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 [2]: # 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 no
        tebook)
        %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 [3]:

```
# Number of houses in the dataset
total_houses = housing_features.shape[0]

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

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

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

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

# 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: The three features that might be significant in my opinion are:

- CRIM: per capita crime rate by town
- RAD: index of accessibility to radial highways
- PTRATIO: pupil-teacher ratio by town

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 [4]:
```
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: The values in client's features corresponding to the three features chosen in Question 1 are:

- CRIM: 11.95
- RAD: 24
- PTRATIO: 20.2

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 the `shuffle_split_data` function is working if the statement "*Successfully shuffled and split the data!*" is printed.

In [5]:
```
# 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 
subsets,
        then returns the training and testing subsets. """

    # Shuffles and splits the data
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_
size=0.3, random_state=12)

    # 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_f
eatures, housing_prices)
    print "Successfully shuffled and split the data!"
except:
    print "Something went wrong with shuffling and splitting the da
ta."
```

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

Question 3

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

Answer: We split the data into training and testing subsets for our model broadly for 2 reasons:

- To evaluate the performance of our model on an independent dataset
- To ensure we are not overfitting with our model

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 the `performance_metric` function is working if the statement "*Successfully performed a metric calculation!*" is printed.

In [6]:
```
# 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 pre
dicted values
        based on a performance metric chosen by the student. """

    error = metrics.mean_squared_error(y_true, y_predict)
    return error


# 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 calculatio
n."
```

```
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: I chose Mean Squared Error (MSE) as the performance metric for predicting housing prices. Accuracy, Precision, Recall and F1 Score are appropriate metrics for classification problems. In our model, since we are making predictions on housing prices which is continuous variable, MSE and MAE are the most appropriate.

Between MSE and MAE, I chose MSE for the following 2 reasons:

- Squaring emphasizes the larger differences between predictions and data
- Mathematically MSE is continuously differentiable and a sufficient statistic for Gaussian distribution

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 the `fit_model` function is working if the statement "*Successfully fit a model to the data!*" is printed.

In [7]:

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

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
    scoring_function = metrics.make_scorer(metrics.mean_squared_err
or, greater_is_better=False)

    # Make the GridSearchCV object
    reg = grid_search.GridSearchCV(regressor, parameters, scoring=s
coring_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.best_estimator_


# 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: Grid search algorithm is a simple way to try multiple combinations of model parameters and to ultimately determine which parameters give the best performance metric as specified. The algortihm is applicable when appropriate model parameters are not known and has an advantage of model evaluation in parallel for large datasets.

However, grid search suffers from the "curse of dimensionality"and may lead to large computation times in large datasets with high number of features. It might not be applicable under such circumstances.

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 is essentially used for model validation and can be defined as a method to assess the applicability of a statistical model to an independent data set.

Typically, cross-validation is performed by dividing a dataset into complementary subsets, then building the statistical model using one subset (training set) and then validate that statistical model on the other subset (testing set). Ideally, several rounds of such cross-validation are performed using different partitions, to get an average validation result over all rounds. This leads to a more accurate assessment of the statistical model.

Cross-validation can be helpful when using grid search because the performance metric from cross-validation for each model parameter combination, could be used to select the best parameter for the statistical model that fits the data. In the case of our Boston housing problem, the model parameter from grid search leading to the least MSE for the cross-validation (on the testing dataset) would be a reasonable best choice for the model.

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 [125]:
```
def learning_curves(X_train, y_train, X_test, y_test):
    """ Calculates the performance of several models with varying s
izes of training data.
        The learning and testing error rates for each model are the
n 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 differe
nt sizes
    sizes = np.rint(np.linspace(1, len(X_train), 50)).astype(int)
    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 t
ree 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], regresso
r.predict(X_train[:s]))

