cs109a_hw8_submit

November 14, 2018

1 CS109A Introduction to Data Science:

1.1 Homework 8: Ensembles: Bagging, Random Forests, and Boosting

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```
In [3]: #RUN THIS CELL
        import requests
        from IPython.core.display import HTML
        styles = requests.get("https://raw.githubusercontent.com/Harvard-IACS/2018-CS109A/mast
        HTML(styles)
```

```
Out[3]: <IPython.core.display.HTML object>
```

1.1.1 INSTRUCTIONS

- To submit your assignment follow the instructions given in Canvas.
- If needed, clarifications will be posted on Piazza.
- This homework can be submitted in pairs.
- If you submit individually but you have worked with someone, please include the name of your **one** partner below.

Name of the person you have worked with goes here: Yajaira Gonzalez Gonzalez

1.2 Learning Objectives

Completing this assignment will demonstrate success at the following objectives:

- Statistical
- Predict when bagging will help model performance.
- Identify how Random Forests improve over bagging.
- Predict when boosting will help model performance.
- Compare and contrast bagging and boosting.
- Coding
- Identify and fix problems in poorly written code
- Communication
- Visually explain a complex concept

```
In [4]: import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt

        from sklearn.model_selection import cross_val_score
        from sklearn.utils import resample
        from sklearn.tree import DecisionTreeClassifier
        from sklearn.ensemble import RandomForestClassifier
        from sklearn.ensemble import AdaBoostClassifier
        from sklearn.metrics import accuracy_score

        %matplotlib inline

        import seaborn as sns
        sns.set(style='whitegrid')
        pd.set_option('display.width', 1500)
        pd.set_option('display.max_columns', 100)
```

Overview: Higgs Boson Discovery

The discovery of the Higgs boson in July 2012 marked a fundamental breakthrough in particle physics. The Higgs boson particle was discovered through experiments at the Large Hadron Collider at CERN, by colliding beams of protons at high energy. A key challenge in analyzing the results of these experiments is to differentiate between collisions that produce Higgs bosons and collisions that produce only background noise. We shall explore the use of ensemble methods for this classification task.

You are provided with data from Monte-Carlo simulations of collisions of particles in a particle collider experiment. The training set is available in `Higgs_train.csv` and the test set is in `Higgs_test.csv`. Each row in these files corresponds to a particle collision described by 28 features (columns 1-28), of which the first 21 features are kinematic properties measured by the particle detectors in the accelerator, and the remaining features are derived by physicists from the first 21 features. The class label is provided in the last column, with a label of 1 indicating that the collision produces Higgs bosons (signal), and a label of 0 indicating that the collision produces other particles (background).

The data set provided to you is a small subset of the HIGGS data set in the UCI machine learning repository. The following paper contains further details about the data set and the predictors used: Baldi et al., Nature Communications 5, 2014.

```
In [5]: # Load data
        data_train = pd.read_csv('Higgs_train.csv')
        data_test = pd.read_csv('Higgs_test.csv')

        print(f"{len(data_train)} training samples, {len(data_test)} test samples")
        print("\nColumns:")
        print(', '.join(data_train.columns))
```

```
5000 training samples, 5000 test samples

Columns:
```

```
lepton pT, lepton eta, lepton phi, missing energy magnitude, missing energy phi, jet 1 pt, jet
```

```
In [6]: display(data_train.head())
        display(data_train.describe())
```

```
   lepton pT  lepton eta  lepton phi  missing energy magnitude  missing energy phi  jet 1 pt  j
0      0.377     -1.5800     -1.7100                     0.991               0.114     1.250
1      0.707      0.0876     -0.4000                     0.919              -1.230     1.170
2      0.617      0.2660     -1.3500                     1.150               1.040     0.955
3      0.851     -0.3810     -0.0713                     1.470              -0.795     0.692
4      0.768     -0.6920     -0.0402                     0.615               0.144     0.749
```

```
         lepton pT   lepton eta   lepton phi  missing energy magnitude  missing energy phi
count  5000.000000  5000.000000  5000.000000               5000.000000         5000.000000  500
mean      0.978645    -0.014280    -0.018956                  1.005793            0.002528
std       0.547025     1.011927     0.997945                  0.591907            1.003337
min       0.275000    -2.410000    -1.740000                  0.010000           -1.740000
25%       0.587000    -0.764250    -0.877500                  0.581000           -0.870000
50%       0.846000    -0.009305    -0.016050                  0.903500            0.001300
75%       1.220000     0.725500     0.837000                  1.300000            0.866000
max       5.330000     2.430000     1.740000                  6.260000            1.740000
```

```
In [7]: # Split into NumPy arrays
        X_train = data_train.iloc[:, data_train.columns != 'class'].values
        y_train = data_train['class'].values
        X_test = data_test.iloc[:, data_test.columns != 'class'].values
        y_test = data_test['class'].values
```

Question 1: A Single Model [20 pts]

We start by fitting a basic model we can compare the other models to. We'll pick a decision tree as the base model, because we'll later include random forests and want a fair comparison. We'll tune the decision tree using cross-validation. As usual, we'll be tuning the maximum tree depth; we refer to this parameter as "depth" for simplicity.

Since we will only be using tree-based methods in this homework, we do not need to standardize or normalize the predictors.

1.1: Fit a decision tree model to the training set. Choose a range of tree depths to evaluate. Plot the estimated performance +/- 2 standard deviations for each depth using 5-fold cross validation. Also include the training set performance in your plot, but set the y-axis to focus on the cross-validation performance.

Hint: use `plt.fill_between` to shade the region.

1.2 Select an appropriate depth and justify your choice. Using your cross-validation estimates, report the mean +/- 2 stdev. Then report the classification accuracy on the test set. (Store the training and test accuracies in variables to refer to in a later question.)

1.3 What is the mechanism by which limiting the depth of the tree avoids over-fitting? What is one downside of limiting the tree depth? Your answer should refer to the bias-variance trade-off.

Answers

1.1

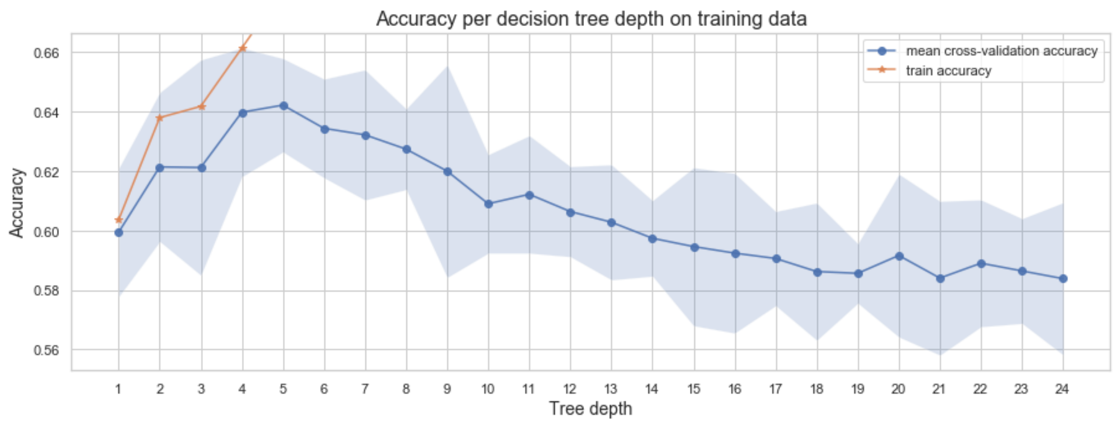
Helper functions for fitting regression trees of depth 1 to 24 on the training data and plotting cross-validation results. The range 1-24 was chosen by experimentation.

