Machine Learning Engineer Nanodegree

Model Evaluation & Validation

Project 1: Predicting Boston Housing Prices

Welcome to the first project of the Machine Learning Engineer Nanodegree! In this notebook, some template code has already been written. You will need to implement additional functionality to successfully answer all of the questions for this project. Unless it is requested, do not modify any of the code that has already been included. In this template code, there are four sections which you must complete to successfully produce a prediction with your model. Each section where you will write code is preceded by a **STEP X** header with comments describing what must be done. Please read the instructions carefully!

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

A description of the dataset can be found here (https://archive.ics.uci.edu/ml/datasets/Housing), which is provided by the **UCI Machine Learning Repository**.

Getting Started

To familiarize yourself with an iPython Notebook, **try double clicking on this cell**. You will notice that the text changes so that all the formatting is removed. This allows you to make edits to the block of text you see here. This block of text (and mostly anything that's not code) is written using Markdown (http://daringfireball.net/projects/markdown/syntax), which is a way to format text using headers, links, italics, and many other options! Whether you're editing a Markdown text block or a code block (like the one below), you can use the keyboard shortcut **Shift + Enter** or **Shift + Return** to execute the code or text block. In this case, it will show the formatted text.

Let's start by setting up some code we will need to get the rest of the project up and running. Use the keyboard shortcut mentioned above on the following code block to execute it. Alternatively, depending on your iPython Notebook program, you can press the **Play** button in the hotbar. You'll know the code block executes successfully if the message *"Boston Housing dataset loaded successfully!"* is printed.

In [43]:
```
# Importing a few necessary libraries
import numpy as np
import matplotlib.pyplot as pl
from sklearn import datasets
from sklearn.tree import DecisionTreeRegressor

# Make matplotlib show our plots inline (nicely formatted in the notebook)
%matplotlib inline

# Create our client's feature set for which we will be predicting a selling price
CLIENT_FEATURES = [[11.95, 0.00, 18.100, 0, 0.6590, 5.6090, 90.00, 1.385, 24, 680.0, 20.20, 332.09, 12.13]]

# Load the Boston Housing dataset into the city_data variable
city_data = datasets.load_boston()

# Initialize the housing prices and housing features
housing_prices = city_data.target
housing_features = city_data.data

print "Boston Housing dataset loaded successfully!"
```

```
Boston Housing dataset loaded successfully!
```

Statistical Analysis and Data Exploration

In this first section of the project, you will quickly investigate a few basic statistics about the dataset you are working with. In addition, you'll look at the client's feature set in `CLIENT_FEATURES` and see how this particular sample relates to the features of the dataset. Familiarizing yourself with the data through an explorative process is a fundamental practice to help you better understand your results.

Step 1

In the code block below, use the imported `numpy` library to calculate the requested statistics. You will need to replace each `None` you find with the appropriate `numpy` coding for the proper statistic to be printed. Be sure to execute the code block each time to test if your implementation is working successfully. The print statements will show the statistics you calculate!

In [44]:
```
# Number of houses in the dataset
total_houses = city_data.data.shape[0]

# Number of features in the dataset
total_features = city_data.data.shape[1]

# Minimum housing value in the dataset
minimum_price = min(housing_prices)

# Maximum housing value in the dataset
maximum_price = max(housing_prices)

# Mean house value of the dataset
mean_price = np.mean(housing_prices)

# Median house value of the dataset
median_price = np.median(housing_prices)

# Standard deviation of housing values of the dataset
std_dev = np.std(housing_prices)

# Show the calculated statistics
print "Boston Housing dataset statistics (in $1000's):\n"
print "Total number of houses:", total_houses
print "Total number of features:", total_features
print "Minimum house price:", minimum_price
print "Maximum house price:", maximum_price
print "Mean house price: {0:.3f}".format(mean_price)
print "Median house price:", median_price
print "Standard deviation of house price: {0:.3f}".format(std_dev)
```

```
Boston Housing dataset statistics (in $1000's):

Total number of houses: 506
Total number of features: 13
Minimum house price: 5.0
Maximum house price: 50.0
Mean house price: 22.533
Median house price: 21.2
Standard deviation of house price: 9.188
```

Question 1

As a reminder, you can view a description of the Boston Housing dataset here (https://archive.ics.uci.edu/ml/datasets/Housing), where you can find the different features under **Attribute Information**. The `MEDV` attribute relates to the values stored in our `housing_prices` variable, so we do not consider that a feature of the data.