            # Find the performance on the testing set
            test_err[i] = performance_metric(y_test, regressor.pred
ict(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', f
ontsize=18, y=1.03)
    fig.tight_layout()
    fig.show()
```

In [84]:

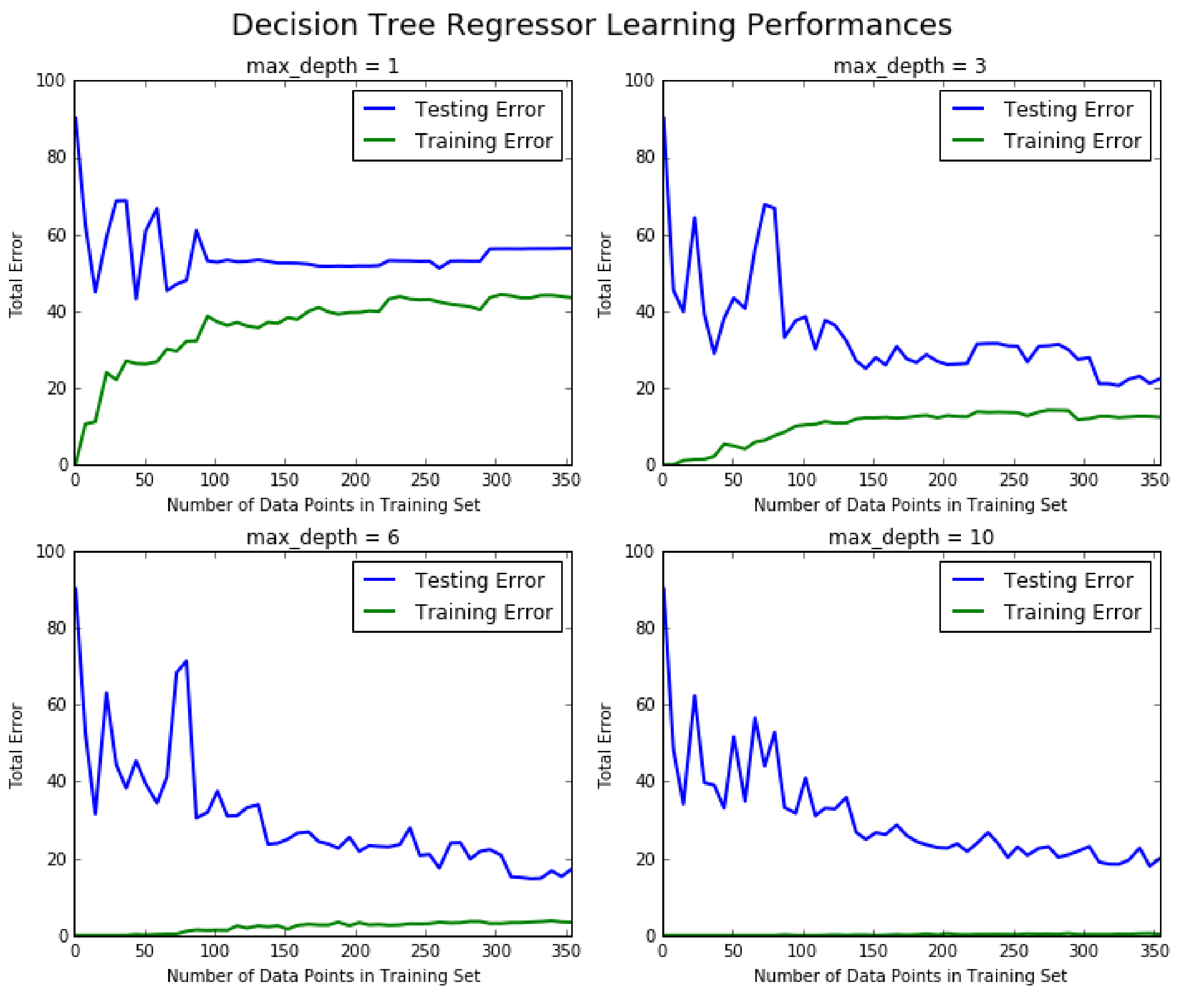
```
def model_complexity(X_train, y_train, X_test, y_test):
    """ Calculates the performance of the model as model complexity
increases.
        The learning and testing errors rates are then plotted. """

    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.predic
t(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 [85]:
```
learning_curves(X_train, y_train, X_test, y_test)
```

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



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: The max depth of the chosen model is 6.

