0, 1), (1, 0.5)):
            sample_weights = np.ones(m)
            plt.sca(axes[subplot])
            for i in range(5):
                svm clf = SVC(kernel="rbf", C=0.05, gamma="scale", random state=42)
                svm_clf.fit(X_train, y_train, sample_weight=sample_weights)
                y pred = svm clf.predict(X train)
                sample weights[v pred != v train] *= (1 + learning rate)
                plot_decision_boundary(svm_clf, X, y, alpha=0.2)
                plt.title("learning_rate = {}".format(learning_rate), fontsize=16)
            if subplot == 0:
                plt.text(-0.7, -0.65, "1", fontsize=14)
                plt.text(-0.6, -0.10, "2", fontsize=14)
                plt.text(-0.5, 0.10, "3", fontsize=14)
                plt.text(-0.4, 0.55, "4", fontsize=14)
                plt.text(-0.3, 0.90, "5", fontsize=14)
            else:
                plt.ylabel("")
        plt.show()
```



The properties of this form of ensemble classifier look like the following.

Gradient Boosting

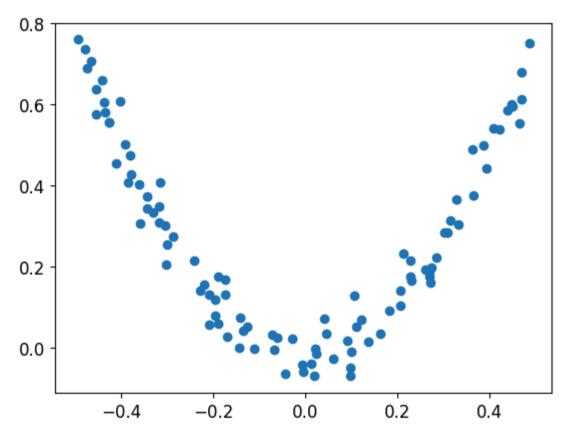
'n_features_in_']

Gradient boosting is a technique whereby we build an ensemble of models where subsequent models try to slightly correct the errors of previous models.

```
In []: np.random.seed(42)
X = np.random.rand(100, 1) - 0.5
y = 3*X[:, 0]**2 + 0.05 * np.random.randn(100)
```

In []: plt.scatter(X, y)

Out[]: <matplotlib.collections.PathCollection at 0x7ce67b68ca10>



Task 7: Gradient Boosting

Task 7a)

In this task, we will be doing the following.

- 1. Initialize a decision tree regressor with max_depth=2 and random_state=42 .
- 2. Fit it to X and y.

- 3. Substract the predicted y from the y values you fitted to in previous step.
- 4. Fit the new classifier with the output values from the previous step.
- 5. Repeat steps 3 and 4 one more time. You should obtain values for y2 and y3.

```
from sklearn.tree import DecisionTreeRegressor
        tree_reg1 = DecisionTreeRegressor(max_depth=2, random_state=42)
        # fit
        tree_reg1.fit(X, y)
Out[]:
                      DecisionTreeRegressor
       DecisionTreeRegressor(max depth=2, random state=42)
In []: y2 = y - tree reg1.predict(X)
        tree reg2 = DecisionTreeRegressor(max depth=2, random state=42)
        tree_reg2.fit(X, y2)
Out[]:
                      DecisionTreeRegressor
       DecisionTreeRegressor(max depth=2, random state=42)
In []: y3 = y2 - tree_reg2.predict(X)
        tree_reg3 = DecisionTreeRegressor(max_depth=2, random_state=42)
        tree_reg3.fit(X, y3)
Out[]:
                      DecisionTreeRegressor
       DecisionTreeRegressor(max_depth=2, random_state=42)
        ተለተለተለተለተለተለተለተለተለተለተለተለተለተለተለተለተለተለ your code goes above this
In [ ]: X_new = np.array([[0.8]])
```

The new predicted y should be the sum of the predictions for the X_new performed by each tree.

