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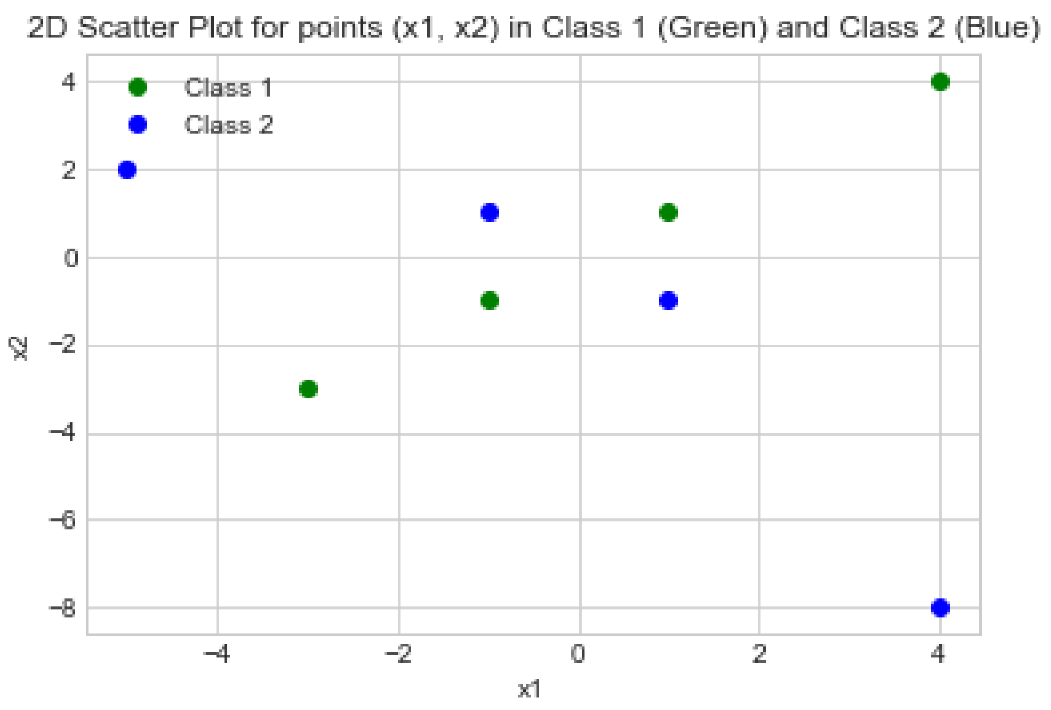
0.1 Problem 1 - Linear Separability

0.1.1 Answer 1.1

```
In [1]: import numpy as np
        import matplotlib.pyplot as plt

        plt.style.use('seaborn-whitegrid')

        %matplotlib inline

In [2]: x_class_1 = np.array([-1, 1, -3, 4])
        y_class_1 = np.array([-1, 1, -3, 4])

        x_class_2 = np.array([-1, 1, -5, 4])
        y_class_2 = np.array([1, -1, 2, -8])

        plt.plot(x_class_1, y_class_1, 'o', color='green', label='Class 1')
        ax = plt.gca()
        ax.set(xlabel = 'x1', ylabel = 'x2')

        plt.plot(x_class_2, y_class_2, 'o', color='blue', label='Class 2')
        ax = plt.gca()
        ax.set(xlabel = 'x1', ylabel = 'x2')

        plt.title('2D Scatter Plot for points (x1, x2) in Class 1 (Green) and Class 2 (Blue)')
        plt.legend()
        plt.show()
```



Let the first set of points belongs to Class 1 and the other set belongs to Class 2.

Green points denote Class 1 while Blue Points denote Class 2. x_1 is the horizontal dimension while x_2 is the vertical one.

We can see from the plot above that the dataset IS NOT LINEARLY SEPARABLE using any linear function/classifier, given only two features $ x_1$ and x_2 (without further transformation into a higher space).

0.1.2 Answer 1.2

Looking at the points from Class 1 and Class 2, we could see that: 1. x_1 and x_2 in Class 1 are of the same sign 2. x_1 and x_2 in Class 2 are of the opposite sign

Thus, we could propose some z such as:

$$z = x_1 * x_2$$

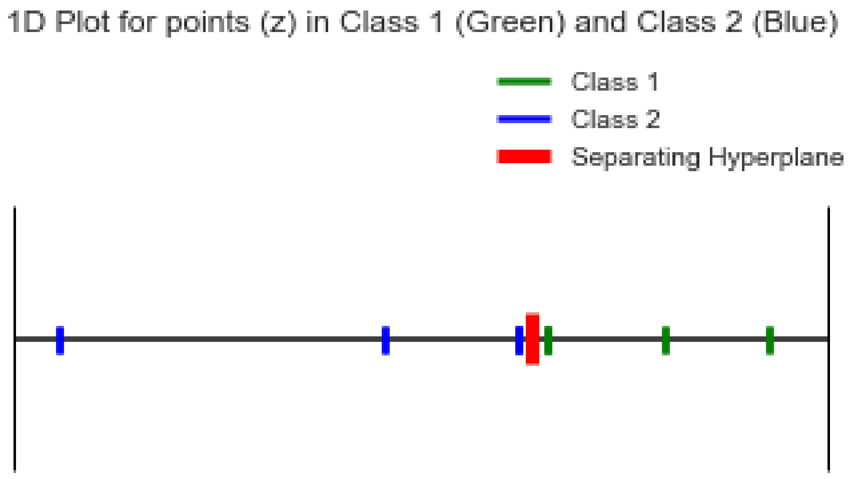
This is linearly separable because Class 1 will all have positive values of z while Class 2 will all have negative values of z.

0.1.3 Answer 1.3

Suppose we have a 1D plane which plots z for Class 1 and Class 2. Green lines denote Class 1 while Blue Points denote Class 2.

The separating hyperplane (or point, because this is 1D) is simply $z = c$, where c is any constant satisfying $-1 < c < 1$. I pick $c = 0$, which is denoted by the thick and short red line in the plot.

```
In [3]: z_class_1 = np.multiply(x_class_1, y_class_1)
        z_class_2 = np.multiply(x_class_2, y_class_2)

        z_class_1 = np.repeat(z_class_1, 2)
        z_class_2 = np.repeat(z_class_2, 2)

        plt.figure()
        plt.hlines(1, -35, 20)

        plt.eventplot(z_class_1, orientation='horizontal', colors='green', linelengths=0.1, line
        plt.eventplot(z_class_2, orientation='horizontal', colors='blue', linelengths=0.1, linew

        plt.eventplot([-35, 20], orientation='horizontal', colors='black', linelengths=1, linewi
        plt.eventplot([0], orientation='horizontal', colors='red', linelengths=0.2, linewidths=5

        plt.axis('off')

        plt.title('1D Plot for points (z) in Class 1 (Green) and Class 2 (Blue)')
        plt.legend()
        plt.show()
```



0.1.4 Answer for Problem 1.4

Question

Explain the importance of nonlinear transformations in classification problems.

Answer

Nonlinear transformations are important to help classifier create a decision boundary for dataset that are not linearly separable. For example, in scikit-learn, there is a package called Kernel SVM which use a Kernel to project the non-linearly separable data in some lower dimension to linearly separable data in some higher dimensions so that the data points belonging to different classes are allocated to different dimensions.

Reference: https://stackabuse.com/implementing-svm-and-kernel-svm-with-pythons-scikit-learn/#:~:text=Rather%2C%20a%20modified%20version%20of,are%20allocated%20to%20different%20dimensio

0.2 Problem 2 - Bias Variance Tradeoff, Regularization

0.2.1 Answer 2.1

$$E[MSE] = E[\frac{1}{t}\sum_{i=1}^{t}(f(x_i) + \epsilon - g(x_i))^2]$$

Introduce terms $E[g(x_i]$ that will cancel each other:

$$E[MSE] = E[\frac{1}{t}\sum_{i=1}^{t}(f(x_i) + \epsilon - g(x_i) + E[g(x_i)] - E[g(x_i)])^2]$$

Using linearity in expectation:

$$E[MSE] = E[\frac{1}{t}\sum_{i=1}^{t}(f(x_i) - E[g(x_i)])^2 + \frac{1}{t}\sum_{i=1}^{t}E[\epsilon^2] + \frac{1}{t}\sum_{i=1}^{t}E[(E[g(x_i)] - g(x_i))^2] + \frac{2}{t}\sum_{i=1}^{t}E[\epsilon(f(x_i) - E[g(x_i)])] + \frac{2}{t}$$