For lower number of data points in the training set (approximately less than 200 data points), the training error increases as the size of training dataset increases. Beyond 200 data points in the dataset, the training error levels off.

Conversely, the overall trend for testing error shows a decline with increasing number of data points (for less than 200 data points in the training set). The noise around this trend is higher compared to the noise around training error trend. As the size of training set increases (beyond approximately 200 data points), the testing error levels off and decreases at a very slow rate

Question 8

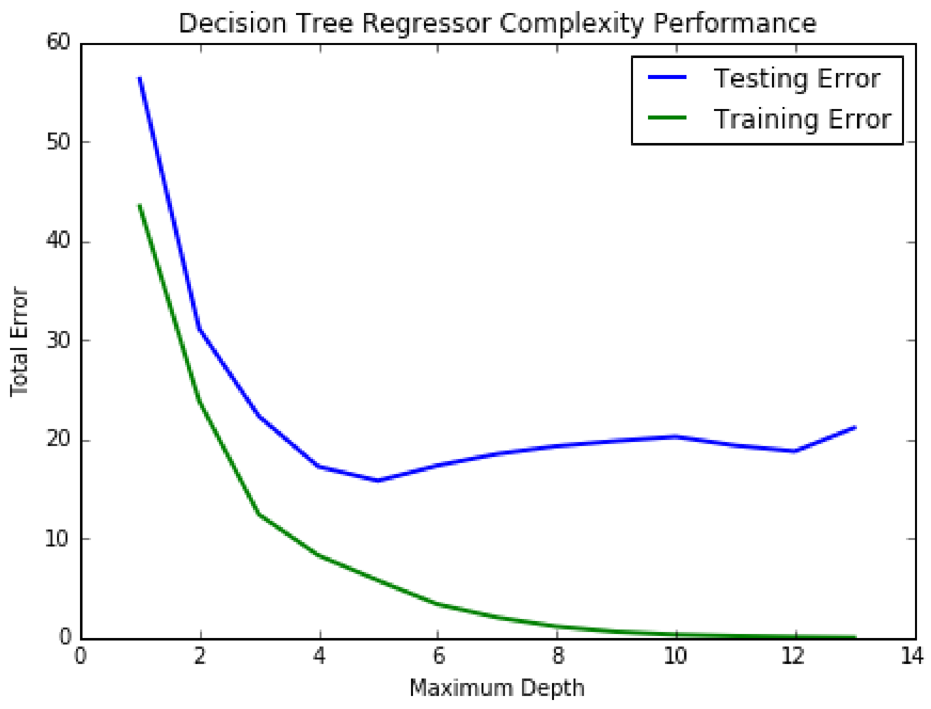
Look at the learning curve graphs for the model with a max depth of 1 and a max depth of 10. When the model is using the full training set, does it suffer from high bias or high variance when the max depth is 1? What about when the max depth is 10?

Answer: For the full training set, when the max depth is 1, the model suffers from high bias. This is highlighted from the learning curve graph for max depth of 1, where more training set data points do not result in any improvement in training error (particularly beyond 100 data points). The model with max depth of 1 is just not complex enough to capture underlying relationships.

For max depth of 10, the model suffers from high variance. The testing error at max depth of 10 for the full training set is higher than the testing error at max depth of 6 for the full training set. This indicates a over-fitting situation at max depth of 10, where the model is unable to generalize its predictions to the independent testing dataset.