```
In [8]: def run_cross_validation_on_trees(X, y, tree_depths, cv=5, scoring='accuracy'):
            cv_scores_list = []
            cv_scores_std = []
            cv_scores_mean = []
            accuracy_scores = []
            for depth in tree_depths:
                tree_model = DecisionTreeClassifier(max_depth=depth)
                cv_scores = cross_val_score(tree_model, X, y, cv=cv, scoring=scoring)
                cv_scores_list.append(cv_scores)
                cv_scores_mean.append(cv_scores.mean())
                cv_scores_std.append(cv_scores.std())
                accuracy_scores.append(tree_model.fit(X, y).score(X, y))
            cv_scores_mean = np.array(cv_scores_mean)
            cv_scores_std = np.array(cv_scores_std)
            accuracy_scores = np.array(accuracy_scores)
            return cv_scores_mean, cv_scores_std, accuracy_scores
```

```
In [11]: def plot_cross_validation_on_trees(depths, cv_scores_mean, cv_scores_std, accuracy_sco
             fig, ax = plt.subplots(1,1, figsize=(15,5))
             ax.plot(depths, cv_scores_mean, '-o', label='mean cross-validation accuracy', alpl
             ax.fill_between(depths, cv_scores_mean-2*cv_scores_std, cv_scores_mean+2*cv_scores
             ylim = plt.ylim()
             ax.plot(depths, accuracy_scores, '-*', label='train accuracy', alpha=0.9)
             ax.set_title(title, fontsize=16)
             ax.set_xlabel('Tree depth', fontsize=14)
             ax.set_ylabel('Accuracy', fontsize=14)
             ax.set_ylim(ylim)
             ax.set_xticks(depths)
             ax.legend()
```

```
In [12]: sm_tree_depths = range(1,25)
         sm_cv_scores_mean, sm_cv_scores_std, sm_accuracy_scores = run_cross_validation_on_tree
```

```
In [13]: plot_cross_validation_on_trees(sm_tree_depths, sm_cv_scores_mean, sm_cv_scores_std, sm
```



1.2

```
In [14]: idx_max = sm_cv_scores_mean.argmax()
         sm_best_tree_depth = sm_tree_depths[idx_max]
         sm_best_tree_cv_score = sm_cv_scores_mean[idx_max]
         sm_best_tree_cv_score_std = sm_cv_scores_std[idx_max]
         print('The depth-{} tree achieves the best mean cross-validation accuracy {} +/- {}% o
```

```
The depth-5 tree achieves the best mean cross-validation accuracy 64.22041 +/- 0.78668% on trai
```

We choose the above tree depth because it achieves the best average accuracy on training data using cross-validation folds with size 5. The lower bound of the confidence interval of the accuracy is high enough to make this value significant. When more nodes are added to the tree, it is clear that the cross-validation accuracy changes towards zero.

The tree of depth 20 achieves perfect accuracy (100%) on the training set, this means that each leave of the tree contains exactly one sample and the class of that sample will be the prediction. That depth-20 tree is overfitting to the training set. The tree depth we chose via cross-validation helps us avoiding overfitting and gives better chance to reproduce the accuracy and generalize the model on test data.

```
In [15]: def run_single_tree(X_train, y_train, X_test, y_test, depth):
             model = DecisionTreeClassifier(max_depth=depth).fit(X_train, y_train)
             accuracy_train = model.score(X_train, y_train)
             accuracy_test = model.score(X_test, y_test)
             print('Single tree depth: ', depth)
             print('Accuracy, Training Set: ', round(accuracy_train*100,5), '%')
             print('Accuracy, Test Set: ', round(accuracy_test*100,5), '%')
             return accuracy_train, accuracy_test
```

```
In [16]: sm_best_tree_accuracy_train, sm_best_tree_accuracy_test = run_single_tree(X_train, y_
```

```
Single tree depth:  5
Accuracy, Training Set:  68.12 %
Accuracy, Test Set:  64.8 %
```

1.3

A full classification tree would split the training data until each leave contains a single observation. This tree would achieves a perfect classification of the training observations and the biais would be 0. In order words, the full tree would overfit to training data. Such a tree would be very sensitive because little changes of training observations would cause the predicted classes to change largely, this means the model variance would be very high.

By reducing the tree depth, we increase the biais (missclassification error on training) but we also reduce the variance. Bias-variance trade-off seeks a compromise between bias and variance, here using cross-validation. By resampling the data many times, splitting the into training and validation folds, fitting trees with different sizes on the training folds and looking at the classification accuracy on the validation folds, we are able to find the tree depth, which gives the best bias-variance trade-off, as we did above. Such a tree does not predict perfectly on the training set (acceptable bias) but its performance will be approximately the same if we change the training set a bit (acceptable variance).

Question 2: Bagging [25 pts]

Bagging is the technique of building the same model on multiple bootstraps from the data and combining each model's prediction to get an overall classification. In this question we build an example by hand and study how the number of bootstrapped datasets impacts the accuracy of the resulting classification.

2.1 Choose a tree depth that will overfit the training set. What evidence leads you to believe that this depth will overfit? Assign your choice to a variable here. (You may want to explore different settings for this value in the problems below.)

2.2 Create 45 bootstrapped replications of the original training data, and fit a decision tree to each. Use the tree depth you just chose in 2.1. Record each tree's prediction. In particular, produce a dataset like those below, where each row is a training (or test) example, each column is one of the trees, and each entry is that tree's prediction for that example. (Labeling the rows and columns is optional.)

Store these results as `bagging_train` and `bagging_test`. Don't worry about visualizing these results yet.

2.3 *Aggregate* all 45 *bootstrapped* models to get a combined prediction for each training and test point: predict a 1 if and only if a majority of the models predict that example to be from class 1. What accuracy does this *bagging* model achieve on the test set? Write an assertion that verifies that this test-set accuracy is at least as good as the accuracy for the model you fit in Question 1.

2.4 We want to know how the number of bootstraps affects our bagging ensemble's performance. Use the `running_predictions` function (given below) to get the model's accuracy score when using only 1,2,3,4,... of the bootstrapped models. Make a plot of training and test set accuracies as a function of number of bootstraps.

On your plot, also include horizontal lines for two baselines: - the test accuracy of the best model from question 1 - the test accuracy of a single tree with the tree depth you chose in 2.1, trained on the full training set.

2.5 Referring to your graph from 2.4, compare the performance of bagging against the baseline of a single depth-10 tree. Explain the differences you see.

2.6 Bagging and limiting tree depth both affect how much the model overfits. Compare and contrast these two approaches. Your answer should refer to your graph in 2.4 and may duplicate something you said in your answer to 1.5.

2.7: In what ways might our bagging classifier be overfitting the data? In what ways might it be underfitting?

Hints - Use `resample` from sklearn to easily bootstrap the x and y data. - use `np.mean` to easily test for majority. If a majority of models vote 1, what does that imply about the mean?

Answers:

2.1

We choose a tree depth for which the classification accuracy on training dataset is 100%, based on the plot we did in question 1. This tree overfits the training set because it always predict a class of a single observation in that set, and not the majority class of a larger region. As shown below it does not generalize well on the test set.