```
In []: y_pred = sum(tree.predict(X_new) for tree in (tree_reg1, tree_reg2, tree_reg3))
In []: y_pred
Out[]: array([0.75026781])
```

Task 7b)

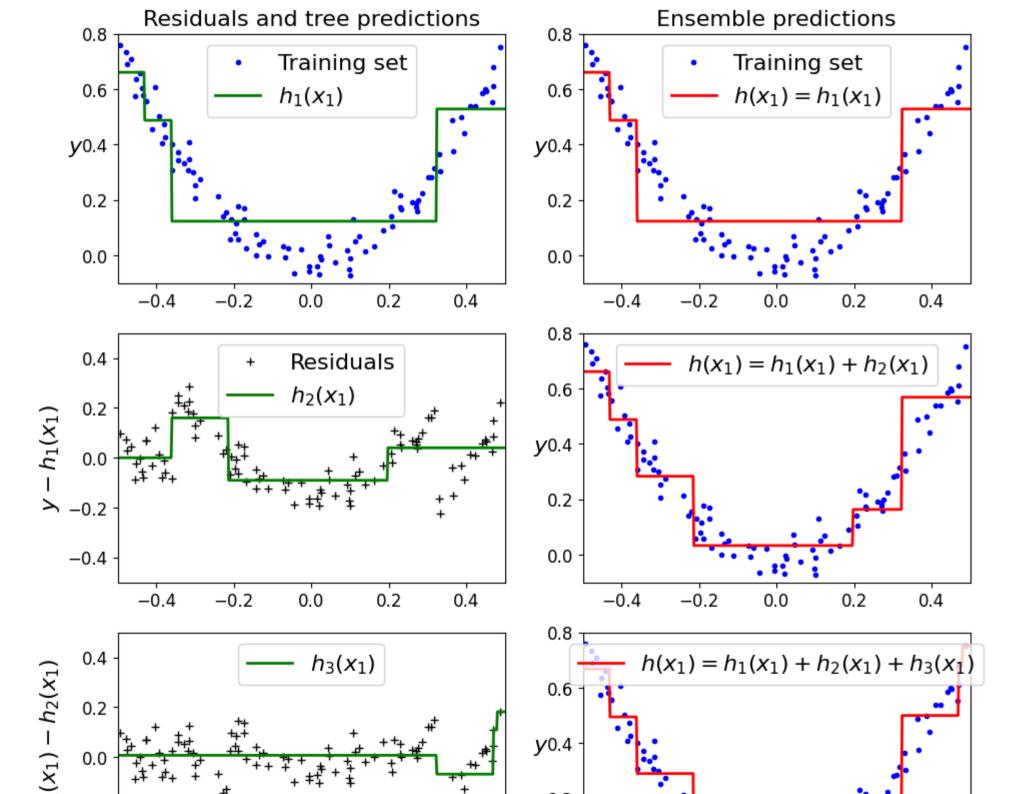
What do plots below show?

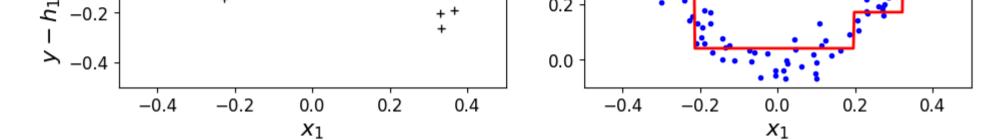
Task 7b) answer:

The plots illustrate the process of Gradient Boosting, showing how weak learners are sequentially trained to minimize the residual errors. The process is iterative and reduces errors step by step. Gradient Boosting incrementally improve predictions by learning from residuals, leading to a strong ensemble model.

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```
In []: plt.figure(figsize=(11,11))
                                          plt.subplot(321)
                                          plot_predictions([tree_reg1], X, y, axes=[-0.5, 0.5, -0.1, 0.8], label="\frac{1(x_1)}{y}, style="g-", data_label="Training set")
                                           plt.ylabel("$y$", fontsize=16, rotation=0)
                                           plt.title("Residuals and tree predictions", fontsize=16)
                                           plt.subplot(322)
                                           plot_predictions([tree_reg1], X, y, axes=[-0.5, 0.5, -0.1, 0.8], label="\frac{h(x_1)}{h(x_1)} = h_1(x_1)", data_label="Training set")
                                           plt.ylabel("$y$", fontsize=16, rotation=0)
                                           plt.title("Ensemble predictions", fontsize=16)
                                           plt.subplot(323)
                                          plot_predictions([tree_reg2], X, y2, axes=[-0.5, 0.5, -0.5, 0.5], label="\frac{h_2(x_1)}{h_2(x_1)}", style="\frac{g}{h_2(x_1)}", data style="\frac{h_2(x_1)}{h_2(x_1)}", style="\frac{g}{h_2(x_1)}", data style="\frac{g}{h_2(x_1)}", style="\frac{g}{h_2(x_1)}", style="\frac{g}{h_2(x_1)}", data style="\frac{g}{h_2(x_1)}", 
                                          plt.ylabel("$y - h_1(x_1)$", fontsize=16)
                                           plt.subplot(324)
                                          plot_predictions([tree_reg1, tree_reg2], X, y, axes=[-0.5, 0.5, -0.1, 0.8], label="\frac{h(x_1) + h(x_1) + h(x_1)
                                          plt.ylabel("$y$", fontsize=16, rotation=0)
                                           plt.subplot(325)
                                           plot_predictions([tree_reg3], X, y3, axes=[-0.5, 0.5, -0.5, 0.5], label="$h_3(x_1)$", style="g_-", data_style="k_+")
```





Task 7c)

We are also going to compare two gradient boosting regressor objects.