In [86]:
```
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: As the max depth increases, training errors decrease exponentially. Testing errors decrease rapidly until max depth = 5 and then start to increase slowly beyond max depth = 6.

max depth = 5 best generalizes the dataset. This max depth is optimal because it reflects the lowest MSE for the testing dataset. Anything higher than max depth = 5 suffers from high variance and over-fitting of training data. Such a model cannot be generalized over other independent datasets. Model with max depth < 5 suffers from bias and does not adequately represent model complexity.

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`. When applying grid search along with cross-validation to optimize your model, it would typically be performed and validated on a training set and subsequently evaluated on a **dedicated test set**. In this project, the optimization below is performed on the *entire dataset* (as opposed to the training set you made above) due to the many outliers in the data. Using the entire dataset for training provides for a less volatile prediction at the expense of not testing your model's performance.

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 [8]:
```
print "Final model has an optimal max_depth parameter of", reg.get_
params()['max_depth']
```

```
Final model has an optimal max_depth parameter of 6
```

Answer: Running the fit model ~20 times, the mean optimal max_depth parameter (rounding to the nearest integer) using grid search on the entire dataset is 6. This is close to the result we got from the complexity graph.

My initial intuition from the original dataset was around 3 to 4 features explaining majority of the variance in the dataset.

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 [9]:
```
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: 20.766
```

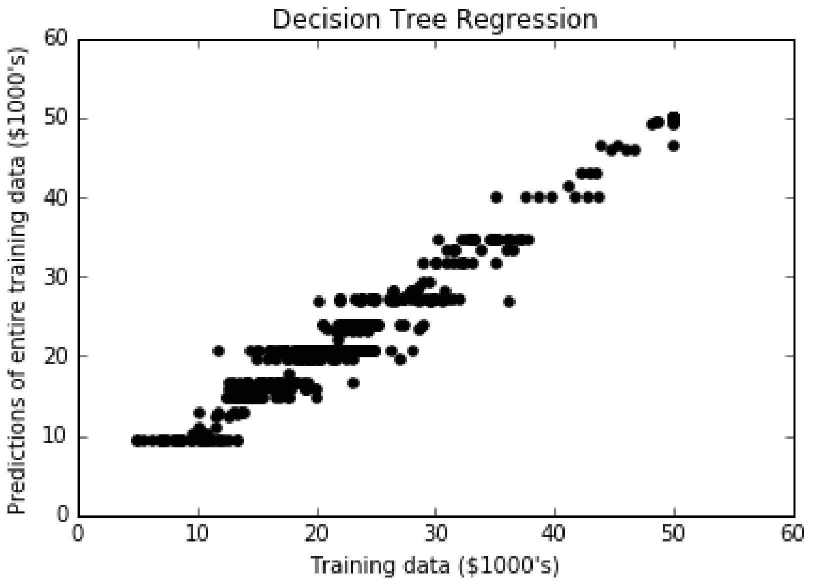
Answer: The best selling price for my client's home with a optimal max_depth parameter of 6 is ~20000. This number is very close to the median house value in the dataset (21000)

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 use this model to predict the selling price. My answer is based on the relatively low MSEs seen for both the training and testing datasets (as seen from the learning and complexity performance for the optimal depth parameter). The scatterplot below of actual v/s predicted housing values (based on the entire training dataset), shows good predictive power for the housing price model.

In [147]:
```
# Scatterplot of predicted v/s actual training dataset
pl.figure()
pl.scatter(housing_prices, reg.predict(housing_features), c="k")
pl.xlabel("Training data ($1000's)")
pl.ylabel("Predictions of entire training data ($1000's)")
pl.title("Decision Tree Regression")
pl.legend()
pl.show()
```



In [12]:
```
from sklearn.neighbors import NearestNeighbors
def find_nearest_neighbor_indexes(x, X):  # x is your vector and X
is the data set.
   neigh = NearestNeighbors( n_neighbors = 15 )
   neigh.fit( X)
   distance, indexes = neigh.kneighbors( x )
   return indexes
indexes = find_nearest_neighbor_indexes(CLIENT_FEATURES, housing_fe
atures)
sum_prices = []
for i in indexes:
    sum_prices.append(housing_prices[i])
neighbor_avg = np.mean(sum_prices)
print "Nearest Neighbors average: " +str(neighbor_avg)
```

```
Nearest Neighbors average: 19.56
```

In [ ]: