Machine Learning Engineer Nanodegree

Model Evaluation & Validation

Project: Predicting Boston Housing Prices

Welcome to the first project of the Machine Learning Engineer Nanodegree! In this notebook, some template code has already been provided for you, and you will need to implement additional functionality to successfully complete this project. You will not need to modify the included code beyond what is requested. Sections that begin with 'Implementation' in the header indicate that the following block of code will require additional functionality which you must provide. Instructions will be provided for each section and the specifics of the implementation are marked in the code block with a 'TODO' statement. Please be sure to read the instructions carefully!

In addition to implementing code, there will be questions that you must answer which relate to the project and your implementation. Each section where you will answer a question is preceded by a 'Question X' header. Carefully read each question and provide thorough answers in the following text boxes that begin with 'Answer:'. Your project submission will be evaluated based on your answers to each of the questions and the implementation you provide.

Note: Code and Markdown cells can be executed using the **Shift + Enter** keyboard shortcut. In addition, Markdown cells can be edited by typically double-clicking the cell to enter edit mode.

Getting Started

In this project, you will evaluate the performance and predictive power of a model that has been trained and tested on data collected from homes in suburbs of Boston, Massachusetts. A model trained on this data that is seen as a *good fit* could then be used to make certain predictions about a home — in particular, its monetary value. This model would prove to be invaluable for someone like a real estate agent who could make use of such information on a daily basis.

The dataset for this project originates from the <u>UCI Machine Learning Repository</u> (https://archive.ics.uci.edu/ml/datasets/Housing). The Boston housing data was collected in 1978 and each of the 506 entries represent aggregated data about 14 features for homes from various suburbs in Boston, Massachusetts. For the purposes of this project, the following preprocessing steps have been made to the dataset:

- 16 data points have an 'MEDV' value of 50.0. These data points likely contain **missing or** censored values and have been removed.
- 1 data point has an 'RM' value of 8.78. This data point can be considered an **outlier** and has been removed.
- The features 'RM', 'LSTAT', 'PTRATIO', and 'MEDV' are essential. The remaining **non-relevant features** have been excluded.
- The feature 'MEDV' has been **multiplicatively scaled** to account for 35 years of market inflation.

Run the code cell below to load the Boston housing dataset, along with a few of the necessary Python libraries required for this project. You will know the dataset loaded successfully if the size of the dataset is reported.

In [39]:

```
# Import libraries necessary for this project
import numpy as np
import pandas as pd
from sklearn.model_selection import ShuffleSplit

# Import supplementary visualizations code visuals.py
import visuals as vs

# Pretty display for notebooks
%matplotlib inline

# Load the Boston housing dataset
data = pd.read_csv('housing.csv')
prices = data['MEDV']
features = data.drop('MEDV', axis = 1)

# Success
print("Boston housing dataset has {} data points with {} variables each.".form
at(*data.shape))
```

Boston housing dataset has 489 data points with 4 variables each.

Data Exploration

In this first section of this project, you will make a cursory investigation about the Boston housing data and provide your observations. Familiarizing yourself with the data through an explorative process is a fundamental practice to help you better understand and justify your results.

Since the main goal of this project is to construct a working model which has the capability of predicting the value of houses, we will need to separate the dataset into **features** and the **target variable**. The **features**, 'RM', 'LSTAT', and 'PTRATIO', give us quantitative information about each data point. The **target variable**, 'MEDV', will be the variable we seek to predict. These are stored in features and prices, respectively.

Implementation: Calculate Statistics

For your very first coding implementation, you will calculate descriptive statistics about the Boston housing prices. Since numpy has already been imported for you, use this library to perform the necessary calculations. These statistics will be extremely important later on to analyze various prediction results from the constructed model.

In the code cell below, you will need to implement the following:

- Calculate the minimum, maximum, mean, median, and standard deviation of 'MEDV', which is stored in prices.
 - Store each calculation in their respective variable.