Both with max_depth=2 and random_state=42, but one will be 'fast' and one will be 'slow'.

For the fast one, set the learning rate to 1 and number of estimators to 3.

For the slow one, set the learning rate to 0.1 and number of estimators to 200.

```
In []: from sklearn.ensemble import GradientBoostingRegressor

gbrt_fast = GradientBoostingRegressor(max_depth=2, n_estimators=3, learning_rate=1.0, random_state=42)

gbrt_slow = GradientBoostingRegressor(max_depth=2, n_estimators=200, learning_rate=0.1, random_state=42)
```

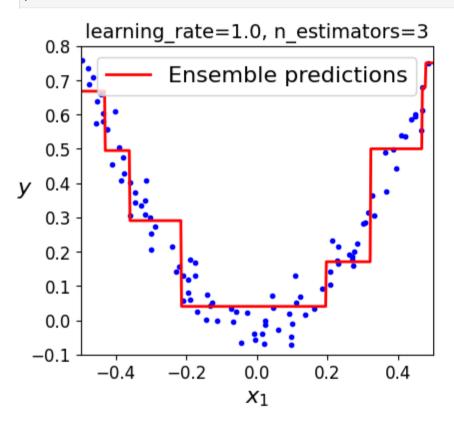
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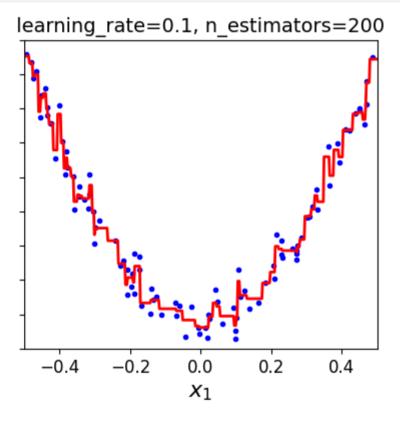
Next, we are fitting them to the data.

```
In [ ]: gbrt_fast.fit(X, y)
   gbrt_slow.fit(X, y)
```

```
Out[]: GradientBoostingRegressor

GradientBoostingRegressor(max_depth=2, n_estimators=200, random_state=42)
```





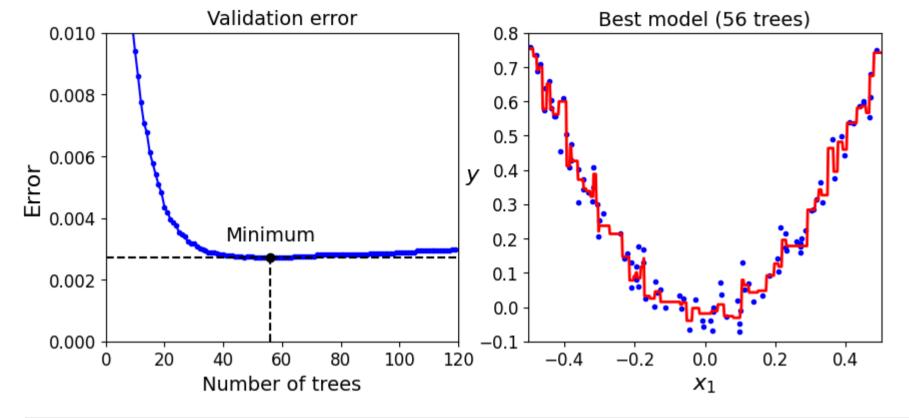
Gradient Boosting with Early stopping

In this section, we are going to be looking for the lowest MSE in a set of boosted trees. Just run the cells below and discuss the results with your group.