Notice that $E[g(x_i)] = g(x_i)$, so that lefts us with:

$$E[MSE] = E[\frac{1}{t}\sum_{i=1}^{t}(f(x_i) - E[g(x_i)])^2 + \frac{1}{t}\sum_{i=1}^{t}E[\epsilon^2] + \frac{1}{t}\sum_{i=1}^{t}E[(E[g(x_i)] - g(x_i))^2]$$

Again, using linearity in expectation:

$$E[MSE] = E[\frac{1}{t}\sum_{i=1}^{t}(f(x_i) - E[g(x_i)])^2] + E[\frac{1}{t}\sum_{i=1}^{t}E[\epsilon^2]] + E[\frac{1}{t}\sum_{i=1}^{t}E[(E[g(x_i)] - g(x_i))^2]$$

$$E[MSE] = \frac{1}{t}\sum_{i=1}^{t}(f(x_i) - E[g(x_i)])^2 + \frac{1}{t}\sum_{i=1}^{t}E[\epsilon^2] + \frac{1}{t}\sum_{i=1}^{t}E[(E[g(x_i)] - g(x_i))^2$$

$$E[MSE] = \frac{1}{t}\sum_{i=1}^{t}(f(x_i) - E[g(x_i)])^2 + \frac{1}{t}\sum_{i=1}^{t}E[(E[g(x_i)] - g(x_i))^2] + \frac{1}{t}(t)E[\epsilon^2]$$

$$E[MSE] = \frac{1}{t}\sum_{i=1}^{t}(f(x_i) - E[g(x_i)])^2 + \frac{1}{t}\sum_{i=1}^{t}E[(E[g(x_i)] - g(x_i))^2] + E[\epsilon^2]$$

Finally:

$$E[MSE] = Bias[g(x)]^2 + Var[g(x)] + Noise$$

where:

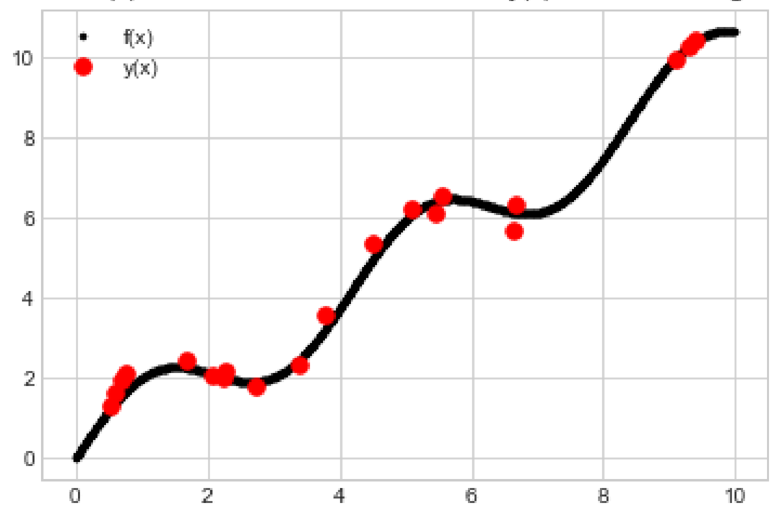
1. $Bias[g(x)]^2 = \frac{1}{t}\sum_{i=1}^{t}(f(x_i) - E[g(x_i)])^2$
2. $Var[g(x)] = \frac{1}{t}\sum_{i=1}^{t} E[(E[g(x_i)] - g(x_i))^2$
3. $Noise = E[\epsilon^2]$

0.2.2 Answer 2.2

The black line plot depicts $f(x)$ while the red dots (20 in total) are the samples drawn from $y(x)$.

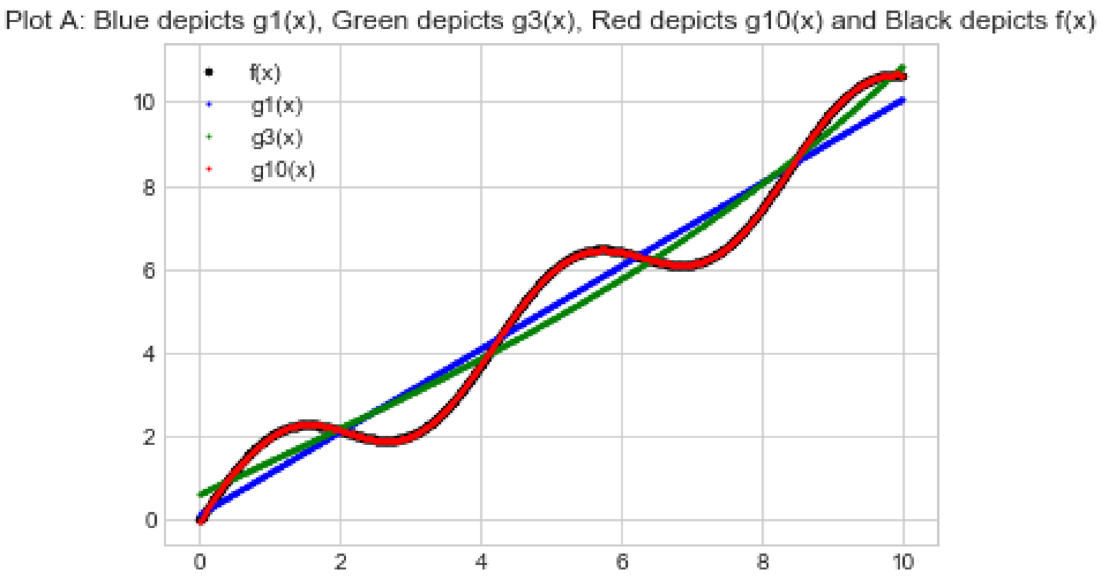
```
In [4]: def f_x(x):
            return x + np.sin((3/2)*x)

        x_smooth = np.arange(0, 10, 0.01)
        f_x_plot_dots = f_x(x_smooth)

        def generate_sample_from_y(x_rand, use_noise):
            y = f_x(x_rand)

            if use_noise:
                y = y + np.random.normal(0, 0.3, len(x_rand))

            return y

        x_rand = np.random.uniform(0, 10, 20)
        y_x_plot_dots = generate_sample_from_y(x_rand, True)


        plt.plot(x_smooth, f_x_plot_dots, 'o', color='black', markersize=2.5, label='f(x)')
        plt.plot(x_rand, y_x_plot_dots, 'o', color='red', markersize=7.5, label='y(x)')

        plt.title('Smooth Line Plot for f(x): Black Line and Scatter Plot for y(x): Red Dots usi
        plt.legend()
        plt.show()
```

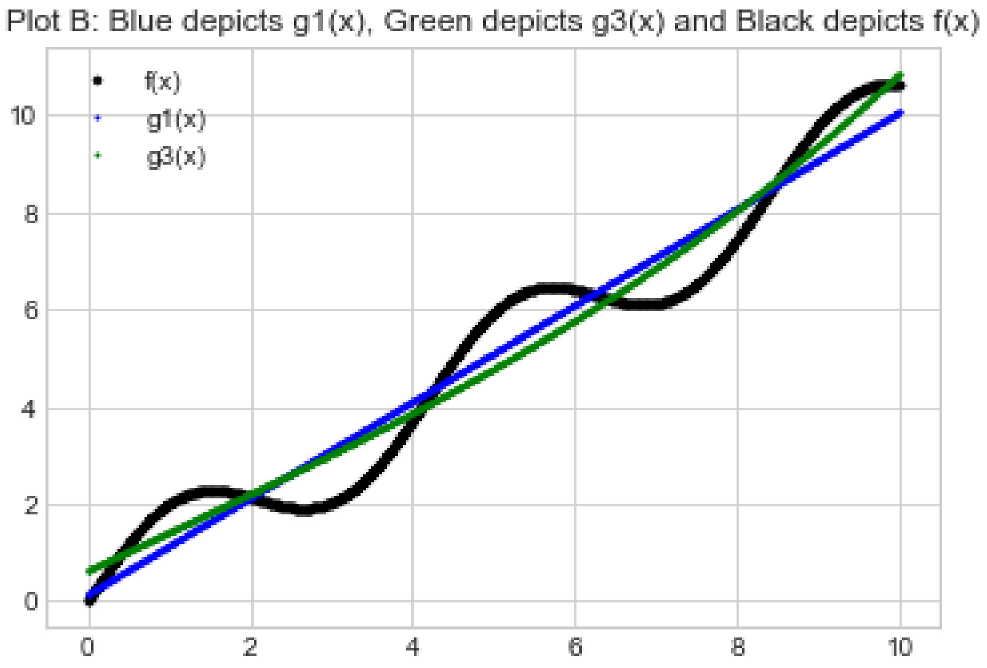
Smooth Line Plot for f(x): Black Line and Scatter Plot for y(x): Red Dots using 20 random points