In [51]:

```
# TODO: Minimum price of the data
minimum price = np.min(prices)
# TODO: Maximum price of the data
maximum price = np.max(prices)
# TODO: Mean price of the data
mean price = np.mean(prices)
# TODO: Median price of the data
median price = np.median(prices)
# TODO: Standard deviation of prices of the data
std price = np.std(prices)
# Show the calculated statistics
print("Statistics for Boston housing dataset:\n")
print("Minimum price: ${}".format(minimum price))
print("Maximum price: ${}".format(maximum_price))
print("Mean price: ${}".format(mean_price))
print("Median price ${}".format(median price))
print("Standard deviation of prices: ${}".format(std price))
```

Statistics for Boston housing dataset:

Minimum price: \$105000.0 Maximum price: \$1024800.0

Mean price: \$454342.9447852761

Median price \$438900.0

Standard deviation of prices: \$165171.13154429474

Question 1 - Feature Observation

As a reminder, we are using three features from the Boston housing dataset: 'RM', 'LSTAT', and 'PTRATIO'. For each data point (neighborhood):

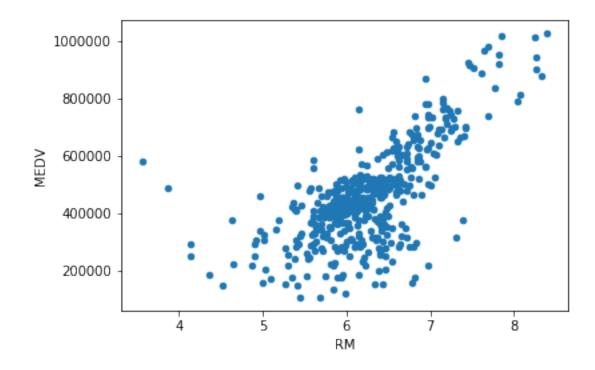
- 'RM' is the average number of rooms among homes in the neighborhood.
- 'LSTAT' is the percentage of homeowners in the neighborhood considered "lower class" (working poor).
- 'PTRATIO' is the ratio of students to teachers in primary and secondary schools in the neighborhood.

Using your intuition, for each of the three features above, do you think that an increase in the value of that feature would lead to an increase in the value of 'MEDV' or a decrease in the value of 'MEDV'? Justify your answer for each.

Hint: This problem can phrased using examples like below.

- Would you expect a home that has an 'RM' value(number of rooms) of 6 be worth more or less than a home that has an 'RM' value of 7?
- Would you expect a neighborhood that has an 'LSTAT' value(percent of lower class workers)
 of 15 have home prices be worth more or less than a neighborhood that has an 'LSTAT' value
 of 20?
- Would you expect a neighborhood that has an 'PTRATIO' value(ratio of students to teachers)
 of 10 have home prices be worth more or less than a neighborhood that has an 'PTRATIO'
 value of 15?

In [69]:



Answer:

The higher 'RM' value, the higher value of 'MEDV'. Houses with more rooms have higher prices. The higher percentage of 'LSTAT', the lower value of 'MEDV'. We can expect that the neighborhood is considered "poor" when 'LSTAT' is large.

Finally, the lower value of 'PTRATIO', the higher value of 'MEDV'. Primary and secondary schools with a lower value of 'PTRATIO' get more 'credits'.

Developing a Model

In this second section of the project, you will develop the tools and techniques necessary for a model to make a prediction. Being able to make accurate evaluations of each model's performance through the use of these tools and techniques helps to greatly reinforce the confidence in your predictions.

Implementation: Define a Performance Metric

It is difficult to measure the quality of a given model without quantifying its performance over training and testing. This is typically done using some type of performance metric, whether it is through calculating some type of error, the goodness of fit, or some other useful measurement. For this project, you will be calculating the <u>coefficient of determination</u> (http://stattrek.com/statistics/dictionary.aspx? definition=coefficient of determination), R², to quantify your model's performance. The coefficient of determination for a model is a useful statistic in regression analysis, as it often describes how "good" that model is at making predictions.

The values for R² range from 0 to 1, which captures the percentage of squared correlation between the predicted and actual values of the **target variable**. A model with an R² of 0 is no better than a model that always predicts the *mean* of the target variable, whereas a model with an R² of 1 perfectly predicts the target variable. Any value between 0 and 1 indicates what percentage of the target variable, using this model, can be explained by the **features**. A model can be given a negative R² as well, which indicates that the model is **arbitrarily worse** than one that always predicts the mean of the target variable.