```
In [17]: sm_overfit_tree_depth = 20
         sm_overfit_accuracy_train, sm_overfit_accuracy_test = run_single_tree(X_train, y_trai
```

```
Single tree depth:  20
Accuracy, Training Set:  100.0 %
Accuracy, Test Set:  60.64 %
```

2.2

Structure of `bagging_train` and `bagging_test`:

`bagging_train`:

	bootstrap model 1's prediction	bootstrap model 2's prediction	...
training row 1	binary value	binary value	...
training row 2	binary value	binary value	...
...	...	...	...

`bagging_test`:

	bootstrap model 1's prediction	bootstrap model 2's prediction	...
test row 1	binary value	binary value	...
test row 2	binary value	binary value	...
...	...	...	...

```
In [18]: def run_bagging(X_train, y_train, X_test, y_test, tree_depth, bagging_size=45):
             bagging_train = np.zeros((X_train.shape[0], bagging_size))
             bagging_test = np.zeros((X_test.shape[0], bagging_size))
             trees = []
             for i in range(bagging_size):
                 X_train_bootstrap, y_train_bootstrap = resample(X_train, y_train)
                 tree = DecisionTreeClassifier(max_depth=tree_depth).fit(X_train_bootstrap, y_
                 bagging_train[:, i] = tree.predict(X_train)
                 bagging_test[:, i] = tree.predict(X_test)
                 trees.append(tree)
             return bagging_train, bagging_test, trees
```

```
In [19]: np.random.seed(0)
         bagging_size = 45
```

```
        bagging_train, bagging_test, bagging_trees = run_bagging(X_train, y_train, X_test, y_
```

2.3

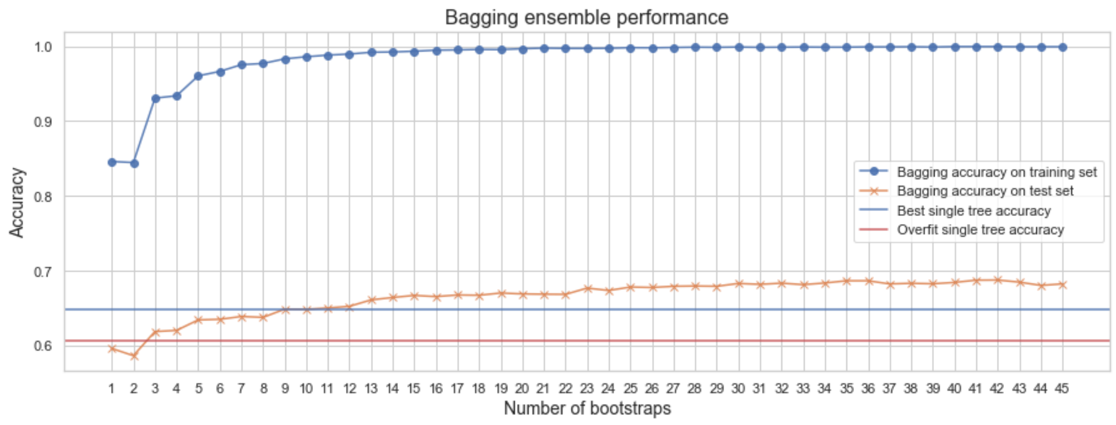
```
In [20]: def aggregate_bagging(bagging):
             return (bagging.sum(axis=1)/bagging.shape[1] > 0.5).astype('int')

In [21]: bagging_accuracy_train = accuracy_score(y_train, aggregate_bagging(bagging_train))
         print('The bagging model achieves classification accuracy {}% on training dataset'.fo

The bagging model achieves classification accuracy 99.96% on training dataset


In [22]: bagging_accuracy_test = accuracy_score(y_test, aggregate_bagging(bagging_test))
         print('The bagging model achieves {}% classification accuracy on test dataset.\nThe be

The bagging model achieves 68.22% classification accuracy on test dataset.
The best single tree model achieved only 64.8% classification accuracy on test.


In [23]: assert bagging_accuracy_test >= sm_best_tree_accuracy_test, "Bagging test accuracy to
```

2.4

```
In [24]: def running_predictions(prediction_dataset, targets):
             """A function to predict examples' class via the majority among trees (ties are p

             Inputs:
               prediction_dataset - a (n_examples by n_sub_models) dataset, where each entry [
                   for example i
               targets - the true class labels

             Returns:
               a vector where vec[i] is the model's accuracy when using just the first i+1 sub
             """

             n_trees = prediction_dataset.shape[1]

             # find the running percentage of models voting 1 as more models are considered
             running_percent_1s = np.cumsum(prediction_dataset, axis=1)/np.arange(1,n_trees+1)

             # predict 1 when the running average is above 0.5
             running_conclusions = running_percent_1s > 0.5

             # check whether the running predictions match the targets
             running_correctnesss = running_conclusions == targets.reshape(-1,1)

             return np.mean(running_correctnesss, axis=0)
             # returns a 1-d series of the accuracy of using the first n trees to predict the
```