0.2.3 Answer 2.3

```
In [5]: from sklearn.preprocessing import PolynomialFeatures
        from sklearn.pipeline import make_pipeline
        from sklearn.linear_model import LinearRegression

        reshape_x_smooth = x_smooth.reshape(-1, 1)

        g_1 = make_pipeline(PolynomialFeatures(1), LinearRegression())
        g_1.fit(reshape_x_smooth, f_x(x_smooth).reshape(-1, 1))

        g_3 = make_pipeline(PolynomialFeatures(3), LinearRegression())
        g_3.fit(reshape_x_smooth, f_x(x_smooth).reshape(-1, 1))

        g_10 = make_pipeline(PolynomialFeatures(10), LinearRegression())
        g_10.fit(reshape_x_smooth, f_x(x_smooth).reshape(-1, 1))

        plt.plot(x_smooth, f_x_plot_dots, 'o', color='black', markersize=2.5, label='f(x)')
        plt.plot(x_smooth, g_1.predict(reshape_x_smooth), 'o', color='blue', markersize=1, label
        plt.plot(x_smooth, g_3.predict(reshape_x_smooth), 'o', color='green', markersize=1, labe
        plt.plot(x_smooth, g_10.predict(reshape_x_smooth), 'o', color='red', markersize=1, label

        plt.title('Plot A: Blue depicts g1(x), Green depicts g3(x), Red depicts g10(x) and Black
        plt.legend()
        plt.show()

        plt.plot(x_smooth, f_x_plot_dots, 'o', color='black', markersize=2.5, label='f(x)')
        plt.plot(x_smooth, g_1.predict(reshape_x_smooth), 'o', color='blue', markersize=1, label
        plt.plot(x_smooth, g_3.predict(reshape_x_smooth), 'o', color='green', markersize=1, labe
        plt.title('Plot B: Blue depicts g1(x), Green depicts g3(x) and Black depicts f(x)')
        plt.legend()
        plt.show()
```





In the first plot, Plot A, we can see that $g_1(x)$ (blue line) and $g_2(x)$ (green line) are underfitting while $g_{10}(x)$ (red line) is overfitting. $f(x)$, which is the black line, is fully overlayed by $g_{10}(x)$, the red line.

To make it clearer, I provide Plot B, in which I get ride of $g_{10}(x)$, i.e. the red line. We can compare that $g_{10}(x)$ resembles $f(x)$ quiet a lot, indicating overfitting.

0.2.4 Answer 2.4

Function to Generate Datasets and to Simulate the Training

```
In [6]: from numpy import polyfit, polyval
        from sklearn.metrics import mean_squared_error

        def generate_dataset(n_sample, x_low, x_high, n_dataset, test_frac, seed):
            np.random.seed(seed)

            x_rand = np.random.uniform(x_low, x_high, n_sample)

            slice_idx = int(test_frac * n_sample)

            x_train = x_rand[:slice_idx]
            x_test = x_rand[slice_idx:]

            # y without noise
            y_x_plot_dots = generate_sample_from_y(x_rand, False)
            y_train = y_x_plot_dots[:slice_idx]
            y_test = y_x_plot_dots[slice_idx:]

            # y with noise
            y_train_sets_noise = []
            y_test_sets_noise = []

            # Generate y_train and y_test
            for i in range(0, n_dataset):
                y_x_plot_dots_noise = generate_sample_from_y(x_rand, True)

                y_train_sets_noise.append(y_x_plot_dots_noise[:slice_idx])
                y_test_sets_noise.append(y_x_plot_dots_noise[slice_idx:])

            return x_train.reshape(-1, 1), x_test.reshape(-1, 1), y_train, y_test, y_train_sets_

        def compute_error(y_test, y_pred):
            y_test = y_test.flatten()
            y_pred = y_pred.flatten()

            assert y_test.shape == (10, )
            assert y_pred.shape == (10, )
            return mean_squared_error(y_pred, y_test)

        def simulate(degree_low, degree_high, x_train, x_test, y_train_sets_noise, y_test_sets_n
            x_train = x_train.flatten() # polyfit needs 1D vector

            y_preds_train = [] # (15, 100, 40, 1)
            y_preds_test = [] # (15, 100, 10, 1)
            test_err = [] # (15, 100, 10, 1)

            models = []

            for degree in range(degree_low - 1, degree_high):
                y_preds_train.append([])
                y_preds_test.append([])
                test_err.append([])

            for i in range(0, len(y_train_sets_noise)):
                y_train_noise = y_train_sets_noise[i].reshape(-1, 1)
                y_test_noise = y_test_sets_noise[i].reshape(-1, 1)

                for degree in range(degree_low - 1, degree_high):
                    model = None
                    # IMPORTANT: Increment the degree by 1 shere so it depicts the real degree
                    # Funny story: I spend almost one hour debugging this offset bug
                    model = polyfit(x_train, y_train_noise, degree + 1)
                    models.append(model)

                    y_pred_test = polyval(model, x_test)
                    y_preds_test[degree].append(y_pred_test)

                    # IMPORTANT: For error, use y WITH NOISE
                    test_err[degree].append(compute_error(y_test_noise, y_pred_test))

            return models, np.array(y_preds_test), np.array(test_err)
```

Function to Compute Bias, Variance and Error

```
In [7]: def compute_squared_bias(y_test, y_preds_test):
            # E[g(x)]
            avg_y_preds_test = y_preds_test.mean(axis=0)

            # Sanity check
            assert avg_y_preds_test.shape == (10, 1)

            # (E[g(x)] - f(x))**2
            # IMPORTANT: Use y WITHOUT NOISE
            # IMPORTANT: FLATTEN the average so it becomes (10, )
            return mean_squared_error(avg_y_preds_test.flatten(), y_test)
```

```
def compute_variance(y_preds_test):
    # IMPORTANT: Remove third dimension, (100, 10, 1) -> (100, 10)
    rows, cols = len(y_preds_test), len(y_preds_test[0])
    y_preds_test = y_preds_test.flatten().reshape(rows, cols)

    # E[g(x)]
    avg_y_preds_test = np.mean(y_preds_test, axis=0)
    # IMPORTANT: Tile to make duplicates, (10, ) -> (100, 10)
    avg_y_preds_test = np.tile(avg_y_preds_test, (100, 1))

    # (g(x) - E[g(x)])**2
    return mean_squared_error(y_preds_test, avg_y_preds_test)
```

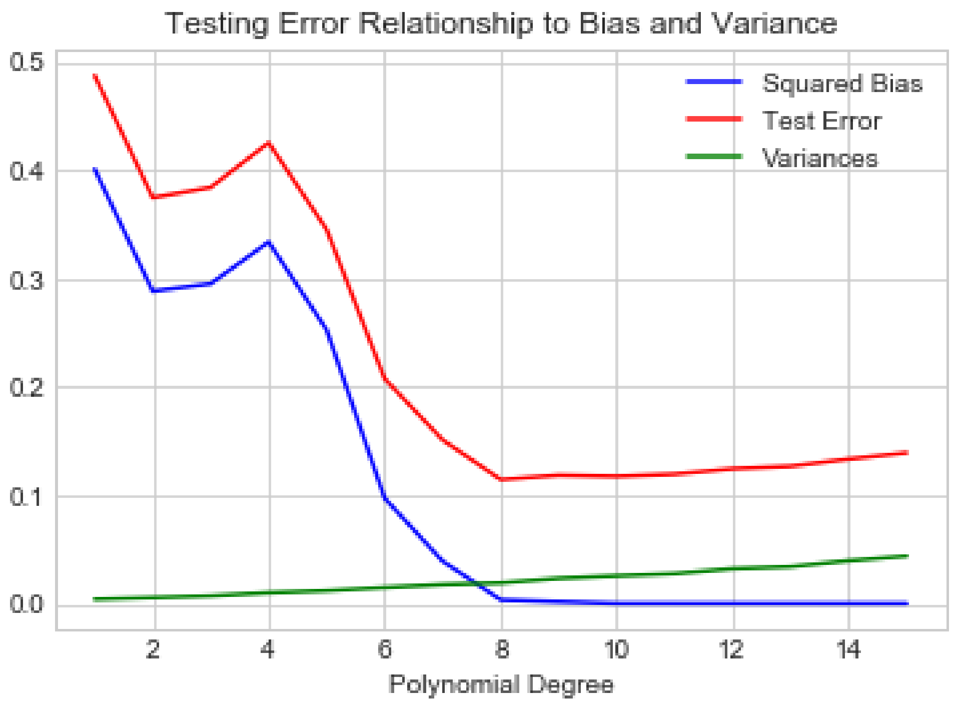
Main Routine to Get the Stats for Each Polynomial Degree

```
In [8]: x_train, x_test, y_train, y_test, y_train_sets_noise, y_test_sets_noise = generate_datas

        models, y_preds_test, test_err = simulate(1, 15, x_train, x_test, y_train_sets_noise, y_

        # Sanity check
        assert y_preds_test.shape == (15, 100, 10, 1)
        assert test_err.shape == (15, 100)

        avg_squared_biases = []
        avg_test_errs = []
        variances = []

        for degree in range(0, 15):
            curr_y_pred_test = y_preds_test[degree]

            avg_squared_biases.append(compute_squared_bias(y_test, curr_y_pred_test))
            avg_test_errs.append(np.mean(test_err[degree]))
            variances.append(compute_variance(curr_y_pred_test))
```