For the performance metric function in the code cell below, you will need to implement the following:

- Use r2_score from sklearn.metrics to perform a performance calculation between y_true and y_predict.
- Assign the performance score to the score variable.

```
In [41]:
```

Question 2 - Goodness of Fit

Assume that a dataset contains five data points and a model made the following predictions for the target variable:

True Value	Prediction		
3.0	2.5		
-0.5	0.0		
2.0	2.1		
7.0	7.8		
4.2	5.3		

Run the code cell below to use the performance_metric function and calculate this model's coefficient of determination.

```
In [42]:
```

```
# Calculate the performance of this model
score = performance_metric([3, -0.5, 2, 7, 4.2], [2.5, 0.0, 2.1, 7.8, 5.3])
print("Model has a coefficient of determination, R^2, of {:.3f}.".format(score))
```

Model has a coefficient of determination, R^2, of 0.923.

- Would you consider this model to have successfully captured the variation of the target variable?
- Why or why not?

Hint: The R2 score is the proportion of the variance in the dependent variable that is predictable from the independent variable. In other words:

- R2 score of 0 means that the dependent variable cannot be predicted from the independent variable.
- R2 score of 1 means the dependent variable can be predicted from the independent variable.
- R2 score between 0 and 1 indicates the extent to which the dependent variable is predictable.
- R2 score of 0.40 means that 40 percent of the variance in Y is predictable from X.

Answer:

A model which has a coefficient of determination of 0.923 is considered to be a good model. That means the predictor explain almost 92 % of the variance in response.

Implementation: Shuffle and Split Data

Your next implementation requires that you take the Boston housing dataset and split the data into training and testing subsets. Typically, the data is also shuffled into a random order when creating the training and testing subsets to remove any bias in the ordering of the dataset.

For the code cell below, you will need to implement the following:

- Use train_test_split from sklearn.cross_validation to shuffle and split the features and prices data into training and testing sets.
 - Split the data into 80% training and 20% testing.
 - Set the random_state for train_test_split to a value of your choice. This
 ensures results are consistent.
- Assign the train and testing splits to X_train, X_test, y_train, and y_test.

In [43]:

```
# TODO: Import 'train_test_split'
from sklearn.cross_validation import train_test_split
# TODO: Shuffle and split the data into training and testing subsets
X_train, X_test, y_train, y_test = train_test_split(features, prices, test_siz e=0.2, random_state=42)
# Success
print("Training and testing split was successful.")
```

Training and testing split was successful.

Question 3 - Training and Testing

 What is the benefit to splitting a dataset into some ratio of training and testing subsets for a learning algorithm?

Hint: Think about how overfitting or underfitting is contingent upon how splits on data is done.

Answer:

We want to create a test partition to provide us honest assessments of the performance of our predictive models. In order to avoid underfitting the test_zise should not be large but if we select the low ratio of test_size, we would face with the problem of overfitting.

Analyzing Model Performance

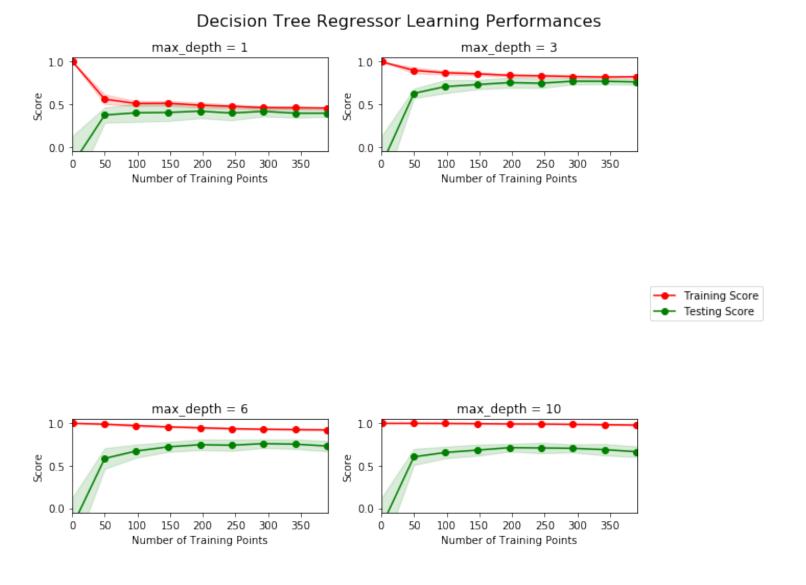
In this third section of the project, you'll take a look at several models' learning and testing performances on various subsets of training data. Additionally, you'll investigate one particular algorithm with an increasing 'max_depth' parameter on the full training set to observe how model complexity affects performance. Graphing your model's performance based on varying criteria can be beneficial in the analysis process, such as visualizing behavior that may not have been apparent from the results alone.