```
In [25]: def plot_bagging_predictions(bagging_size, bagging_train, y_train, bagging_test, y_tes
                                      sm_best_tree_accuracy_test, sm_overfit_accuracy_test, ti
             bagging_accuracy_train = running_predictions(bagging_train, y_train)
             bagging_accuracy_test = running_predictions(bagging_test, y_test)
             fig, ax = plt.subplots(1,1, figsize=(15,5))
             bagging_sizes = range(1, bagging_size+1)
             ax.plot(bagging_sizes, bagging_accuracy_train, '-o', label='Bagging accuracy on tr
             ax.plot(bagging_sizes, bagging_accuracy_test, '-x', label='Bagging accuracy on tes
             ax.axhline(y=sm_best_tree_accuracy_test, label='Best single tree accuracy', alpha=
             ax.axhline(y=sm_overfit_accuracy_test, label='Overfit single tree accuracy', c='r
             ax.set_title(title, fontsize=16)
             ax.set_xlabel('Number of bootstraps', fontsize=14)
             ax.set_ylabel('Accuracy', fontsize=14)
             ax.set_xticks(bagging_sizes)
             ax.legend()
             #ax.grid(False)
```

```
In [26]: plot_bagging_predictions(bagging_size, bagging_train, y_train, bagging_test, y_test, s
```



2.5

```
In [27]: print('The single depth-{} tree picked in 2.1 achieves {}% classification accuracy on
         print('Bagging with depth-{} tree achieves {}% classification accuracy on training se
         print('The single depth-{} tree chosen in 1.5 achieves {}% classification accuracy on
```

```
The single depth-20 tree picked in 2.1 achieves 100.0% classification accuracy on training set
Bagging with depth-20 tree achieves 99.96% classification accuracy on training set and 68.22% o
The single depth-5 tree chosen in 1.5 achieves 68.12% classification accuracy on training set a
```

Looking at the plot from 2.4, by fitting a depth-20 tree on 3 or more bootstraps of the training set and averaging their classifications by majority vote, we achieve better classification accuracy on test (orange line) compared to using a single depth-20 tree (red line).

With bagging we are averaging the variances introduced by overfitting the original depth-20 tree to training data. This results in less overfitting, and better performance on test, even better than the best single tree tuned via cross-validation.

2.6

- **limiting tree depth**: the big depth-20 tree from 2.1 has a high number of parameters and overfits training data, especially because we end up with a tree where each leave is classifying one training sample (accuracy 100%). In order to avoid overfitting and reduce variance, we can stop building the tree when the leaves are pure, or when leaves have a specific size or when the gain of adding nodes is less than a given threshold. Ultimately we found the best 5-depth tree via cross-validation in 1.2.
- **bagging**: by sampling with replacement, bagging creates several large low-bias depth-20 trees fitted to bootstraped training data. Assuming that the trees are independent, we averaged their predictions in order to reduce variance and solve overfitting. The large tree size captures most information in the training dataset, resulting in low bias. Bagging with 20 or more trees improves test accuracy (68.22%), compared to a single 5-depth tree (64.8%), as shown in 2.4.

2.7

Even with bagging we can still overfit the data, especially when the trees are correlated. In such case, the total variance is not just the average of individual variances, but a whole buch of covariance terms are also taken into consideration. This is because Bagging will most probably pick the same predictors at the beginning for the first split of the trees. Random forests come into play to solve this issue.

Bagging can also underfit. This is the case when the tree depth is too low. Additionally since through boostrap we do not use all data for training, we can end up with underfitting to the whole training dataset. The out-of-bag samples can however be used to validate the trees.

It is to be noted that bagging will not help if we have very high biais.

Question 3: Random Forests [15 pts]

Random Forests are closely related to the bagging model we built by hand in question 2. In this question we compare our by-hand results with the results of using `RandomForestClassifier` directly.

3.1 Fit a `RandomForestClassifier` to the original `X_train` data using the same tree depth and number of trees that you used in Question 2.2. Evaluate its accuracy on the test set.

3.2 For each of the decision trees you fit in the bagging process, how many times is each feature used at the top node? How about for each tree in the random forest you just fit? What about the process of training the Random Forest causes this difference? What implication does this observation have on the accuracy of bagging vs Random Forest?

Hint: A decision tree's top feature is stored in `model.tree_.feature[0]`. A random forest object stores its decision trees in its `.estimators_` attribute.

3.3: Make a table of the training and test accuracy for the following models:

- Single tree with best depth chosen by cross-validation (from Question 1)
- A single overfit tree trained on all data (from Question 2, using the depth you chose there)
- Bagging 45 such trees (from Question 2)
- A Random Forest of 45 such trees (from Question 3.1)

(This problem should not require fitting any new models, though you may need to go back and store the accuracies from models you fit previously.)

What is the relative performance of each model on the training set? On the test set? Comment on how these relationships make sense (or don't make sense) in light of how each model treats the bias-variance trade-off.

Answers:

3.1

```
In [28]: def run_random_forest(X_train, y_train, X_test, y_test, size, depth):
             randomf = RandomForestClassifier(n_estimators=size, max_depth=depth).fit(X_train,
             accuracy_train = randomf.score(X_train, y_train)
             accuracy_test = randomf.score(X_test, y_test)
             print('RANDOM FOREST')
             print('Number of trees: ', size)
             print('Tree depth: ', depth)
             print('Accuracy, Training Set: ', round(accuracy_train*100,5), '%')
             print('Accuracy, Test Set: ', round(accuracy_test*100,5), '%')
             return accuracy_train, accuracy_test, randomf
```

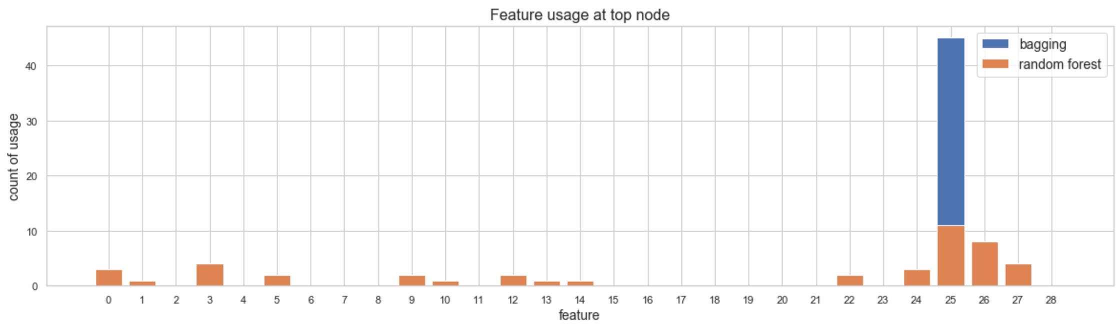
```
In [29]: rf_accuracy_train, rf_accuracy_test, randomf = run_random_forest(X_train, y_train, X_
```