Plot Testing Error, Bias and Variance against Model Complexity

```
In [9]: fig, ax = plt.subplots()

        x_plots = np.arange(1, 16, 1)
        y_plots = avg_squared_biases
        ax.plot(x_plots, y_plots, color='blue', label='Squared Bias')

        x_plots = np.arange(1, 16, 1)
        y_plots = avg_test_errs
        ax.plot(x_plots, y_plots, color='red', label='Test Error')

        x_plots = np.arange(1, 16, 1)
```

```
y_plots = variances
ax.plot(x_plots, y_plots, color='green', label='Variances')

ax.set_xlabel('Polynomial Degree')

ax.set_title('Testing Error Relationship to Bias and Variance')
ax.legend()
ax.grid(True)

plt.show()
```



Identifying the Best Model

```
In [10]: best_performing_degree = np.argmin(avg_test_errs) + 1
         best_performing_degree
```

```
Out[10]: 8
```

The best performing model is the one with the lowest testing error, which is Polynomial Degree 8. We can also see that from the graph that this model seems to have a good balance between its bias and variance at Polynomial Degree 8.

0.2.5 Answer 2.5

Ridge Regression is Used to Apply L2 Regularization

```
In [11]: def warn(*args, **kwargs):
             pass

         import warnings
         warnings.warn = warn

         from sklearn.linear_model import Ridge
         from sklearn.preprocessing import PolynomialFeatures
         from sklearn.pipeline import make_pipeline

         degree = 10

         # Polynomial Degree 10 model from 2.4
         model_10 = models[degree - 1]

         # Ridge Regression, e.g. LinearRegression with L2 regularization
         # Use alpha=1.0, meaning we optimize bias and norm equally
         model_10_L2 = make_pipeline(PolynomialFeatures(degree), Ridge(alpha=1.0))

         y_preds_test_L2 = []
         test_err_L2 = []

         # Simulation Loop
         for i in range(0, len(y_train_sets_noise)):
             y_train_noise = y_train_sets_noise[i].reshape(-1, 1)
             y_test_noise = y_test_sets_noise[i].reshape(-1, 1)

             model_10_L2.fit(x_train, y_train_noise)

             y_pred_test = model_10_L2.predict(x_test)
             y_preds_test_L2.append(y_pred_test)

             # IMPORTANT: For error, use y WITH NOISE
             test_err_L2.append(compute_error(y_test_noise, y_pred_test))

         y_preds_test_L2 = np.array(y_preds_test_L2)
         test_err_L2 = np.array(test_err_L2)

         avg_squared_bias_L2 = compute_squared_bias(y_test, y_preds_test_L2)
         avg_test_err_L2 = np.mean(test_err_L2)
         variance_L2 = compute_variance(y_preds_test_L2)

         print('Model without Regularization:')
         print('Squared Bias: {}'.format(avg_squared_biases[degree-1]))
         print('MSE: {}'.format(avg_test_errs[degree-1]))
         print('Variance: {}'.format(variances[degree-1]))

         print('-----------------------------')
```

```
        print('-----------------------------')

        print('Model with L2 Regularization:')
        print('Squared Bias: {}'.format(avg_squared_bias_L2))
        print('MSE: {}'.format(avg_test_err_L2))
        print('Variance: {}'.format(variance_L2))

        print('-----------------------------')
        print('-----------------------------')
```

```
Model without Regularization:
Squared Bias: 0.00032542725998055356
MSE: 0.11739956779615142
Variance: 0.025728605869716047
-----------------------------
-----------------------------
Model with L2 Regularization:
Squared Bias: 0.06944578350660215
MSE: 0.1744139448742389
Variance: 0.01537534620983641
-----------------------------
-----------------------------
```

Explanation for Bias and MSE Comparison

From the report above, we could see:

1. The regularized model have a significantly higher bias (0.0694 vs 0.0003)
2. The regularized model also has a higher MSE (0.1744 vs 0.1174)
3. However, the regularized model has a lower variance, although not significant (0.0154 vs 0.0257)

The explanations are:

1. The regularized model has lower variance because it takes into account the solution norm, L2 to be specific, into its loss function. Its loss function is roughly: $||y - Xw||_2^2 + alpha * ||w||_2^2$ where it is an addition of bias (like normal linear regression) and the L2 norm of the solution w to some extent of alpha. I use alpha equals 1 that means we optimize both terms equally. Thus, not only the regularized model minimizes the bias, but it tries to also minimize the L2 norm at the same time, resulting in a simpler model with lower variance.

2. The consequences of having to minimize both bias and L2 norms are that we might not get the solution with optimal (minimum) bias. Hence, with L2 regularization, we frequently have lower bias and MSE.

0.3 Problem 3

0.3.1 Answer 3.1

Two datasets picked:

1. energy-efficiency (https://www.openml.org/d/1472)
2. optdigits (https://www.openml.org/d/28)

```
In [12]: import numpy as np
         import pandas as pd

         d1_path = 'data/energy-efficiency.csv'
         d1_name = 'Energy Efficiency'

         t_df = pd.read_csv(d1_path)
         t_df.head()
```

```
Out[12]:      V1     V2     V3      V4   V5  V6   V7  V8  y1  y2
         0  0.98  514.5  294.0  110.25  7.0   2  0.0   0   7  11
         1  0.98  514.5  294.0  110.25  7.0   3  0.0   0   7  11
         2  0.98  514.5  294.0  110.25  7.0   4  0.0   0   7  11
         3  0.98  514.5  294.0  110.25  7.0   5  0.0   0   7  11
         4  0.90  563.5  318.5  122.50  7.0   2  0.0   0  12  18
```

```
In [13]: d2_path = 'data/optdigits.csv'
         d2_name = 'Opt Digits'

         i_df = pd.read_csv(d2_path)
         i_df.head()
```

```
Out[13]:    input1  input2  input3  input4  input5  input6  input7  input8  input9  \
         0       0       1       6      15      12       1       0       0       0
         1       0       0      10      16       6       0       0       0       0
         2       0       0       8      15      16      13       0       0       0
         3       0       0       0       3      11      16       0       0       0
         4       0       0       5      14       4       0       0       0       0

            input10  ...  input56  input57  input58  input59  input60  input61  \
         0        7  ...        0        0        0        6       14        7
         1        7  ...        0        0        0       10       16       15
         2        1  ...        0        0        0        9       14        0
         3        0  ...        0        0        0        0        1       15
         4        0  ...        0        0        0        4       12       14

            input62  input63  input64  class
         0        1        0        0      0
         1        3        0        0      0
         2        0        0        0      7
         3        2        0        0      4
```

```
4        7        0        0      6

[5 rows x 65 columns]
```

Function to Summarize Attributes from a Dataset

```
In [14]: def get_attribute_summary(df, class_column, dname):
             df_info = {}

             df_info['num_features'] = len(df.columns) - 1 # excluding label column
             df_info['num_instances'] = len(df)
             df_info['num_classes'] = len(np.unique(df[class_column]))

             df_info['num_numerical_features'] = 0
             df_info['num_categorical_features'] = 0

             df_info['categorical_indexes'] = []

             idx = 0
             for column in df:
                 if column != class_column:
                     if str(df[column].dtypes) == 'category':
                         df_info['num_categorical_features'] = df_info['num_categorical_features
                         df_info['categorical_indexes'].append(idx)
                     else:
                         df_info['num_numerical_features'] = df_info['num_numerical_features'] +

                     idx = idx + 1

             # Some sanity check
             assert df_info['num_numerical_features'] + df_info['num_categorical_features'] == d

             print('Summary of {} dataset attributes: '.format(dname))
             print('Number of features: {}'.format(df_info['num_features']))
             print('Number of instances: {}'.format(df_info['num_instances']))
             print('Number of classes: {}'.format(df_info['num_classes']))
             print('Number of numerical features: {}'.format(df_info['num_numerical_features']))
             print('Number of categorical features: {}'.format(df_info['num_categorical_features

             return df_info
```