Learning Curves

The following code cell produces four graphs for a decision tree model with different maximum depths. Each graph visualizes the learning curves of the model for both training and testing as the size of the training set is increased. Note that the shaded region of a learning curve denotes the uncertainty of that curve (measured as the standard deviation). The model is scored on both the training and testing sets using R², the coefficient of determination.

Run the code cell below and use these graphs to answer the following question.

Produce learning curves for varying training set sizes and maximum depths vs.ModelLearning(features, prices)



Question 4 - Learning the Data

- Choose one of the graphs above and state the maximum depth for the model.
- What happens to the score of the training curve as more training points are added? What about the testing curve?
- Would having more training points benefit the model?

Hint: Are the learning curves converging to particular scores? Generally speaking, the more data you have, the better. But if your training and testing curves are converging with a score above your benchmark threshold, would this be necessary? Think about the pros and cons of adding more training points based on if the training and testing curves are converging.

Answer:

max_depth=3.

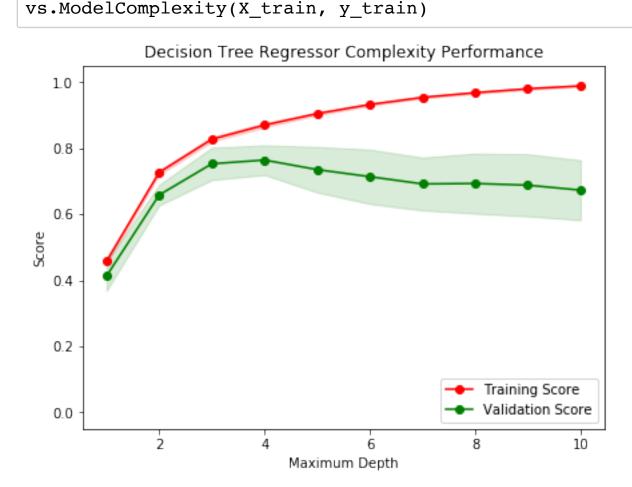
The score of the training curve decreases when more training points are added. But at some point, the training curve start decreasing slightly. The same situation with the testing curve, firstly the score increases and at some point the curve start decreasing slightly. In general, the more data you have, the better. But if the curve reaches the benchmark, it would not be necessary adding more data. At the point of 300 training points, the curves almost converged.

Complexity Curves

The following code cell produces a graph for a decision tree model that has been trained and validated on the training data using different maximum depths. The graph produces two complexity curves — one for training and one for validation. Similar to the **learning curves**, the shaded regions of both the complexity curves denote the uncertainty in those curves, and the model is scored on both the training and validation sets using the performance metric function.

Run the code cell below and use this graph to answer the following two questions Q5 and Q6.

In [45]:



Question 5 - Bias-Variance Tradeoff

- When the model is trained with a maximum depth of 1, does the model suffer from high bias or from high variance?
- How about when the model is trained with a maximum depth of 10? What visual cues in the graph justify your conclusions?

Hint: High bias is a sign of underfitting(model is not complex enough to pick up the nuances in the data) and high variance is a sign of overfitting(model is by-hearting the data and cannot generalize well). Think about which model(depth 1 or 10) aligns with which part of the tradeoff.