Of the features available for each data point, choose three that you feel are significant and give a brief description for each of what they measure.

Remember, you can **double click the text box below** to add your answer!

Answer: My three chosen featers are: CRIM, RM, and DIS. House prices tend to be higher in areas with lower per capita crime rates (CRIM). The average number of rooms per dwelling positively impact the housing prices. Short distance to the main employment centers (DIS) also contribute to higher housing prices.

Question 2

Using your client's feature set `CLIENT_FEATURES`, which values correspond with the features you've chosen above?
Hint: Run the code block below to see the client's data.

In [45]:
```
print CLIENT_FEATURES
```

```
[[11.95, 0.0, 18.1, 0, 0.659, 5.609, 90.0, 1.385, 24, 680.0, 20.2, 332.
09, 12.13]]
```

Answer: CRIM : 11.95 , RM : 5.609 , DIS : 1.385

Evaluating Model Performance

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

Step 2

In the code block below, you will need to implement code so that the `shuffle_split_data` function does the following:

- Randomly shuffle the input data `X` and target labels (housing values) `y`.
- Split the data into training and testing subsets, holding 30% of the data for testing.

If you use any functions not already acessible from the imported libraries above, remember to include your import statement below as well!
Ensure that you have executed the code block once you are done. You'll know if the `shuffle_split_data` function is working if the statement *"Successfully shuffled and split the data!"* is printed.

In [46]:
```
# Put any import statements you need for this code block here
from sklearn.utils import shuffle
from sklearn.cross_validation import train_test_split

def shuffle_split_data(X, y):
    """ Shuffles and splits data into 70% training and 30% testing subse
ts,
        then returns the training and testing subsets. """

    # Shuffle and split the data
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=
0.3, random_state=0)

    # Return the training and testing data subsets
    return X_train, y_train, X_test, y_test


# Test shuffle_split_data
try:
    X_train, y_train, X_test, y_test = shuffle_split_data(housing_featur
es, housing_prices)
    print "Successfully shuffled and split the data!"
except:
    print "Something went wrong with shuffling and splitting the data."
```

```
Successfully shuffled and split the data!
```

Question 4

Why do we split the data into training and testing subsets for our model?

Answer: We separate training and testing sets so we can get a better idea whether the model can generalize to unseen data rather than fit to the data just seen (overfitting). It also gives estimates of performance of our model on an independent data.

Step 3

In the code block below, you will need to implement code so that the `performance_metric` function does the following:

- Perform a total error calculation between the true values of the `y` labels `y_true` and the predicted values of the `y` labels `y_predict`.

You will need to first choose an appropriate performance metric for this problem. See the sklearn metrics documentation (http://scikit-learn.org/stable/modules/classes.html#sklearn-metrics-metrics) to view a list of available metric functions. **Hint:** Look at the question below to see a list of the metrics that were covered in the supporting course for this project.

Once you have determined which metric you will use, remember to include the necessary import statement as well!
Ensure that you have executed the code block once you are done. You'll know if the `performance_metric` function is working if the statement *"Successfully performed a metric calculation!"* is printed.

In [47]:
```
# Put any import statements you need for this code block here
from sklearn import metrics

def performance_metric(y_true, y_predict):
    """ Calculates and returns the total error between true and predicte
d values
        based on a performance metric chosen by the student. """

    return metrics.mean_squared_error(y_true, y_predict) #evaluate perfo
rmance

# Test performance_metric
try:
    total_error = performance_metric(y_train, y_train)
    print "Successfully performed a metric calculation!"
except:
    print "Something went wrong with performing a metric calculation."
```

```
Successfully performed a metric calculation!
```

Question 4

Which performance metric below did you find was most appropriate for predicting housing prices and analyzing the total error. Why?

- *Accuracy*
- *Precision*
- *Recall*
- *F1 Score*
- *Mean Squared Error (MSE)*
- *Mean Absolute Error (MAE)*

Answer: For regression type of problems, as it is with Boston housing prices, we are dealing with model that make predictions on continuous data. In this case we care more about how close the prediction is. We can use either MSE or MAE. Accuracy, Precision, Recall and F1 Score can be used with Classification problems.

The Mean Absolute Error penalizes mistakes by averaging the mistakes in. The Mean Squared Error penalizes mistakes even more by squaring the difference before averaging them. Basically MAE is more robust to outlier than is MSE. MAE assigns equal weight to the data whereas MSE emphasizes the extremes. That was the reason for choosing MSE as performance metric.