Attribute Summary for Dataset 1

```
In [15]: d1_classname = 'y1'

         # Even though y2 contains integer, but it is stated as a nominal variable
         # in the dataset explanation (see https://www.openml.org/d/1472)
         # Thus, I add some string prefix so it will count as nominal
```

```
        # t_df['y2'] = 'str' + t_df['y2'].astype(str)
        t_df['y2'] = t_df['y2'].astype('category')

        d1_info = get_attribute_summary(t_df, d1_classname, d1_name)
```

```
Summary of Energy Efficiency dataset attributes:
Number of features: 9
Number of instances: 768
Number of classes: 37
Number of numerical features: 8
Number of categorical features: 1
```

Attribute Summary for Dataset 2

```
In [16]: d2_classname = 'class'
         d2_info = get_attribute_summary(i_df, d2_classname, d2_name)
```

```
Summary of Opt Digits dataset attributes:
Number of features: 64
Number of instances: 5620
Number of classes: 10
Number of numerical features: 64
Number of categorical features: 0
```

0.3.2 Answer 3.2

Convert Categorical Features in Both Dataset, Both Train and Test

```
In [17]: t_df = pd.get_dummies(t_df)
         i_df = pd.get_dummies(i_df)

         # print(t_df.shape) # (768, 47)
         # print(i_df.shape) # (5620, 65)
```

Split Both Dataset into Train and Test

```
In [18]: from sklearn.model_selection import train_test_split

         t_X_train, t_X_test, t_y_train, t_y_test = train_test_split(t_df.drop(columns=[d1_class
         i_X_train, i_X_test, i_y_train, i_y_test = train_test_split(i_df.drop(columns=[d2_class
```

Generate 10 Different Train Sets

```
In [19]: def generate_ten_subsamples(X_train, y_train):
             X_train_sets = []
             y_train_sets = []
```

```
    for i in range(1, 11):
        frac = i * 10 / 100

        # Use the same random state so that we get matching X_train and y_train
        X_train_sets.append(X_train.sample(frac=frac, random_state=28))
        y_train_sets.append(y_train.sample(frac=frac, random_state=28))

    return X_train_sets, y_train_sets

t_X_train_sets, t_y_train_sets = generate_ten_subsamples(t_X_train, t_y_train)
i_X_train_sets, i_y_train_sets = generate_ten_subsamples(i_X_train, i_y_train)
```

Function to Train Dataset using Random Forests and Gradient Boosting

```
In [20]: from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
         from datetime import datetime, timedelta

         def run_train_scenario(dname, X_train_sets, y_train_sets):
             i = 0

             rf_models = []
             gb_models = []

             rf_training_times = []
             gb_training_times = []

             for X_train, y_train in list(zip(X_train_sets, y_train_sets)):
                 rf = RandomForestClassifier(n_estimators=20, max_depth=5, random_state=28)
                 gb = GradientBoostingClassifier(n_estimators=20, max_depth=5, random_state=28)

                 start = datetime.now()
                 rf.fit(X_train, y_train)
                 rf_training_times.append((datetime.now() - start).total_seconds())
                 rf_models.append(rf)

                 start = datetime.now()
                 gb.fit(X_train, y_train)
                 gb_training_times.append((datetime.now() - start).total_seconds())
                 gb_models.append(gb)

                 i = i + 1
                 total_time_elapsed = rf_training_times[len(rf_training_times) - 1] + gb_trainin
         #          print('Finished {} training for subsample {}, total time elapsed: {}'.format(

             return rf_models, gb_models, rf_training_times, gb_training_times
```

Run Training on Dataset 1

```
In [21]: t_rf_models, t_gb_models, t_rf_training_times, t_gb_training_times = run_train_scenario
```

Run Training with Dataset 2

```
In [22]: i_rf_models, i_gb_models, i_rf_training_times, i_gb_training_times = run_train_scenario
```

Create function to Compute Accuracies on Test Set

```
In [23]: from sklearn.metrics import accuracy_score

         def calculate_test_accuracies(clf_list, X_test, y_test):
             accuracies = []

             for clf in clf_list:
                 y_pred = clf.predict(X_test)
                 accuracies.append(accuracy_score(y_test, y_pred))

             return accuracies
```

Compute Test Accuracies on Dataset 1

```
In [24]: t_rf_accuracies = calculate_test_accuracies(t_rf_models, t_X_test, t_y_test)
         t_gb_accuracies = calculate_test_accuracies(t_gb_models, t_X_test, t_y_test)
```

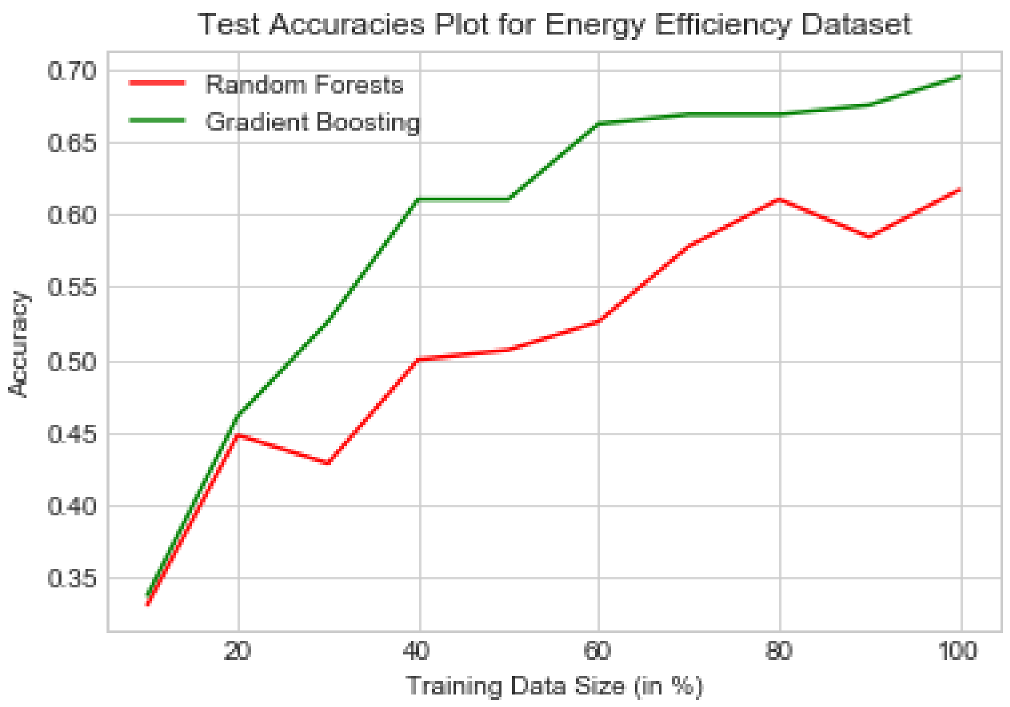
Compute Test Accuracy on Dataset 2

```
In [25]: i_rf_accuracies = calculate_test_accuracies(i_rf_models, i_X_test, i_y_test)
         i_gb_accuracies = calculate_test_accuracies(i_gb_models, i_X_test, i_y_test)
```