Answer:

When max_depth=10, the model is overfitting the data, the model has a low level of bias but when we apply this model to the test data sets, the validation score would be poor because the model did not generalize the training data. As a result at max_depth=10 we have a higher variance.

At the depth of 1, the model has a high level of bias and as a result the model is underfitting. When a model has a high bias, the model doesn't take into account nuances in the data and predictions would be poor. The higher depth, the more model tries fitting the model and as a result overfitting. With the high level of depth, the model is good at the training set but if the model is applied to the test set, it would have a 'poor' validation score. The same thing with variance, the more flexible model becomes, the higher variance and vice versa. In general, the goal is to achive the low variance and bias simultaneously. We can notice that max_depth=3 is the benchmark, after that point the bias starts decreasing and the variance increasing.

However, if a method has high variance then small changes in the training data can result in large changes in the test data. In general, more flexible statistical methods have higher variance. As we use more flexible methods, the variance will increase and the bias will decrease. Generally, more flexible methods result in less bias.

Question 6 - Best-Guess Optimal Model

- Which maximum depth do you think results in a model that best generalizes to unseen data?
- What intuition lead you to this answer?

Hint: Look at the graph above Question 5 and see where the validation scores lie for the various depths that have been assigned to the model. Does it get better with increased depth? At what point do we get our best validation score without overcomplicating our model? And remember, Occams Razor states "Among competing hypotheses, the one with the fewest assumptions should be selected."

Answer:

max_depth=3. At this level, the model achives low variance and low bias simultaneously. After that level, the model starts overfitting the data and as a result, the variance starts increasing and the bias decreasing.

Evaluating Model Performance

In this final section of the project, you will construct a model and make a prediction on the client's feature set using an optimized model from fit model.

Question 7 - Grid Search

- What is the grid search technique?
- How it can be applied to optimize a learning algorithm?

Hint: When explaining the Grid Search technique, be sure to touch upon why it is used, what the 'grid' entails and what the end goal of this method is. To solidify your answer, you can also give an example of a parameter in a model that can be optimized using this approach.

Answer:

Grid search means we have a set of models (which differ from each other in their parameter values, which lie on a grid), an example was shown in the graph above. We train each of the models and evaluate it using cross-validation. Then select the one that performed the best. For example, these parameters max_depth, min_samples_split, min_samples_leaf, we can choose different values for them in order to achive the best model(e.g, max_depth=[1,2,3,4,5,10], etc.

Question 8 - Cross-Validation

- What is the k-fold cross-validation training technique?
- What benefit does this technique provide for grid search when optimizing a model?

Hint: When explaining the k-fold cross validation technique, be sure to touch upon what 'k' is, how the dataset is split into different parts for training and testing and the number of times it is run based on the 'k' value.

When thinking about how k-fold cross validation helps grid search, think about the main drawbacks of grid search which are hinged upon **using a particular subset of data for training or testing** and how k-fold cv could help alleviate that. You can refer to the <u>docs (http://scikit-learn.org/stable/modules/cross_validation.html#cross-validation)</u> for your answer.

Answer: In k-fold cross-validation, the data is divided into k subsets. Now the method is repeated k times, such that each time, one of the k subsets is used as the test set/validation set and the other k-1 subsets are put together to form a training set. Usually we don't have enough data and removing a part of it, for purposes of the test set, causes the problem of underfitting. By reducing the training data, we risk losing important patterns in data set, which increases bias. This approach allows using most of the data for fitting, and most of the data is also being used in validation set.

Implementation: Fitting a Model

Your final implementation requires that you bring everything together and train a model using the **decision tree algorithm**. To ensure that you are producing an optimized model, you will train the model using the grid search technique to optimize the 'max_depth' parameter for the decision tree. The 'max_depth' parameter can be thought of as how many questions the decision tree algorithm is allowed to ask about the data before making a prediction. Decision trees are part of a class of algorithms called *supervised learning algorithms*.