```
RANDOM FOREST
Number of trees:  45
Tree depth:  20
Accuracy, Training Set:  99.96 %
Accuracy, Test Set:  68.34 %
```

3.2

```
In [30]: top_features_occurencies = np.zeros((data_train.shape[1], 2))
         for i in range(bagging_size):
             bagging_top_feature_idx = bagging_trees[i].tree_.feature[0]
             randomf_top_feature_idx = randomf.estimators_[i].tree_.feature[0]
             top_features_occurencies[bagging_top_feature_idx, 0] += 1
             top_features_occurencies[randomf_top_feature_idx, 1] += 1
```

```
In [31]: fig, ax = plt.subplots(1,1,figsize=(20,5))
         ax.bar(np.arange(data_train.shape[1]),top_features_occurencies[:,0], label='bagging')
         ax.bar(np.arange(data_train.shape[1]),top_features_occurencies[:,1], label='random fo
         ax.set_xticks(np.arange(data_train.shape[1]))
         ax.set_xlabel('feature', fontsize=14)
         ax.set_ylabel('count of usage', fontsize=14)
         ax.legend(fontsize=14)
         ax.set_title('Feature usage at top node', fontsize=16);
```



Bagging tends to always choose the same feature nr. 25 (**m_bb**) as root feature for all 45 bootstrap trees. Feature nr. 25 provides the best first split of data in two regions with minimal Gini impurity. Therefore the trees will all be correlated, at least at their top nodes. This results in overfitting to training data by bagging and lost of classification accuracy on test.

Random Forest does not use the full set of 29 features as bagging does. At each split when fitting the trees, random forest rather selects a subset of predictors, randomly. It then search for the feature within that subset, as well as a threshold value that provides the most optimal split (via Gini, entropy, etc.). The size of the random subset, usually the sqrt of the total number of features, can be found via cross-validation using the unused samples after bootstrapping (out-of-bag). As a result with Random Forest, 15 out of 29 features appear at the top of our 45 trees. A down-side of random forests is: if many of our 29 features are irrelevant, Random Forest might end up choosing the less relevant ones, resulting in a poor tree. In such case we might want to do some pre-check using cross-correlation and features selection.

Random Forest achieves slightly better classification accuracy on test, compared to bagging. This is because Random Forest de-correlates the trees and aids reducing the variance in the results, even more than bagging, since with random forest covariance terms between trees are reduced.

3.3

Fill in the following table (ideally in code, but ok to fill in this Markdown cell).

classifier	training accuracy	test accuracy
single tree with best depth chosen by CV		
single depth-X tree		
bagging 45 depth-X trees		
Random Forest of 45 depth-X trees		

```
In [32]: classifier = ['single tree with best depth-5 chosen by CV','single depth-20 tree','bag
         training_accuracy = [sm_best_tree_accuracy_train, sm_overfit_accuracy_train, bagging_a
         test_accuracy = [sm_best_tree_accuracy_test, sm_overfit_accuracy_test, bagging_accurac
         models_benchmark_df = pd.DataFrame({'classifier':classifier, 'training accuracy': trai
         models_benchmark_df
```

```
Out[32]:                                    classifier  training accuracy  test accuracy
         0  single tree with best depth-5 chosen by CV             0.6812         0.6480
         1                        single depth-20 tree             1.0000         0.6064
         2                     bagging 45 depth-20 trees           0.9996         0.6822
```

```
        3          Random Forest of 45 depth-20 trees              0.9996          0.6834
```

Performance

The fully grown depth-20 tree leads to almost 100% accuracy on training set (also with bagging and random forest), in contrast to the single tree with best depth-5 chosen by CV, which achieves only 68.12% accuracy on training set. The bottom side of the CV approach is that by stopping too soon, we missed out some information in the training dataset and we end up with high bias (only 64.8% test accuracy with depth-5 tree).

Bagging and random forest reduce overfitting and improves the accuracy on test set.

Bias-variance trade-off

- CV provides the lowest variance (less overfit to training set) at the cost of highest bias. The low tree depth did not allow to catch additional information in the data; we stopped building the tree too early.
- The depth-20 tree is not robust and leads to too much variance. Bagging and random forest reduce variance and lead to the lower bias, compared to the single depth-5 tree.

Question 4: Boosting [15 pts]

In this question we explore a different kind of ensemble method, boosting, where each new model is trained on a dataset weighted towards observations that the current set of models predicts incorrectly.

We'll focus on the AdaBoost flavor of boosting and examine what happens to the ensemble model's accuracy as the algorithm adds more predictors to the ensemble.

4.1 We'll motivate AdaBoost by noticing patterns in the errors that a single classifier makes. Fit `tree1`, a decision tree with depth 3, to the training data. For each predictor, make a plot that compares two distributions: the values of that predictor for examples that `tree1` classifies correctly, and the values of that predictor for examples that `tree1` classifies incorrectly. Do you notice any predictors for which the distributions are clearly different?

4.2 The following code attempts to implement a simplified version of boosting using just two classifiers (described below). However, it has both stylistic and functionality flaws. First, imagine that you are a grader for a Data Science class; write a comment for the student who submitted this code. Then, imagine that you're the TF writing the solutions; make an excellent example implementation. Finally, use your corrected code to compare the performance of `tree1` and the boosted algorithm on both the training and test set.

4.3 Now let's use the sklearn implementation of AdaBoost: Use `AdaBoostClassifier` to fit another ensemble to `X_train`. Use a decision tree of depth 3 as the base learner and a learning rate 0.05, and run the boosting for 800 iterations. Make a plot of the effect of the number of estimators/iterations on the model's train and test accuracy.

Hint: The `staged_score` method provides the accuracy numbers you'll need. You'll need to use `list()` to convert the "generator" it returns into an ordinary list.

4.4 Repeat the plot above for a base learner with depth of (1, 2, 3, 4). What trends do you see in the training and test accuracy?

(It's okay if your code re-fits the depth-3 classifier instead of reusing the results from the previous problem.)

4.5 Based on the plot you just made, what combination of base learner depth and number of iterations seems optimal? Why? How does the performance of this model compare with the performance of the ensembles you considered above?

Answers

4.1

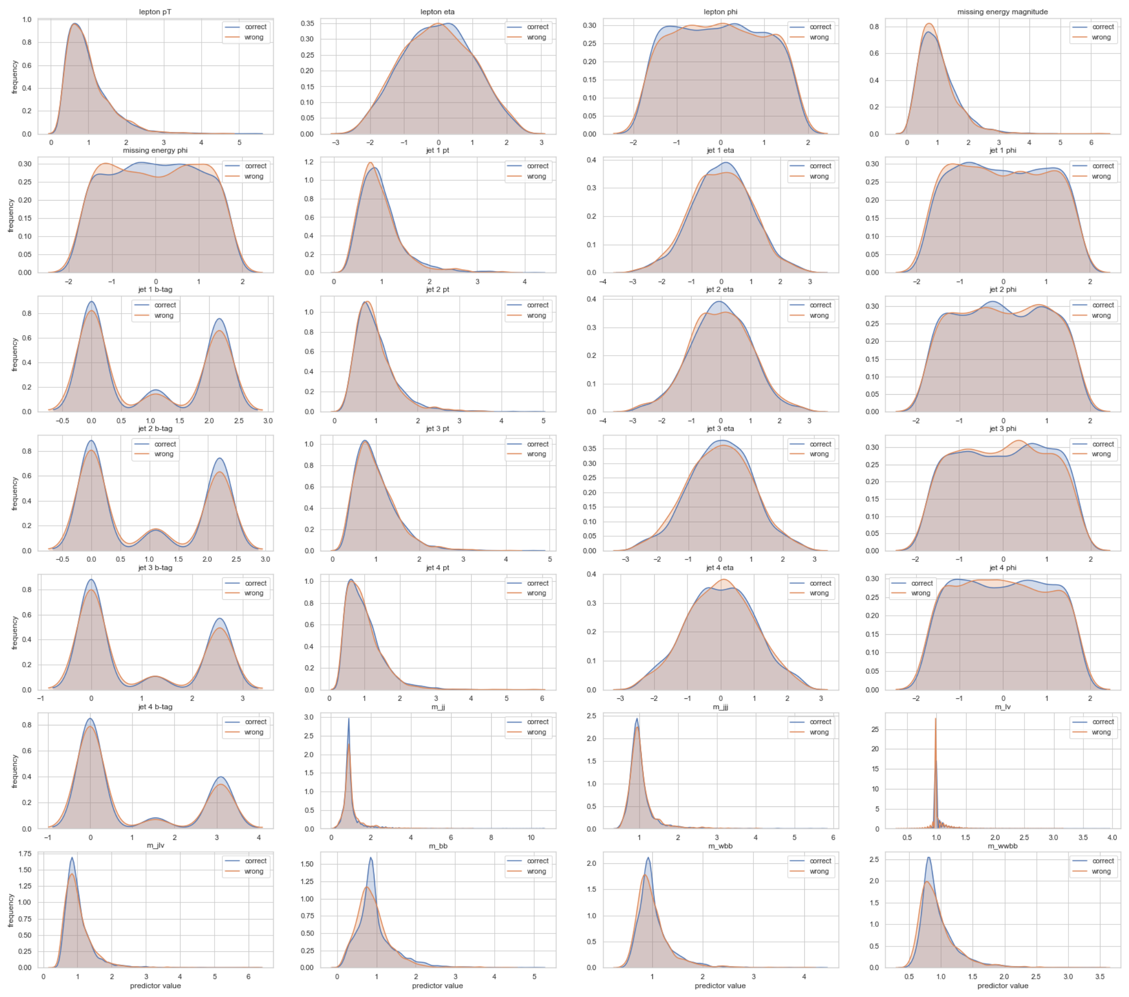
Hints: - If you have `fig, axs = plt.subplots(...)`, then `axs.ravel()` gives a list of each plot in reading order. - `sns.kdeplot` takes `ax` and `label` parameters.