Plot Test Accuracies and Training Times for Dataset 1

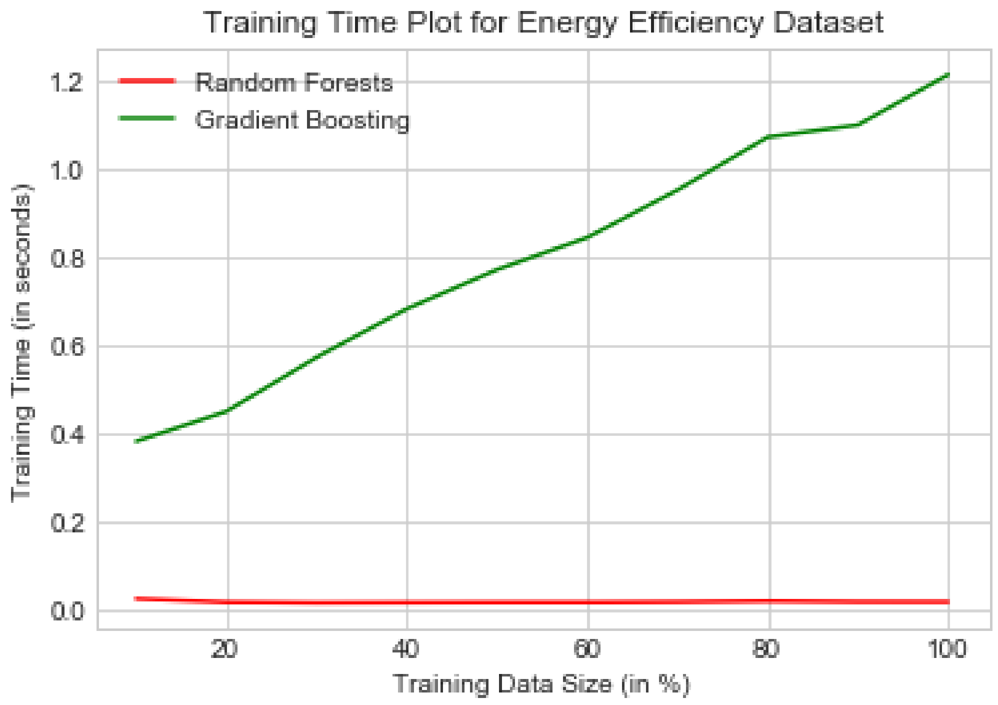
Test Accuracies

```
In [26]: fig, ax = plt.subplots()

         x_plots = np.arange(10, 110, 10)
         y_plots = t_rf_accuracies
         ax.plot(x_plots, y_plots, color='red', label='Random Forests')

         x_plots = np.arange(10, 110, 10)
         y_plots = t_gb_accuracies
         ax.plot(x_plots, y_plots, color='green', label='Gradient Boosting')

         ax.set_xlabel('Training Data Size (in %)')
         ax.set_ylabel('Accuracy')

         ax.set_title('Test Accuracies Plot for ' + d1_name + ' Dataset')
         ax.legend()
         ax.grid(True)

         plt.show()
```



Training Times

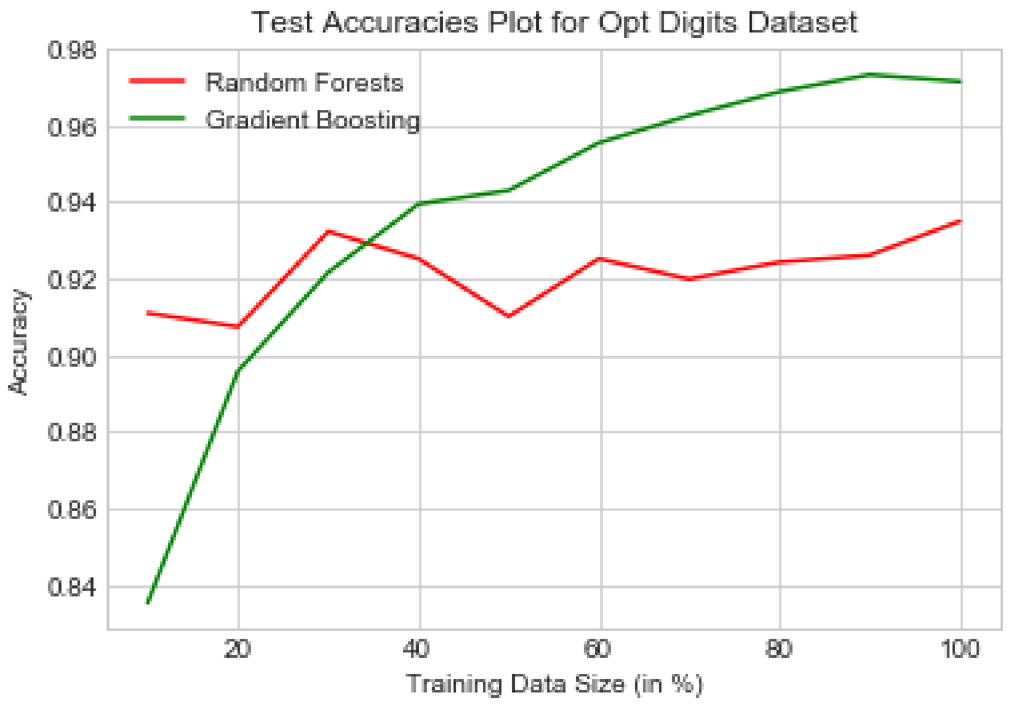
```
In [27]: fig, ax = plt.subplots()

         x_plots = np.arange(10, 110, 10)
         y_plots = t_rf_training_times
         ax.plot(x_plots, y_plots, color='red', label='Random Forests')

         x_plots = np.arange(10, 110, 10)
         y_plots = t_gb_training_times
         ax.plot(x_plots, y_plots, color='green', label='Gradient Boosting')

         ax.set_xlabel('Training Data Size (in %)')
         ax.set_ylabel('Training Time (in seconds)')

         ax.set_title('Training Time Plot for ' + d1_name + ' Dataset')
         ax.legend()
         ax.grid(True)

         plt.show()
```



Plot Test Accuracies and Training Times for Dataset 2

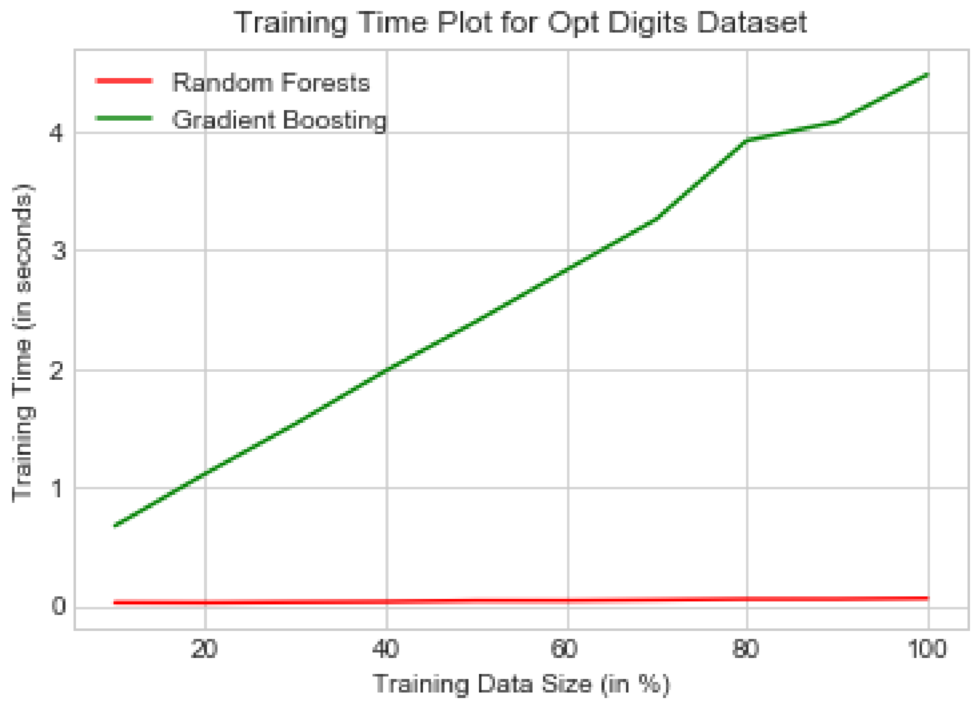
Test Accuracies

```
In [28]: fig, ax = plt.subplots()

         x_plots = np.arange(10, 110, 10)
         y_plots = i_rf_accuracies
         ax.plot(x_plots, y_plots, color='red', label='Random Forests')

         x_plots = np.arange(10, 110, 10)
         y_plots = i_gb_accuracies
         ax.plot(x_plots, y_plots, color='green', label='Gradient Boosting')

         ax.set_xlabel('Training Data Size (in %)')
         ax.set_ylabel('Accuracy')

         ax.set_title('Test Accuracies Plot for ' + d2_name + ' Dataset')
         ax.legend()
         ax.grid(True)

         plt.show()
```



Training Times

```
In [29]: fig, ax = plt.subplots()

         x_plots = np.arange(10, 110, 10)
         y_plots = i_rf_training_times
         ax.plot(x_plots, y_plots, color='red', label='Random Forests')

         x_plots = np.arange(10, 110, 10)
         y_plots = i_gb_training_times
         ax.plot(x_plots, y_plots, color='green', label='Gradient Boosting')

         ax.set_xlabel('Training Data Size (in %)')
         ax.set_ylabel('Training Time (in seconds)')

         ax.set_title('Training Time Plot for ' + d2_name + ' Dataset')
         ax.legend()
         ax.grid(True)

         plt.show()
```



0.3.3 Answer 3.3

For context, I'm limiting the n_estimators to 20 and max_depth to 3 for both algorithm (Random Forests and Gradient Boosting).

There are three main observations that I find:

1. For both dataset, the training time of Random Forests is constant, it is not affected by the training data size. Meanwhile, the training time for Gradient Boosting grows linearly with the increase in training data size.
2. For dataset with many features (64 features for Opt Digits, Dataset 2), Random Forests doesn't do well, i.e. the increase in training size doesn't boost performance on test set. For dataset with small features (9 features for), Random Forests are still quite on par with Gradient Boosting (accuracy doesn't differ significantly).
3. Gradient Boosting, while being limited to small max_depth and n_estimators, still performs well on both dataset, meaning it is robust to significant increase in features.

Thus, in general, Gradient Boosting wins performance wise, i.e. it gives better accuracy, meanwhile Random Forest wins speed wise, i.e. it has shorter training time.

0.4 Problem 4

0.4.1 Answer 4.1

Question 1

Does true negative matter for both ROC and PR curve?

Answer

True Negative (TN) matters for ROC curve, but not for PR curve. True Negative matters for ROC curve because its x-axis is FPR (False Positive Rate). We know that FPR is obtained as below:

$$FPR = \frac{FP}{N} = \frac{FP}{FP + TN}$$

We can see that TN is involved in the formula, thus TN matters for PR curve.

Question 2

Argue why each point on ROC curve corresponds to a unique point on PR curve?

Answer

Let's limit the scope for binary classification. Recall the concept that a point on ROC curve defines a certain, unique, confusion matrix given that the dataset is fixed, i.e. we know how many positive and negative examples are there in the dataset.

In PR curve, TN is not used, so each point in PR curve might lead to some different confusion matrices. But, if the dataset is fixed, and we know the other three statistics, which are TP, FP and FN, then TN is unique. If TN is unique, then it is proved that each point on ROC curve corresponds to a unique point on PR. One additional condition would be that the Recall of the model should be greater than zero, otherwise we couldn't compute FP and consequently, TN is not unique.

0.4.2 Answer 4.2

Load Dataset I use wdbc dataset (https://www.openml.org/d/1510)

```
In [30]: d4_path = 'data/wdbc.csv'
         d4_name = 'WDBC'
         d4_classname = 'Class'

         df4 = pd.read_csv(d4_path)
         df4.head()
```

```
Out[30]:       V1     V2      V3      V4       V5       V6      V7       V8      V9  \
         0  17.99  10.38  122.80  1001.0  0.11840  0.27760  0.3001  0.14710  0.2419
         1  20.57  17.77  132.90  1326.0  0.08474  0.07864  0.0869  0.07017  0.1812
         2  19.69  21.25  130.00  1203.0  0.10960  0.15990  0.1974  0.12790  0.2069
         3  11.42  20.38   77.58   386.1  0.14250  0.28390  0.2414  0.10520  0.2597
         4  20.29  14.34  135.10  1297.0  0.10030  0.13280  0.1980  0.10430  0.1809

                V10  ...    V22     V23     V24     V25     V26     V27     V28  \
         0  0.07871  ...  17.33  184.60  2019.0  0.1622  0.6656  0.7119  0.2654
         1  0.05667  ...  23.41  158.80  1956.0  0.1238  0.1866  0.2416  0.1860
         2  0.05999  ...  25.53  152.50  1709.0  0.1444  0.4245  0.4504  0.2430
         3  0.09744  ...  26.50   98.87   567.7  0.2098  0.8663  0.6869  0.2575
         4  0.05883  ...  16.67  152.20  1575.0  0.1374  0.2050  0.4000  0.1625

               V29      V30  Class
         0  0.4601  0.11890      2
         1  0.2750  0.08902      2
         2  0.3613  0.08758      2
         3  0.6638  0.17300      2
         4  0.2364  0.07678      2

         [5 rows x 31 columns]
```

Attribute Summary

```
In [31]: get_attribute_summary(df4, d4_classname, d4_name)
```

```
Summary of WDBC dataset attributes:
Number of features: 30
Number of instances: 569
Number of classes: 2
Number of numerical features: 30
Number of categorical features: 0
```

```
Out[31]: {'categorical_indexes': [],
          'num_categorical_features': 0,
          'num_classes': 2,
          'num_features': 30,
          'num_instances': 569,
          'num_numerical_features': 30}
```

Class Distribution

```
In [32]: df4[d4_classname].value_counts()
```

```
Out[32]: 1    357
         2    212
         Name: Class, dtype: int64
```

Preprocessing

1. Change label from {1, 2} to {1, 0}. Notice that I do this because Class 1 has more instances, so I assume it's the positive one.
2. Train Test Split

```
In [33]: df4[d4_classname] = df4[d4_classname].astype('int')
         df4[d4_classname] = df4[d4_classname].replace(2, 0)

         X_train, X_test, y_train, y_test = train_test_split(df4.drop(columns=[d4_classname]), d
```

Class Distribution in Train and Test

```
In [34]: print(y_train.value_counts())
         print(y_test.value_counts())
```

```
1    284
0    171
Name: Class, dtype: int64
1    73
0    41
Name: Class, dtype: int64
```

Train on Both Classifiers I limit the n_estimators to 3 for Adaboost and max_iter to 20 for Logistic Regression.

```
In [35]: from sklearn.ensemble import AdaBoostClassifier
         from sklearn.linear_model import LogisticRegression

         a_clf = AdaBoostClassifier(n_estimators=3, random_state=28)
         a_clf.fit(X_train, y_train)

         l_clf = LogisticRegression(max_iter=20, random_state=28)
         l_clf.fit(X_train, y_train)
```

```
Out[35]: LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
                            intercept_scaling=1, l1_ratio=None, max_iter=20,
                            multi_class='auto', n_jobs=None, penalty='l2',
                            random_state=28, solver='lbfgs', tol=0.0001, verbose=0,
                            warm_start=False)
```

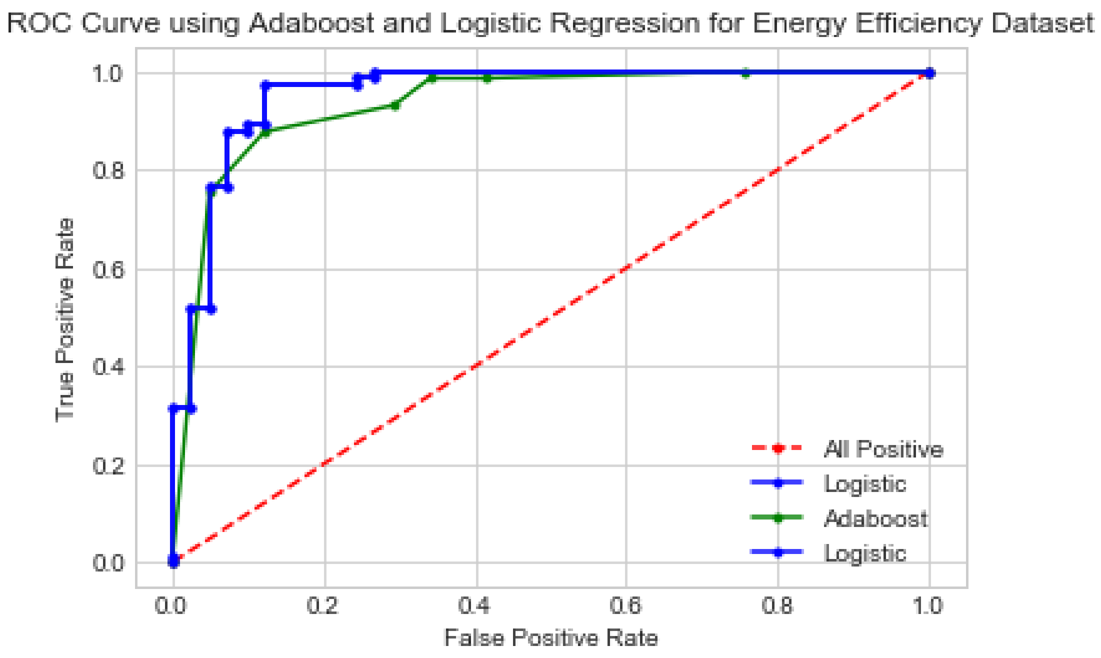
Get Prediction and Its Probabilities (Only for Positive/Majority Class)

```
In [36]: a_pred_probs = a_clf.predict_proba(X_test) #192, 2
         l_pred_probs = l_clf.predict_proba(X_test) #192, 2

         a_pos_probs = a_pred_probs[:, 1]
         l_pos_probs = l_pred_probs[:, 1]
```

```
        a_y_preds = a_clf.predict(X_test)
        l_y_preds = l_clf.predict(X_test)

        # An all positive classifier, always predicts 1
        ap_pos_probs = [float(1.0) for _ in range(len(y_test))]
        ap_y_preds = [int(1) for _ in range(len(y_test))]
```