In addition, you will find your implementation is using ShuffleSplit() for an alternative form of cross-validation (see the 'cv_sets' variable). While it is not the K-Fold cross-validation technique you describe in **Question 8**, this type of cross-validation technique is just as useful!. The ShuffleSplit() implementation below will create 10 ('n_splits') shuffled sets, and for each shuffle, 20% ('test_size') of the data will be used as the *validation set*. While you're working on your implementation, think about the contrasts and similarities it has to the K-fold cross-validation technique.

Please note that ShuffleSplit has different parameters in scikit-learn versions 0.17 and 0.18. For the fit model function in the code cell below, you will need to implement the following:

- Use <u>DecisionTreeRegressor</u> (http://scikitlearn.org/stable/modules/generated/sklearn.tree.DecisionTreeRegressor.html) from sklearn.tree to create a decision tree regressor object.
 - Assign this object to the 'regressor' variable.
- Create a dictionary for 'max_depth' with the values from 1 to 10, and assign this to the 'params' variable.
- Use make_scorer (http://scikit-learn.org/stable/modules/generated/sklearn.metrics.make_scorer.html) from sklearn.metrics to create a scoring function object.
 - Pass the performance metric function as a parameter to the object.
 - Assign this scoring function to the 'scoring fnc' variable.
- Use <u>GridSearchCV (http://scikit-learn.org/0.17/modules/generated/sklearn.grid_search.GridSearchCV.html)</u> from sklearn.grid_search to create a grid search object.
 - Pass the variables 'regressor', 'params', 'scoring_fnc', and 'cv_sets' as parameters to the object.
 - Assign the GridSearchCV object to the 'grid' variable.

```
In [82]:
```

```
# TODO: Import 'make_scorer', 'DecisionTreeRegressor', and 'GridSearchCV'
from sklearn.metrics import make scorer
from sklearn.tree import DecisionTreeRegressor
from sklearn.grid search import GridSearchCV
def fit model(X, y):
    """ Performs grid search over the 'max_depth' parameter for a
        decision tree regressor trained on the input data [X, y].
    # Create cross-validation sets from the training data
    # sklearn version 0.18: ShuffleSplit(n splits=10, test size=0.1, train siz
e=None, random state=None)
    # sklearn versiin 0.17: ShuffleSplit(n, n iter=10, test size=0.1, train si
ze=None, random state=None)
    cv sets = ShuffleSplit(n splits=10, test size = 0.20, random state = 0)
    cv sets=cv sets.get n splits(X)
    # TODO: Create a decision tree regressor object
    regressor = DecisionTreeRegressor()
    # TODO: Create a dictionary for the parameter 'max depth' with a range fro
m 1 to 10
    params = {'max depth': list(range(1, 11))}
    # TODO: Transform 'performance metric' into a scoring function using 'make
scorer'
    scoring fnc = make scorer(performance metric)
    # TODO: Create the grid search cv object --> GridSearchCV()
    # Make sure to include the right parameters in the object:
    # (estimator, param grid, scoring, cv) which have values 'regressor', 'par
ams', 'scoring fnc', and 'cv sets' respectively.
    grid = GridSearchCV(regressor, param grid=params, scoring=scoring fnc, cv=
cv sets)
    # Fit the grid search object to the data to compute the optimal model
    grid = grid.fit(X, y)
    # Return the optimal model after fitting the data
```

Making Predictions

return grid.best estimator

Once a model has been trained on a given set of data, it can now be used to make predictions on new sets of input data. In the case of a *decision tree regressor*, the model has learned *what the best questions to ask about the input data are*, and can respond with a prediction for the **target variable**. You can use these predictions to gain information about data where the value of the target variable is unknown — such as data the model was not trained on.

Question 9 - Optimal Model

 What maximum depth does the optimal model have? How does this result compare to your guess in Question 6?

Run the code block below to fit the decision tree regressor to the training data and produce an optimal model

```
In [83]:
```

```
# Fit the training data to the model using grid search
reg = fit_model(X_train, y_train)

# Produce the value for 'max_depth'
print("Parameter 'max_depth' is {} for the optimal model.".format(reg.get_para
ms()['max_depth']))
```

Parameter 'max_depth' is 4 for the optimal model.

Hint: The answer comes from the output of the code snipped above.