Step 4 (Final Step)

In the code block below, you will need to implement code so that the `fit_model` function does the following:

- Create a scoring function using the same performance metric as in **Step 2**. See the sklearn `make_scorer` documentation (http://scikit-learn.org/stable/modules/generated/sklearn.metrics.make_scorer.html).
- Build a GridSearchCV object using `regressor`, `parameters`, and `scoring_function`. See the sklearn documentation on GridSearchCV (http://scikit-learn.org/stable/modules/generated/sklearn.grid_search.GridSearchCV.html).

When building the scoring function and GridSearchCV object, *be sure that you read the parameters documentation thoroughly.* It is not always the case that a default parameter for a function is the appropriate setting for the problem you are working on.

Since you are using `sklearn` functions, remember to include the necessary import statements below as well!
Ensure that you have executed the code block once you are done. You'll know if the `fit_model` function is working if the statement *"Successfully fit a model to the data!"* is printed.

In [48]:
```
# Put any import statements you need for this code block
from sklearn.grid_search import GridSearchCV

def fit_model(X, y):
    """ Tunes a decision tree regressor model using GridSearchCV on the
input data X
        and target labels y and returns this optimal model. """

    # Create a decision tree regressor object
    regressor = DecisionTreeRegressor()

    # Set up the parameters we wish to tune
    parameters = {'max_depth':(1,2,3,4,5,6,7,8,9,10)}

    # Make an appropriate scoring function
    # functions ending with _error or _loss return a value to minimize,
the lower the better
    scoring_function = metrics.make_scorer(metrics.mean_squared_error, g
reater_is_better=False)

    # Make the GridSearchCV object
    reg = GridSearchCV(regressor, param_grid = parameters, scoring = sco
ring_function)

    # Fit the learner to the data to obtain the optimal model with tuned
parameters
    reg.fit(X, y)

    # Return the optimal model
    return reg


# Test fit_model on entire dataset
try:
    reg = fit_model(housing_features, housing_prices)
    print "Successfully fit a model!"
except:
    print "Something went wrong with fitting a model."
```

```
Successfully fit a model!
```

Question 5

What is the grid search algorithm and when is it applicable?

Answer: In the context of machine learning, hyperparameter optimization or model selection is the problem of choosing a set of hyperparameters for a learning algorithm, usually with the goal of optimizing a measure of the algorithm's performance on an independent data set.

The traditional way of performing hyperparameter optimization has been grid search, or a parameter sweep, which is simply an exhaustive searching through a manually specified subset of the hyperparameter space of a learning algorithm.

Question 6

What is cross-validation, and how is it performed on a model? Why would cross-validation be helpful when using grid search?

Answer: A classic and popular approach for estimating the generalization performance of machine learning models is holdout cross-validation. Using the holdout method, we split our initial dataset into a separate training and test dataset— the former is used for model training, and the latter is used to estimate its performance. A better way of using the holdout method for model selection is to separate the data into 3 parts, a training set, a validation set, and a test set. The training set is used to fit the different models, and the performances on the validation set is then used for the model selection.

However, by partitioning the available data into three sets, we drastically reduce the number of samples which can be used for learning the model, and the results can depend on a particular random choice for the pair of (train, validation) sets.

A solution to this problem is a procedure called cross-validation. A test set should still be held out for final evaluation, but the validation set is no longer needed when doing CV. In the basic approach, called k-fold CV, the training set is split into k smaller sets.

In K-fold cross validation, we randomly split the training dataset into k folds, where k-1 folds are used for model training and one fold is used for testing. The procedure is repeated k times so that we obtain k models and performance estimates. We then calculate the average performance of the models based on the different independent folds to obtain a performance estimate that is less sensitive to the sub-partitioning of training data compared to holdout method.

Using K-fold cross validation in combination with Grid Search is a useful approach for fine-tuning the performance of machine learning model by varying its hyperparameters values.

Checkpoint!

You have now successfully completed your last code implementation section. Pat yourself on the back! All of your functions written above will be executed in the remaining sections below, and questions will be asked about various results for you to analyze. To prepare the **Analysis** and **Prediction** sections, you will need to intialize the two functions below. Remember, there's no need to implement any more code, so sit back and execute the code blocks! Some code comments are provided if you find yourself interested in the functionality.