```
In [33]: tree1 = DecisionTreeClassifier(max_depth=3).fit(X_train, y_train)

         y_train_predicted_tree1 = tree1.predict(X_train)

         y_train_predicted_tree1_bool = y_train_predicted_tree1 == y_train
         X_train_correct = X_train[y_train_predicted_tree1_bool]
         X_train_wrong = X_train[np.logical_not(y_train_predicted_tree1_bool)]
```

```
In [34]: fig, axs = plt.subplots(7, 4, figsize=(30, 27))
         i = 0;
         for ax in axs.ravel():
             sns.kdeplot(X_train_correct[:,i], ax=ax, shade=True, label='correct')
             sns.kdeplot(X_train_wrong[:,i], ax=ax, shade=True, label='wrong')
             ax.set_title(data_train.columns[i])
             if i >= 24:
                 ax.set_xlabel('predictor value')
             if i%4 == 0:
                 ax.set_ylabel('frequency')
             i += 1
         fig.suptitle("Distribution of predictors' values per classification success", fontsiz
```

```
C:\ProgramData\Anaconda3\lib\site-packages\scipy\stats\stats.py:1713: FutureWarning: Using a no
  return np.add.reduce(sorted[indexer] * weights, axis=axis) / sumval
```

Distribution of predictors' values per classification success



The distribution of samples' values for correct vs. wrong predictions is almost identical. This evidence suggests that the likeliwood that a sample could be missclassified does not depend on its value. Therefore we can improve the predictive capability of the tree by combining it with another tree trained on miss-classification information. This is the motivation behind doing boosting.

4.2

The intended functionality is the following: 1. Fit `tree1`, a decision tree with max depth 3. 2. Construct an array of sample weights. Give a weight of 1 to samples that `tree1` classified correctly, and 2 to samples that `tree1` misclassified. 3. Fit `tree2`, another depth-3 decision tree, using those sample weights. 4. To predict, compute the probabilities that `tree1` and `tree2` each assign to the positive class. Take the average of those two probabilities as the prediction probability.

```
In [35]: def boostmeup():
             tree = DecisionTreeClassifier(max_depth=3)
             tree1 = tree.fit(X_train, y_train)
```

```
        sample_weight = np.ones(len(X_train))
        q = 0
        for idx in range(len(X_train)):
          if tree1.predict([X_train[idx]]) != y_train[idx]:
             sample_weight[idx] = sample_weight[idx] * 2
             q = q + 1
        print("tree1 accuracy:", 1-q / len(X_train))
        tree2 = tree.fit(X_train, y_train, sample_weight=sample_weight)

    # Train
        q = 0
        for idx in range(len(X_train)):
            t1p = tree1.predict_proba([X_train[idx]])[0][1]
            t2p = tree2.predict_proba([X_train[idx]])[0][1]
            m = (t1p + t2p) / 2
            if m > .5:
                if y_train[idx] == True:
                    q = q + 0
                else:
                    q = q + 1
            else:
                if y_train[idx] == True:
                    q = q + 1
                else:
                    q = 0
        print("Boosted accuracy:", q / len(X_train))