Answer: max_depth=4

Question 10 - Predicting Selling Prices

Imagine that you were a real estate agent in the Boston area looking to use this model to help price homes owned by your clients that they wish to sell. You have collected the following information from three of your clients:

Feature	Client 1	Client 2	Client 3
Total number of rooms in home	5 rooms	4 rooms	8 rooms
Neighborhood poverty level (as %)	17%	32%	3%
Student-teacher ratio of nearby schools	15-to-1	22-to-1	12-to-1

- What price would you recommend each client sell his/her home at?
- Do these prices seem reasonable given the values for the respective features?

Hint: Use the statistics you calculated in the **Data Exploration** section to help justify your response. Of the three clients, client 3 has has the biggest house, in the best public school neighborhood with the lowest poverty level; while client 2 has the smallest house, in a neighborhood with a relatively high poverty rate and not the best public schools.

Run the code block below to have your optimized model make predictions for each client's home.

```
In [48]:
```

```
Predicted selling price for Client 1's home: $403,025.00 Predicted selling price for Client 2's home: $237,478.72 Predicted selling price for Client 3's home: $931,636.36
```

Answer: As discussed earlier, we expect that houses with a higher number of rooms, lower level of LSTAT and a lower PTRATIO(e.g 12-to-1) would have higher prices. As we can see from the output of the model, the results seem to be reasonable.

Sensitivity

An optimal model is not necessarily a robust model. Sometimes, a model is either too complex or too simple to sufficiently generalize to new data. Sometimes, a model could use a learning algorithm that is not appropriate for the structure of the data given. Other times, the data itself could be too noisy or contain too few samples to allow a model to adequately capture the target variable — i.e., the model is underfitted.

Run the code cell below to run the fit_model function ten times with different training and testing sets to see how the prediction for a specific client changes with respect to the data it's trained on.

```
In [49]:
```

Range in prices: \$29,438.89

```
vs.PredictTrials(features, prices, fit_model, client_data)

Trial 1: $391,183.33

Trial 2: $411,417.39

Trial 3: $415,800.00

Trial 4: $420,622.22

Trial 5: $413,334.78

Trial 6: $411,931.58

Trial 7: $399,663.16

Trial 8: $407,232.00

Trial 9: $402,531.82

Trial 10: $413,700.00
```

Question 11 - Applicability

 In a few sentences, discuss whether the constructed model should or should not be used in a real-world setting.

Hint: Take a look at the range in prices as calculated in the code snippet above. Some questions to answering:

- How relevant today is data that was collected from 1978? How important is inflation?
- Are the features present in the data sufficient to describe a home? Do you think factors like
 quality of apppliances in the home, square feet of the plot area, presence of pool or not etc
 should factor in?
- Is the model robust enough to make consistent predictions?
- Would data collected in an urban city like Boston be applicable in a rural city?
- Is it fair to judge the price of an individual home based on the characteristics of the entire neighborhood?

In [50]:

performance metric(prices, reg.predict(features)) #r2 score

Out[50]:

0.8582276931365317

Answer:

According to the Bureau of Labor Statistics consumer price index, the dollar experienced an average inflation rate of 3.45% per year. Prices in 2017 are 275.4% higher than prices in 1978. As prices in the data were multiplicatively scaled to account for 35 years of market inflation, we can make predictions, although, new data would give us better predictions.

Our features(RM, LSTAT, PTRATIO) play an important role in the predictions of the prices. Further, we can improve our model by adding more features such as square feet of the plot area, presence of pool or not, year built, baths, home type, etc.

The model has R2=0.86, which means the predictors explain 86 % of the variance in response.

The model defined for Boston would not be a good model for a rural city. Predictors may play a different role in predicting prices for a rural city.

If the predictors can explain ~99% of the variance in response, it would be fair to judge the price of an individual home. In this case we have a lower rate of the R2 but on average the predictions would be close to the real price.

Note: Once you have completed all of the code implementations and successfully answered each question above, you may finalize your work by exporting the iPython Notebook as an HTML document. You can do this by using the menu above and navigating to

File -> Download as -> HTML (.html). Include the finished document along with this notebook as your submission.