In [49]:
```
def learning_curves(X_train, y_train, X_test, y_test):
    """ Calculates the performance of several models with varying sizes of training data.
        The learning and testing error rates for each model are then plotted. """

    print "Creating learning curve graphs for max_depths of 1, 3, 6, and 10. . ."

    # Create the figure window
    fig = pl.figure(figsize=(10,8))

    # We will vary the training set size so that we have 50 different sizes
    sizes = np.round(np.linspace(1, len(X_train), 50))
    train_err = np.zeros(len(sizes))
    test_err = np.zeros(len(sizes))

    # Create four different models based on max_depth
    for k, depth in enumerate([1,3,6,10]):

        for i, s in enumerate(sizes):

            # Setup a decision tree regressor so that it learns a tree with max_depth = depth
            regressor = DecisionTreeRegressor(max_depth = depth)

            # Fit the learner to the training data
            regressor.fit(X_train[:s], y_train[:s])

            # Find the performance on the training set
            train_err[i] = performance_metric(y_train[:s], regressor.predict(X_train[:s]))

            # Find the performance on the testing set
            test_err[i] = performance_metric(y_test, regressor.predict(X_test))

        # Subplot the learning curve graph
        ax = fig.add_subplot(2, 2, k+1)
        ax.plot(sizes, test_err, lw = 2, label = 'Testing Error')
        ax.plot(sizes, train_err, lw = 2, label = 'Training Error')
        ax.legend()
        ax.set_title('max_depth = %s'%(depth))
        ax.set_xlabel('Number of Data Points in Training Set')
        ax.set_ylabel('Total Error')
        ax.set_xlim([0, len(X_train)])

    # Visual aesthetics
    fig.suptitle('Decision Tree Regressor Learning Performances', fontsize=18, y=1.03)
    fig.tight_layout()
    fig.show()
```

In [50]:
```
def model_complexity(X_train, y_train, X_test, y_test):
    """ Calculates the performance of the model as model complexity incr
eases.
        The learning and testing errors rates are then plotted. """

    print "Creating a model complexity graph. . . "

    # We will vary the max_depth of a decision tree model from 1 to 14
    max_depth = np.arange(1, 14)
    train_err = np.zeros(len(max_depth))
    test_err = np.zeros(len(max_depth))

    for i, d in enumerate(max_depth):
        # Setup a Decision Tree Regressor so that it learns a tree with
depth d
        regressor = DecisionTreeRegressor(max_depth = d)

        # Fit the learner to the training data
        regressor.fit(X_train, y_train)

        # Find the performance on the training set
        train_err[i] = performance_metric(y_train, regressor.predict(X_t
rain))

        # Find the performance on the testing set
        test_err[i] = performance_metric(y_test, regressor.predict(X_tes
t))

    # Plot the model complexity graph
    pl.figure(figsize=(7, 5))
    pl.title('Decision Tree Regressor Complexity Performance')
    pl.plot(max_depth, test_err, lw=2, label = 'Testing Error')
    pl.plot(max_depth, train_err, lw=2, label = 'Training Error')
    pl.legend()
    pl.xlabel('Maximum Depth')
    pl.ylabel('Total Error')
    pl.show()
```

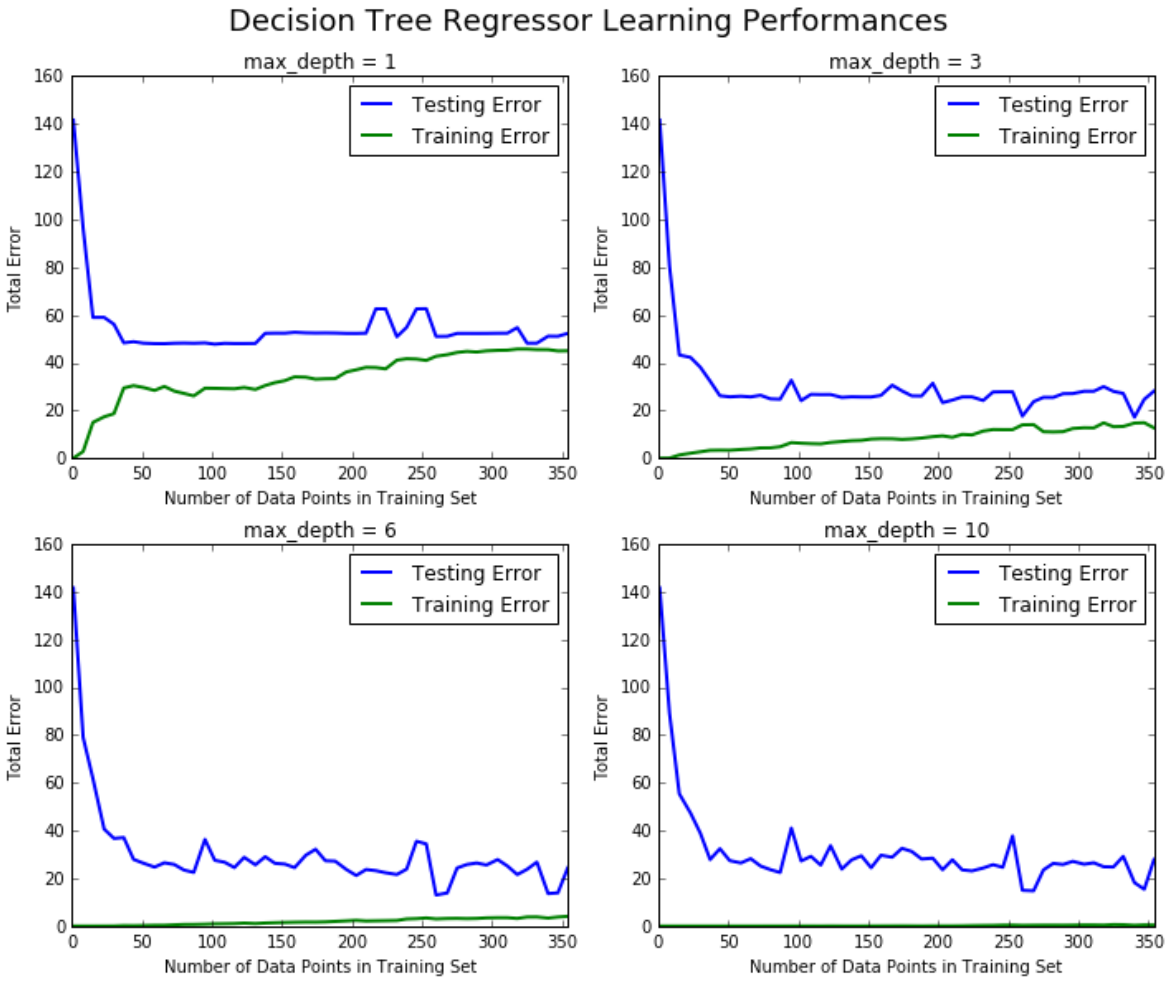
Analyzing Model Performance

In this third section of the project, you'll take a look at several models' learning and testing error rates 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 learning and testing errors. 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.

In [51]:
```
learning_curves(X_train, y_train, X_test, y_test)
```

```
Creating learning curve graphs for max_depths of 1, 3, 6, and 10. . .

C:\Anaconda2\lib\site-packages\ipykernel\__main__.py:24: DeprecationWar
ning: using a non-integer number instead of an integer will result in a
n error in the future
C:\Anaconda2\lib\site-packages\ipykernel\__main__.py:27: DeprecationWar
ning: using a non-integer number instead of an integer will result in a
n error in the future
```



Question 7

Choose one of the learning curve graphs that are created above. What is the max depth for the chosen model? As the size of the training set increases, what happens to the training error? What happens to the testing error?

Answer: My chosen model has max depth of 3. As the training set increases, the training error increases and the testing error decreases.

Question 8

Look at the learning curve graphs for the model with a max depth of 1 and a max depth of 10. When the model is using the full training set, does it suffer from high bias or high variance when the max depth is 1? What about when the max depth is 10?

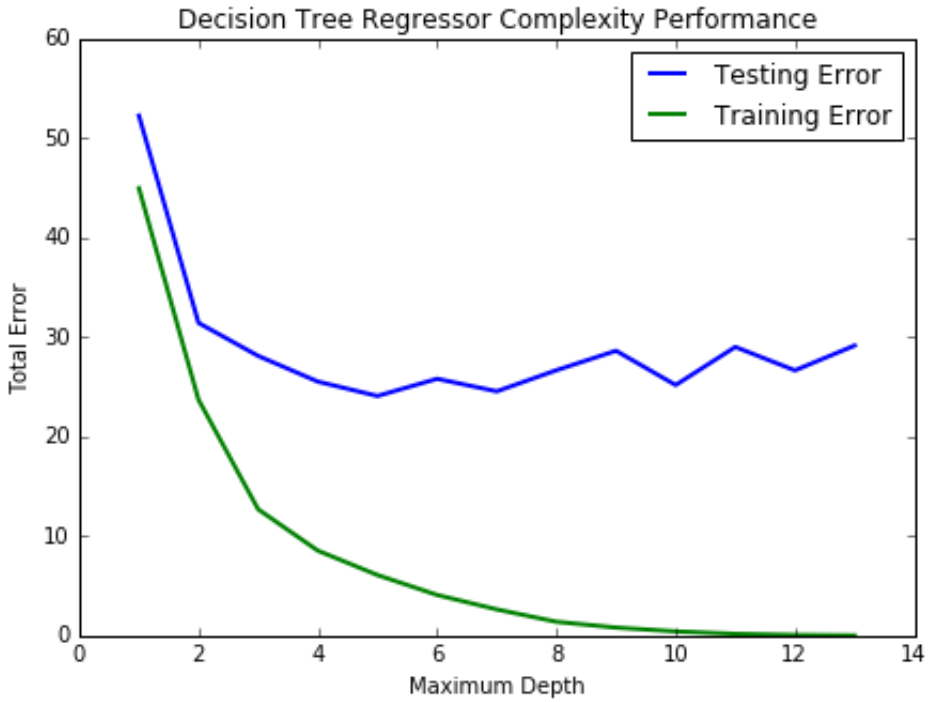
Answer: Models that are too complex tend to have high variance and low bias, while models that are too simple will tend to have high bias and low variance.

Model with max depth 1 is suffering from high bias and low variance. The training and testing errors converge and they are quite high. No matter how much data we feed it, the model cannot represent the underlying relationship and therefore has systematic high errors.

The model with max depth 10 is suffering from the low bias and high variance. we have a large gap between the training and testing error and the training error is very low. Unlike a bias model, models that suffer from variance can generally improve if we have more data to learn from or we can simplify the model representing the most important features of the data.

In [52]:
```
model_complexity(X_train, y_train, X_test, y_test)
```

```
Creating a model complexity graph. . .
```



Question 9

From the model complexity graph above, describe the training and testing errors as the max depth increases. Based on your interpretation of the graph, which max depth results in a model that best generalizes the dataset? Why?

Answer: We see here that as the model complexity (or max depth) increases, the error calculated on the training set continues to decrease, where as the testing error decreases for max depth of below 5 and plateau at the max depth of 5 and above. We showed above that error calculated on the testing set is the true indicator of how well an estimator will generalize to new data points. The error calculated on the training set strongly disagrees with the error calculated on the testing set after the optimal model complexity has been reached.

Model Prediction

In this final section of the project, you will make a prediction on the client's feature set using an optimized model from `fit_model`. *To answer the following questions, it is recommended that you run the code blocks several times and use the median or mean value of the results.*

Question 10

Using grid search on the entire dataset, what is the optimal `max_depth` parameter for your model? How does this result compare to your intial intuition?
Hint: Run the code block below to see the max depth produced by your optimized model.

In [53]:
```
print "Final model optimal parameters:", reg.best_params_
```

```
Final model optimal parameters: {'max_depth': 6}
```

Answer: Optimal max depth : 6

My initial intuition was max depth of 5 and the optimal max calculated above is 6.

Question 11

With your parameter-tuned model, what is the best selling price for your client's home? How does this selling price compare to the basic statistics you calculated on the dataset?

Hint: Run the code block below to have your parameter-tuned model make a prediction on the client's home.

In [54]:
```
sale_price = reg.predict(CLIENT_FEATURES)
print "Predicted value of client's home: {0:.3f}".format(sale_price[0])
print "Mean Price: {0:.3f}".format(mean_price)
print "Median Price: {0:.3f}".format(median_price)
print "Standart Deviation: {0:.3f}".format(std_dev)
```

```
Predicted value of client's home: 20.766
Mean Price: 22.533
Median Price: 21.200
Standart Deviation: 9.188
```

Answer: Best selling price is : 20.766

This prediction's value is well within the range of the mean and standard deviation, and it is close to the median price.

Question 12 (Final Question):

In a few sentences, discuss whether you would use this model or not to predict the selling price of future clients' homes in the Greater Boston area.

Answer: I would plot the residual graph which is to plot the predicted values versus the observed values for the entire dataset. Ideally the residual plot should have the following characteristics:

(1) they're pretty symmetrically distributed, tending to cluster towards the middle of the plot

(2) they're clustered around the lower single digits of the y-axis (e.g., 0.5 or 1.5, not 30 or 50)

If the above conditions are met, I would use the model for the future predictions.