    # Test
        q = 0
        for idx in range(len(X_test)):
            t1p = tree1.predict_proba([X_test[idx]])[0][1]
            t2p = tree2.predict_proba([X_test[idx]])[0][1]
            m = (t1p + t2p) / 2
            if m > .5:
                if y_train[idx] == True:
                    q = q + 0
                else:
                    q = q + 1
            else:
                if y_train[idx] == True:
                    q = q + 1
                else:
                    q = 0
        print("Boosted accuracy:", q / len(X_test))

    boostmeup()
```

```
tree1 accuracy: 0.6417999999999999
```

```
Boosted accuracy: 0.0008
Boosted accuracy: 0.002
```

- the predictions can be made outside the for loop for the whole training dataset instead of sample-wise
- the weight 2 could be assigned directly instead of doing a multiplication 1 * 2
- the count of successfully predicted samples can be done using boolean arrays
- the tree accuracy appears to be the misscalssification rate. It might be better to use the sklearn accuracy_score function.
- the whole for loop can be replace by np array operations, which are faster
- the X_train and y_train can be given as function parameters

```
In [40]: tree1 = DecisionTreeClassifier(max_depth=3).fit(X_train, y_train)

         y_train_predicted_tree1 = tree1.predict(X_train)
         y_test_predicted_tree1 = tree1.predict(X_test)

         y_train_predicted_tree1_bool = y_train_predicted_tree1 == y_train

         sample_weights = np.ones(len(X_train))
         sample_weights[np.logical_not(y_train_predicted_tree1_bool)] = 2

         tree2 = DecisionTreeClassifier(max_depth=3).fit(X_train, y_train, sample_weight=sampl
         y_train_predicted_tree2 = tree2.predict(X_train)
         y_test_predicted_tree2 = tree2.predict(X_test)

         y_train_predicted_boosted = ((tree1.predict_proba(X_train)[:,1] + tree2.predict_proba
         y_test_predicted_boosted = ((tree1.predict_proba(X_test)[:,1] + tree2.predict_proba(X
```

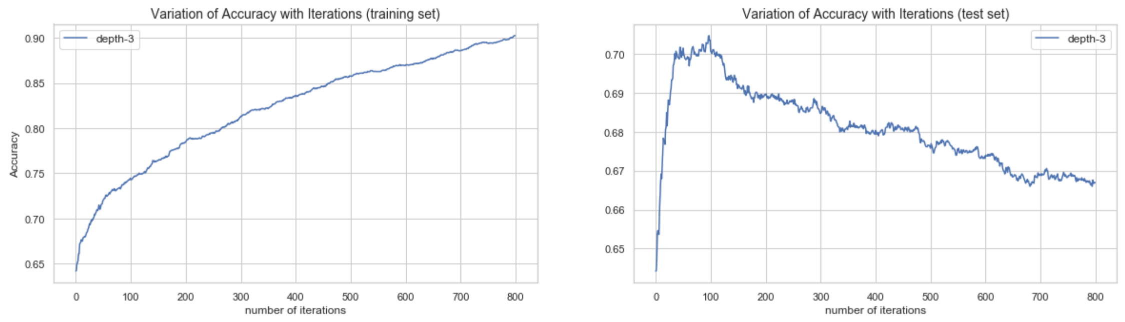
```
In [42]: models_benchmark_df = models_benchmark_df.append(pd.DataFrame({'classifier':['single
                       'training accuracy': [accuracy_score(y_train, y_train_predicted_tree1),
                                             accuracy_score(y_train, y_train_predicted_tree2),
                                             accuracy_score(y_train, y_train_predicted_boosted
                       'test accuracy': [accuracy_score(y_test, y_test_predicted_tree1),
                                             accuracy_score(y_test, y_test_predicted_tree2),
                                             accuracy_score(y_test, y_test_predicted_boosted)]
         models_benchmark_df.drop_duplicates()
```

```
Out[42]:                                    classifier  training accuracy  test accuracy
         0  single tree with best depth-5 chosen by CV             0.6812         0.6480
         1                          single depth-20 tree             1.0000         0.6064
         2                       bagging 45 depth-20 trees             0.9996         0.6822
         3               Random Forest of 45 depth-20 trees             0.9996         0.6834
         0                           single depth-3 tree             0.6418         0.6442
         1      single depth-3 tree with updated weights             0.6134         0.6088
         2                 manually boosted depth-3 tree             0.6488         0.6510
```

4.3

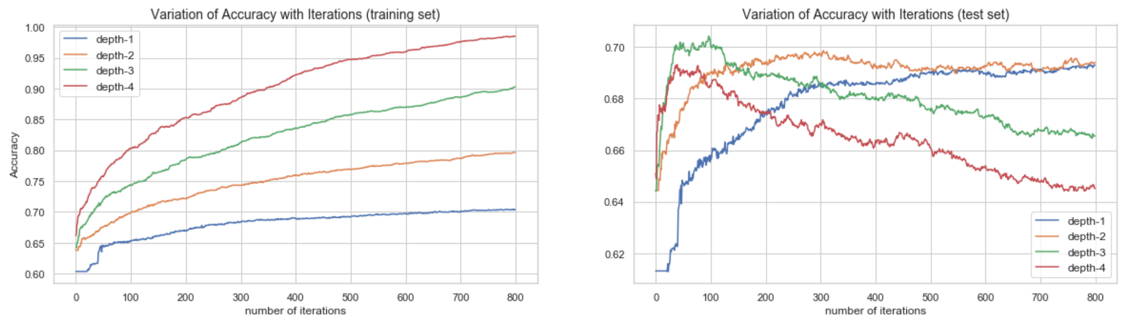
```
In [43]: def run_adaboosting(X_train, y_train, X_test, y_test, depths=[3], iterations=800, lr=(
             fig, ax = plt.subplots(1,2,figsize=(20,5))
             ab_train_scores = np.zeros((iterations, len(depths)))
             ab_test_scores = np.zeros((iterations, len(depths)))
             for i, depth in enumerate(depths):
                 ab_model = AdaBoostClassifier(base_estimator=DecisionTreeClassifier(max_depth=
                 ab_model.fit(X_train, y_train);
                 train_scores = list(ab_model.staged_score(X_train,y_train))
                 test_scores = list(ab_model.staged_score(X_test, y_test))
                 ab_train_scores[:, i] = np.array(train_scores)
                 ab_test_scores[:, i] = np.array(test_scores)
                 ax[0].plot(train_scores,label='depth-{}'.format(depth))
                 ax[1].plot(test_scores,label='depth-{}'.format(depth))
             ax[0].set_xlabel('number of iterations', fontsize=12)
             ax[1].set_xlabel('number of iterations', fontsize=12)
             ax[0].set_ylabel('Accuracy', fontsize=12)
             ax[0].set_title("Variation of Accuracy with Iterations (training set)", fontsize=1
             ax[1].set_title("Variation of Accuracy with Iterations (test set)", fontsize=14)
             ax[0].legend(fontsize=12);
             ax[1].legend(fontsize=12);
             return ab_train_scores, ab_test_scores
```