ROC Curves

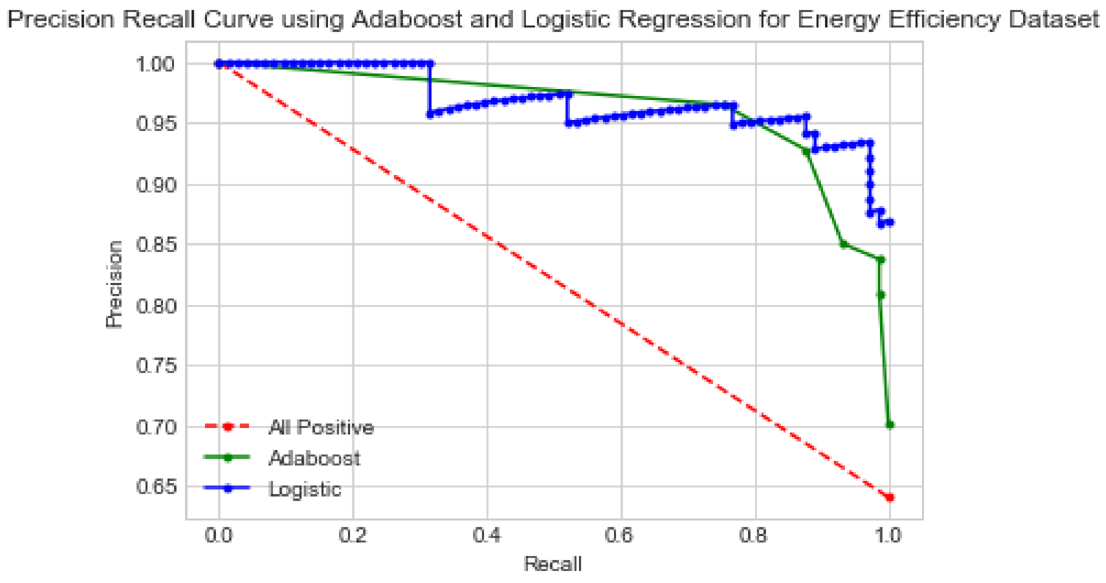
```
In [37]: from sklearn.metrics import roc_curve

         ap_fp_rate, ap_tp_rate, _ = roc_curve(y_test, ap_pos_probs)
         a_fp_rate, a_tp_rate, _ = roc_curve(y_test, a_pos_probs)
         l_fp_rate, l_tp_rate, _ = roc_curve(y_test, l_pos_probs)

         fig, ax = plt.subplots()

         x_plots = ap_fp_rate
         y_plots = ap_tp_rate
         ax.plot(x_plots, y_plots, color='red', marker='.', label='All Positive', linestyle='das

         x_plots = l_fp_rate
         y_plots = l_tp_rate
         ax.plot(x_plots, y_plots, color='blue', marker='.', label='Logistic')

         x_plots = a_fp_rate
         y_plots = a_tp_rate
         ax.plot(x_plots, y_plots, color='green', marker='.', label='Adaboost')

         x_plots = l_fp_rate
         y_plots = l_tp_rate
         ax.plot(x_plots, y_plots, color='blue', marker='.', label='Logistic')

         ax.set_xlabel('False Positive Rate')
         ax.set_ylabel('True Positive Rate')

         ax.set_title('ROC Curve using Adaboost and Logistic Regression for ' + d1_name + ' Data
         ax.legend()
         ax.grid(True)
```



PR Curves

```
In [38]: from sklearn.metrics import precision_recall_curve

         ap_precision, ap_recall, _ = precision_recall_curve(y_test, ap_pos_probs)
         a_precision, a_recall, _ = precision_recall_curve(y_test, a_pos_probs)
         l_precision, l_recall, _ = precision_recall_curve(y_test, l_pos_probs)

         fig, ax = plt.subplots()

         x_plots = ap_recall
         y_plots = ap_precision
         ax.plot(x_plots, y_plots, color='red', marker='.', label='All Positive', linestyle='das

         x_plots = a_recall
         y_plots = a_precision
         ax.plot(x_plots, y_plots, color='green', marker='.', label='Adaboost')

         x_plots = l_recall
         y_plots = l_precision
         ax.plot(x_plots, y_plots, color='blue', marker='.', label='Logistic')

         ax.set_xlabel('Recall')
         ax.set_ylabel('Precision')
```

```
        ax.set_title('Precision Recall Curve using Adaboost and Logistic Regression for ' + d1_
        ax.legend()
        ax.grid(True)
```



0.4.3 Answer 4.3

Calculate AUROC

```
In [39]: from sklearn.metrics import roc_auc_score

         a_auroc = roc_auc_score(y_test, a_pos_probs)
         l_auroc = roc_auc_score(y_test, l_pos_probs)

         print('AUROC value for Adaboost: {}'.format(a_auroc))
         print('AUROC value for Logistic Regression: {}'.format(l_auroc))
```

```
AUROC value for Adaboost: 0.9343468092215168
AUROC value for Logistic Regression: 0.9565653190778483
```

AUROC value for Logistice Regression is slightly greater than that of Adaboost, with ~0.02 difference.

Calculate AUPR

```
In [40]: from sklearn.metrics import average_precision_score

         a_aupr = average_precision_score(y_test, a_pos_probs)
         l_aupr = average_precision_score(y_test, l_pos_probs)

         print('AUPR value for Adaboost: {}'.format(a_aupr))
         print('AUPR value for Logistic Regression: {}'.format(l_aupr))
```

```
AUPR value for Adaboost: 0.9434076960517591
AUPR value for Logistic Regression: 0.9683464053796522
```

AUPR value for Logistice Regression is slightly greater than that of Adaboost, with ~0.025 difference.

For AUPRG, I'm going to use prg package (https://github.com/meeliskull/prg)

```
In [41]: !pip install pyprg
```

```
Requirement already satisfied: pyprg in /Library/Frameworks/Python.framework/Versions/3.6/lib/py
Requirement already satisfied: matplotlib in /Library/Frameworks/Python.framework/Versions/3.6/l
Requirement already satisfied: numpy in /Library/Frameworks/Python.framework/Versions/3.6/lib/py
Requirement already satisfied: python-dateutil>=2.1 in /Library/Frameworks/Python.framework/Vers
Requirement already satisfied: pyparsing!=2.0.4,!=2.1.2,!=2.1.6,>=2.0.1 in /Library/Frameworks/P
Requirement already satisfied: kiwisolver>=1.0.1 in /Library/Frameworks/Python.framework/Version
Requirement already satisfied: cycler>=0.10 in /Library/Frameworks/Python.framework/Versions/3.6
Requirement already satisfied: six>=1.5 in /Library/Frameworks/Python.framework/Versions/3.6/lib
Requirement already satisfied: setuptools in /Library/Frameworks/Python.framework/Versions/3.6/l
```

Calculate AUPRG

```
In [42]: from prg.prg import create_prg_curve, calc_auprg

         a_prg_curve = create_prg_curve(y_test, a_pos_probs)
         l_prg_curve = create_prg_curve(y_test, l_pos_probs)

         a_auprg = calc_auprg(a_prg_curve)
         l_auprg = calc_auprg(l_prg_curve)

         print('AUPRG value for Adaboost: {}'.format(a_auprg))
         print('AUPRG value for Logistic Regression: {}'.format(l_auprg))
```

```
AUPRG value for Adaboost: 0.8812399596400051
AUPRG value for Logistic Regression: 0.8926037279876874
```

AUROC value for Logistice Regression is slightly greater than that of Adaboost, with ~0.01 difference.

Question

Do you agree with the conclusion of NIPS paper that practitioners should use PR gain curves rather than PR curves?

Answer

Yes, I agree with the author. There are several reasons:

1. The author experimentally proves that the conventional AUPR is not accurate in measuring the expected F1 score, i.e. it can favor models with lower expected F1 score amongst other models.

2. AUPRG is an easier metric to calculate, compared to AUPR, due to linear interpolation.

3. Traditional PR curves don't have some properties that are desirable (like that of ROC). One example would be that the PR curve has some uninterpretable areas. AUPR is not meaningful because it's merely a geometric expected precision when uniformly varying the recall. Also, as we could see in 4.2, PR curve has unreachable region at the lower RHS (right hand side) of the plot, which area depends on the class distribution.