Again, the important thing here is to understand the plots. Don't worry about trying to understand all of the code.

```
In []: import numpy as np
        from sklearn.model selection import train test split
        from sklearn.metrics import mean squared error
        from sklearn.ensemble import GradientBoostingRegressor
        X_train, X_val, y_train, y_val = train_test_split(X, y, random_state=49)
        gbrt = GradientBoostingRegressor(max depth=2, n estimators=120, random state=42)
        gbrt.fit(X train, y train)
        errors = [mean squared error(y val, y pred)
                  for y pred in qbrt.staged predict(X val)]
        bst n estimators = np.argmin(errors) + 1
        gbrt best = GradientBoostingRegressor(max depth=4, n estimators=bst n estimators, random state=42)
        gbrt_best.fit(X_train, y_train)
Out[]:
                               GradientBoostingRegressor
        GradientBoostingRegressor(max depth=4, n estimators=56, random state=42)
In [ ]: min error = np.min(errors)
In []: plt.figure(figsize=(10, 4))
        plt.subplot(121)
        plt.plot(errors, "b.-")
        plt.plot([bst_n_estimators, bst_n_estimators], [0, min_error], "k--")
        plt.plot([0, 120], [min error, min error], "k--")
        plt.plot(bst_n_estimators, min_error, "ko")
        plt.text(bst n estimators, min error*1.2, "Minimum", ha="center", fontsize=14)
        plt.axis([0, 120, 0, 0.01])
        plt.xlabel("Number of trees")
        plt.ylabel("Error", fontsize=16)
        plt.title("Validation error", fontsize=14)
        plt.subplot(122)
        plot_predictions([gbrt_best], X, y, axes=[-0.5, 0.5, -0.1, 0.8])
        plt.title("Best model (%d trees)" % bst_n_estimators, fontsize=14)
        plt.ylabel("$y$", fontsize=16, rotation=0)
        plt.xlabel("$x_1$", fontsize=16)
```

plt.show()



```
In []: gbrt = GradientBoostingRegressor(max_depth=4, warm_start=True, random_state=42)

min_val_error = float("inf")
error_going_up = 0
for n_estimators in range(1, 120):
    gbrt.n_estimators = n_estimators
    gbrt.fit(X_train, y_train)
    y_pred = gbrt.predict(X_val)
    val_error = mean_squared_error(y_val, y_pred)
    if val_error < min_val_error:
        min_val_error = val_error
        error_going_up = 0
    else:
        error_going_up += 1
        if error_going_up == 5:
            break # early stopping</pre>
```

In []: print(gbrt.n_estimators)

```
In [ ]: print("Minimum validation MSE:", min_val_error)
```

Minimum validation MSE: 0.0030785999080668687

Using XGBoost

Task 8

Finally, we move to an XGBoost regressor - arguably one of the most popular and widely-used algorithms nowadays. **At low depths and low estimators**, XGBoost can actually perform **worse than a normal gradient-boosted tree** because of the way the data is binned into histograms by the model **but can scale better** than a standard gradient-boosted tree allowing for overall better results.

First, make sure you have it installed.

```
In []: !pip install xgboost
    Requirement already satisfied: xgboost in /usr/local/lib/python3.11/dist-packages (2.1.4)
    Requirement already satisfied: numpy in /usr/local/lib/python3.11/dist-packages (from xgboost) (1.26.4)
    Requirement already satisfied: nvidia-nccl-cu12 in /usr/local/lib/python3.11/dist-packages (from xgboost) (2.21.5)
    Requirement already satisfied: scipy in /usr/local/lib/python3.11/dist-packages (from xgboost) (1.13.1)

In []: import xgboost

In []: xgb_reg = xgboost.XGBRegressor(n_estimators=100, max_depth=2, random_state=42)
    xgb_reg.fit(X_train, y_train)
    y_pred = xgb_reg.predict(X_val)
    val_error = mean_squared_error(y_val, y_pred) # Not shown
    print("Validation MSE:", val_error) # Not shown

Validation MSE: 0.003860706105008133
```

Task 8

Do the same thing as above but while fitting, add a validation sets and set $early_stopping_rounds=2$. To do that, you want to add the $eval_set$ parameter and set $[(X_val, y_val)]$ value there.

```
In [ ]: val errors with stop = []
        xqb reg = xqboost.XGBRegressor(n_estimators=100, max_depth=2, random_state=42, early_stopping_rounds=2)
        # add the validation set and an early stopping, fit
        xgb req.fit(X train, y train, eval set=[(X val, y val)])
        val errors with stop = xqb req.evals result()['validation 0']['rmse']
        y_pred = xgb_reg.predict(X_val)
        val error = mean_squared_error(y_val, y_pred) # Not shown
        print("Validation MSE:", val error)
                                                        # Not shown
       [0]
               validation 0-rmse:0.16431
       [1]
               validation 0-rmse:0.12752
       [2]
               validation 0-rmse:0.10129
       [3]
               validation 0-rmse:0.08966
       [4]
               validation 0-rmse:0.07659
       [5]
               validation_0-rmse:0.06950
       [6]
               validation 0-rmse:0.06822
       [7]
               validation 0-rmse:0.06925
       [8]
               validation 0-rmse:0.06551
       [9]
               validation 0-rmse:0.06206
       [10]
               validation 0-rmse:0.06053
       [11]
               validation 0-rmse:0.06227
       [12]
               validation_0-rmse:0.06063
       Validation MSE: 0.003664239897742551
```

 \uparrow your code goes above this