```
In [44]: ab_train_scores, ab_test_scores = run_adaboosting(X_train, y_train, X_test, y_test)
```



4.4

```
In [45]: tree_depths = [1,2,3,4]
         ab_train_scores, ab_test_scores = run_adaboosting(X_train, y_train, X_test, y_test, de
```



With boosting we learn from the residuals of the previous tree in each new iteration, therefore we observe an increasing training set accuracy until we will overfit the data and observe a steady state close to 100%.

The tree depth affects the trends pretty much. The training set accuracy is higher with bigger trees, regardless the number of iterations. The variation of test set accuracy is not consistent for different tree depths. Depth-1 and depth-2 trees can be considered as very slow learners, which require a higher number of iterations. Depth-3 and depth-4 trees are learning faster; the test set accuracy increases steadily during the first iterations until it reaches a peak, then it decreases with increasing number of iterations. While depth-1 and depth-2 trees underfit the data, depth-4 tree overfits the most. The lowest variance and lowest biais is suggested by depth 3.

4.5

```
In [46]: best_nb_iterations = np.array([ab_test_scores[:,i].argmax() for i in range(len(tree_de
         best_test_scores = np.array([ab_test_scores[best_nb_iterations[i],i] for i in range(le
         optimal_tree_depth_idx = best_test_scores.argmax()
         optimal_nb_iterations = best_nb_iterations[optimal_tree_depth_idx]
         optimal_tree_depth = tree_depths[optimal_tree_depth_idx]
         optimal_test_score = ab_test_scores[optimal_nb_iterations, optimal_tree_depth_idx]
         optimal_train_score = ab_train_scores[optimal_nb_iterations, optimal_tree_depth_idx]
         print('The combination of base learner depth {} and {} iterations achieves the best ac
```

```
The combination of base learner depth 3 and 97 iterations achieves the best accuracy 70.42% on
```

```
In [47]: models_benchmark_df = models_benchmark_df.append(pd.DataFrame({'classifier':['ada-boos
                              'training accuracy': [optimal_train_score],
                              'test accuracy': [optimal_test_score]}))
```

Ada-boosted depth-3 decisision tree classifier obtained after 97 boosting iterations seems optimal in terms of low variance and low bias. Ada-boosting achieves better accuracy than the manually boosted depth-3 tree using updated weights in question 4.2. The improved accuracy suggests that ada-boosting actually helps quite much.

Question 5: Understanding [15 pts]

This question is an overall test of your knowledge of this homework's material. You may need to refer to lecture notes and other material outside this homework to answer these questions.

5.1 How do boosting and bagging relate: what is common to both, and what is unique to each?

5.2 Reflect on the overall performance of all of the different classifiers you have seen throughout this assignment. Which performed best? Why do you think that may have happened?

5.3 What is the impact of having too many trees in boosting and in bagging? In which instance is it worse to have too many trees?

5.4 Which technique, boosting or bagging, is better suited to parallelization, where you could have multiple computers working on a problem at the same time?

5.5 Which of these techniques can be extended to regression tasks? How?

Answers:

5.1

Bagging and boosting are so-called 'ensemble' techniques, which by aggregating many weak-learner models such as single decision trees, substantially improve the predictive accuracy.

Bagging works by fitting a weak-learner to multiple boostraps of the same data and aggregating their predictions into a single outcome. Although bagging can be parallelized, boosting works sequentially by starting with a weak-learner and adding up a new model trained on residuals of the weak-learner. This process is repeated several times and each model is trained by a modified version of the original dataset, regularized using a learning rate.

5.2

```
In [48]: models_benchmark_df.drop_duplicates()
```

```
Out[48]:                             classifier  training accuracy  test accuracy
         0  single tree with best depth-5 chosen by CV             0.6812         0.6480
         1                          single depth-20 tree             1.0000         0.6064
         2                      bagging 45 depth-20 trees            0.9996         0.6822
         3              Random Forest of 45 depth-20 trees           0.9996         0.6834
         0                           single depth-3 tree             0.6418         0.6442
         1        single depth-3 tree with updated weights           0.6134         0.6088
         2                   manually boosted depth-3 tree           0.6488         0.6510
         0                         ada-boosted depth-3 tree          0.7428         0.7042
```

Ada-boosting performs the best. Instead of fitting a single large decision tree to the data with potentially overfitting, our Ada-boosted model learns slowly on updated versions of training data using a smaller tree.

5.3

Unlike bagging, boosting can overfit if the number of trees is too large. This overfit can be avoid by choosing number of trees via cross-validation. The number of trees is no a critical parameter for bagging, a large number will not lead to overfitting because of the aggregation. With bagging we are able to squeeze out the variance. With boosting a large number of trees we fit down to each single residual and end up fitting the model to each single sample of the training set. This overfitting can be avoided by regularization or by early stopping as soon as the validation loss starts raizing.

5.4

Each tree in bagging can be trained independently of the others. Therefore bagging technique is better suited to parallelization for example on a multi-core CPU computer. Boosting is sequential since each tree is built using the previous one.

5.5

Bagging can improve prediction for many regression methods such as least-square linear regression, by fitting a linear regression model to multiple training datasets obtained via bootstrap and averaging the resulting predictions. Moreover the out-of-bag samples can be used for validation.

Boosting can be applied to regression tasks as well. Here we do not work on boostraped data, instead we fit a model on the original data, the next model is fit on the residuals obtained; the predictions of both models are weighted with the learning rate and summed up.

Question 6: Explaining Complex Concepts Clearly [10 pts]

One of the core skills of a data scientist is to be able to explain complex concepts clearly. To practice this skill, you'll make a short presentation of one of the approaches we have recently studied.

Choose one of the following topics:

- Decision Trees
- Random Forests
- Bagging
- Boosting
- Simple Neural Nets (like the MLP we saw in Homework 6)
- (other topics are possible, but get staff approval first)

Make 3 slides explaining the concept.

- Focus on **clear explanations**, NOT aesthetic beauty. Photos of pen-and-paper sketches are fine if they're legible.
- For your audience, choose **future CS109A students**.
- You may take inspiration from anywhere, but explain in **your own words** and **make your own illustrations**.

Submit your slides as a PDF and the source format (`.pptx`, Google Slides, etc.)

NOTE: If you would be okay with us using your slides for future classes (with attribution, of course), please include a note to that effect. This will not affect your grade either way.

1.3 Google Slides presentation

The presentation can be used for future classes.

https://docs.google.com/presentation/d/1ggM5kmSSOOcY4x8-ecluDQOpybIb3uJv2Ev-AvNlnXU/