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 [5]:
```
# 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 [15]:
```
# Number of houses in the dataset
total_houses = np.size(housing_prices, 0)

# Number of features in the dataset
total_features = np.size(housing_features, 1)

# Minimum housing value in the dataset
minimum_price = np.amin(housing_prices)

# Maximum housing value in the dataset
maximum_price = np.amax(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

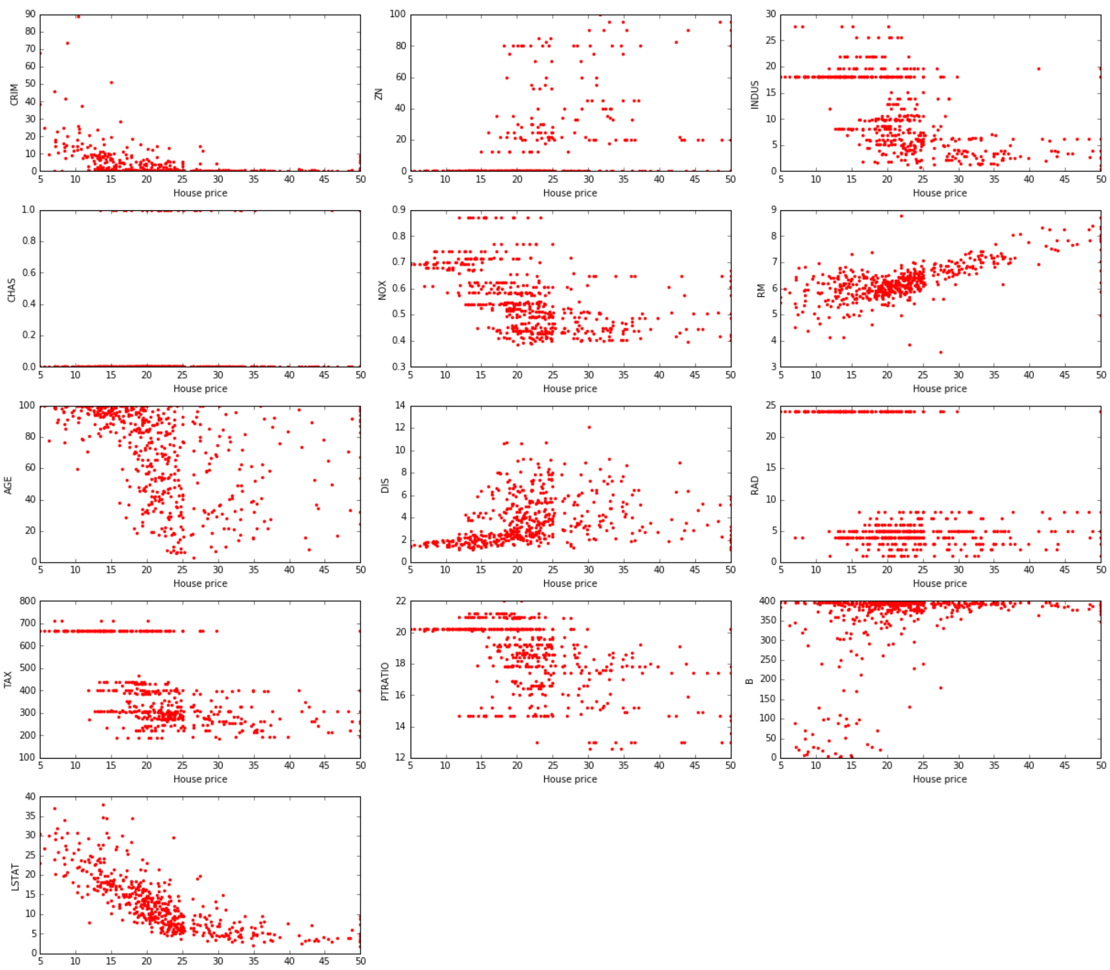
As a reminder, you can view a description of the Boston Housing dataset here (https://archive.ics.uci.edu/ml/datasets/Housing), where you can find the different features under **Attribute Information**. The `MEDV` attribute relates to the values stored in our `housing_prices` variable, so we do not consider 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: I built a raster plots of features vs house price (see below). Based on these plots, I would choose RM, LSTAT and NOX features. RM is an average number of rooms per property and it demonstrates clear positive correlation with property price. The other two features: LSTAT (socio economic status) and NOX (nitric oxides concentration) demonstrate negative correlation with price. Other features shows either less correlative dependence with property price (like CHAS) or even bimodal distribution (like RAD).

In [16]:
```
pl.figure(figsize=(17,15))
for i in range(0, total_features) :
    pl.subplot(5, 3, i+1)
    pl.plot(housing_prices, housing_features[:,i], 'r.')
    pl.legend()
    pl.label = ''
    pl.xlabel('House price')
    pl.ylabel(str(city_data.feature_names[i]))
    pl.tight_layout()
pl.show()
```



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 [8]:
```
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: NOX - 0.659, RM - 5.6, LSTAT - 12.13,

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 [17]:
```
# Put any import statements you need for this code block here
from sklearn import cross_validation

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

    # Shuffle and split the data
    X_train, X_test, y_train, y_test = cross_validation.train_test_split(
        X, y, test_size=0.3, random_state=42)

    # 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_features, housi
ng_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 3

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

Answer: To perform non-bias analysis of the data and avoid underfitting or overfitting issues, we build a model and tune parameters of regression analysis on training set and check performance on test set. The division of the data into train and test sets must be executed carefully to avoid introducing any systematic differences between learn and test. For example, we would never want to select the first half of the data for learning since there is a risk that data was ordered in a specific way.

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)](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 [18]:

```
# Put any import statements you need for this code block here
from sklearn.metrics import mean_squared_error

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



# 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: First 4 metrics are used for binary classification, while Mean Squered Error (MSE) and Mean Absolute Error (MAE) are used for regression analysis on continuous data. MSE analysis make use of squared distances between data and fit, thus large errors have relatively greater influence on MSE than do the smaller error. MAE is more robust to outliers since it does not make use of square. On the other hand, MSE is more useful if we are concerned about large errors whose consequences are much bigger than equivalent smaller ones. Thus in a given analysis I will implement MSE 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 [19]:

```
# Put any import statements you need for this code block
from sklearn.metrics import make_scorer
from sklearn import grid_search

def fit_model(X, y):
    """ Tunes a decision tree regressor model using GridSearchCV on the input dat
a 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 ->
    scoring_function = make_scorer(performance_metric, greater_is_better = False)

    # Make the GridSearchCV object ->
    reg = grid_search.GridSearchCV(regressor, parameters, scoring=scoring_functio
n)

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

    # Return the optimal model
    return reg


# Test fit_model
try:
    reg = fit_model(X_train, y_train)
    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:

Some learning algorithms use additional parameters that have to be setted up outside of training procedure. SVM algorithm for example requires setting up misclassification penalty term. Grid search (GS) algorithm is a way of systematically working through multiple combinations of these parameters, it picks out a grid of parameter values, evaluates every one of them, and returns the best.

Limitations of GS:

- GS is non-reliable in high dimensional spaces (> 3d)
- It may find different hyperparameter values on different training sets
- GS computationally is less efficient then random search 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: Cross validation (CV) is a model evaluation method. When we split data into train and test parts, the evaluation may depend on the amount of data and on which data points end up in the training set and which end up in the test set. To overcome these potential issues, CV method suggest to split data in to *k* parts, and run analysis *k*, where each time we use *k-1* parts for training and 1 part for testing. This way we increase *k* times amount of data we use for testing and we remove potential bias due to the choosing of test data. In a limiting *k* may be equal to *N* - number of data points in the set. In this case the training runs *N* times, each time on *N-1* data point and the last point is used for test.

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 [20]:
```
def learning_curves(X_train, y_train, X_test, y_test):
    """ Calculates the performance of several models with varying sizes of traini
ng 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_d
epth = 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_tr
ain[: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 [13]:
```
def model_complexity(X_train, y_train, X_test, y_test):
    """ Calculates the performance of the model as model complexity increases.
        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_train))

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

    # 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()
```

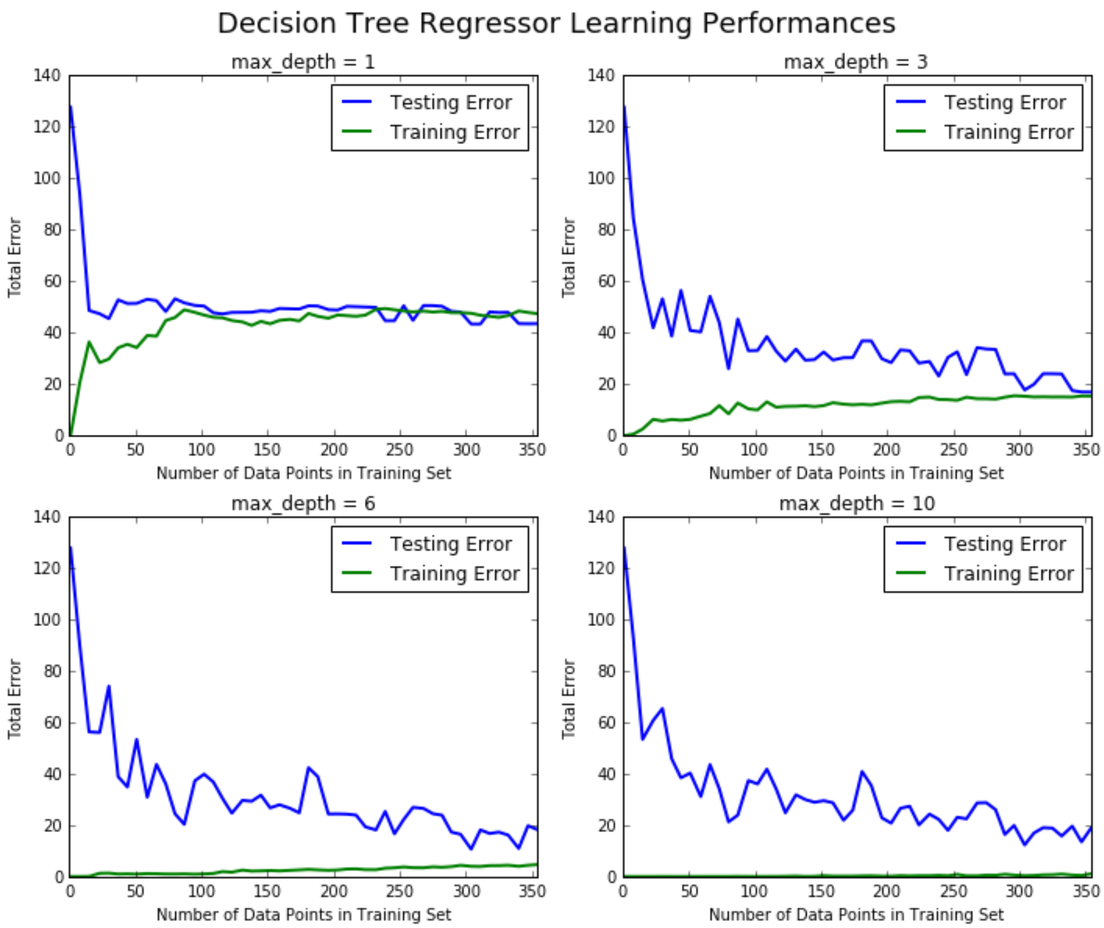
Analyzing Model Performance

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 [21]:
```
learning_curves(X_train, y_train, X_test, y_test)
```

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

/Users/Roma/Library/Enthought/Canopy_64bit/User/lib/python2.7/site-packages/ipyk
ernel/__main__.py:23: DeprecationWarning: using a non-integer number instead of
an integer will result in an error in the future
/Users/Roma/Library/Enthought/Canopy_64bit/User/lib/python2.7/site-packages/ipyk
ernel/__main__.py:26: DeprecationWarning: using a non-integer number instead of
an integer will result in an 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: Let's focus for example on error plot for max depth 6. As the training size increases, the training error increases slightly, the test error decreases and the model begins to predict better. THere is a gap between training and test errors curves which means that there is a high variance problem: the algorithm overfits data. Increasing amount of data set is likely to help.

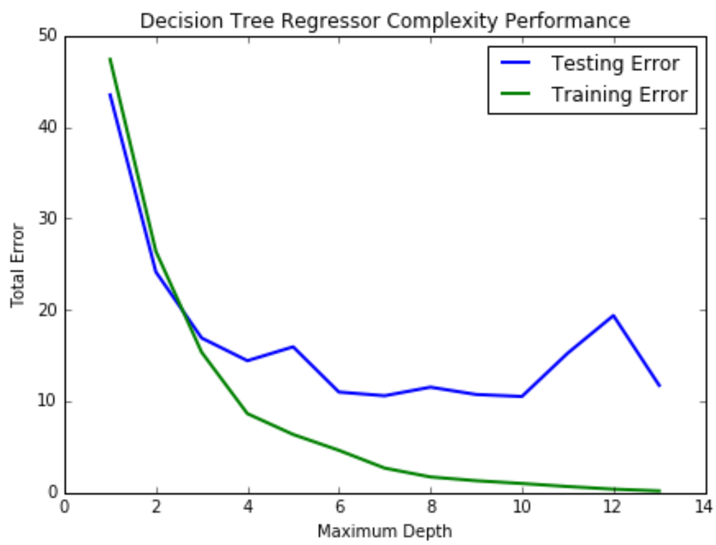
Question 8

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: With max depth 1, model suffers from high bias: both the training and test dataset has high errors and flattens out very fast. With max depth 10, model suffers from high variance: there is a significant gap between test and train erorrs which doesn't disappear with increasing number of data points in trining set.

In [67]:
```
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: With increase of max depth number, the training error keep decreasing but testing error leveled off (reaches steady minimum) for max depth of ~ 5-6. Therefore this is the max depths that best generalizes the data set: further increase in max depth will lead to increase in model complexity but won't improve model performance

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, 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 [68]:
```
print "Final model optimal parameters:", reg.best_params_
```

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

Answer: The average of *max_depth* parameter is about 5.8, which corresponds to the dependence of total error on max_depth value.

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 [69]:
```
sale_price = reg.predict(CLIENT_FEATURES)
print "Predicted value of client's home: {0:.3f}".format(sale_price[0])
```

```
Predicted value of client's home: 21.445
```

Answer: The model prediction of my client's home value is ~214K which is very close to to the median value of the property -212K in the database.

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: The model is not good enougth for predicting the selling price. The reason for my conclusion: even for the optimal max depth parameter, there is a gap between training and testing error which points on overfitting problem. To overcome this issue we have either perform cross validation analysis or if possible, increase data points.