Polynomial regression

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June 12, 2019

1 Polynomial regression

When dealing with regression (linear or not) problems, it is usually necessary to solve an optimization problem. When we fit a model, we need to find some parameters that better approximate our data. In the course of this exercise, we will use two different kinds of optimization techniques:

- **gradient descent**, which is an iterative algorithm;
- **normal equation**, which is an analytical method.

The differences between the two approaches are that the former requires a phase of features scaling when they have values with a different order of magnitude. The latter doesn't require any scaling, but it can be slower since it has to calculate the inverse of a matrix that can be huge if there are a lot of features.

It is up to us to choose the best optimization method to use, considering the data-set over which we will optimize the model.

1.1 Imports and definitions

Let's first import the packages we need and let's define the standard functions used in the previous exercises:

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

        import pandas as pd
        import seaborn as sns

        %matplotlib inline

        from sklearn.datasets import load_boston
        from sklearn.linear_model import LinearRegression
        from sklearn.metrics import mean_squared_error

        boston_dataset = load_boston()
```

```
In [2]: def gradient_descent_vectorized(x, y, theta = [[0], [0]],
                                alpha = 0.01, num_iters = 400, epsilon = 0.0001):
            J_history = np.zeros((num_iters))
```

```
        early_stop = -1;
        for k in range(num_iters):
            h = x.dot(theta)
            theta = theta - (alpha/m)*(x.T.dot(h-y))
            J_history[k] = compute_cost_vectorized(x, y, theta)
        return theta, J_history
    def compute_cost_vectorized(x, y, theta):
        h = x.dot(theta)
        J = (h-y).T.dot(h-y)
        return J/(2*m)
    def find_flat(history, epsilon = 0.001):
        for k in range(1, history.size):
            if (history[k-1] - history[k] < epsilon):
                return k;
        return -1
    def normal_equations(x, y):
        return np.linalg.pinv(x.T.dot(x)).dot(x.T).dot(y)
    def polynomial_features(x, degree):
        for i in range(1, degree):
            label = VARIABLE + '_%d'%(i+1)
            x[label] = x[VARIABLE]**(i+1)
        return x
```

Let's see the name of the features in the dataset:

```
In [3]: print(boston_dataset.keys())
```

```
dict_keys(['data', 'target', 'feature_names', 'DESCR', 'filename'])
```

We can access to the description of the dataset and the explanation of the features in it.

```
In [4]: print(boston_dataset.DESCR)
```

```
.. _boston_dataset:

Boston house prices dataset
---------------------------

**Data Set Characteristics:**

    :Number of Instances: 506

    :Number of Attributes: 13 numeric/categorical predictive. Median Value (attribute 14)
    is usually the target.

    :Attribute Information (in order):
        - CRIM     per capita crime rate by town
        - ZN       proportion of residential land zoned for lots over 25,000 sq.ft.
```

```
        - INDUS     proportion of non-retail business acres per town
        - CHAS      Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
        - NOX       nitric oxides concentration (parts per 10 million)
        - RM        average number of rooms per dwelling
        - AGE       proportion of owner-occupied units built prior to 1940
        - DIS       weighted distances to five Boston employment centres
        - RAD       index of accessibility to radial highways
        - TAX       full-value property-tax rate per $10,000
        - PTRATIO   pupil-teacher ratio by town
        - B         1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
        - LSTAT     % lower status of the population
        - MEDV      Median value of owner-occupied homes in $1000's

    :Missing Attribute Values: None

    :Creator: Harrison, D. and Rubinfeld, D.L.

This is a copy of UCI ML housing dataset.
https://archive.ics.uci.edu/ml/machine-learning-databases/housing/


This dataset was taken from the StatLib library which is maintained at Carnegie
Mellon University.

The Boston house-price data of Harrison, D. and Rubinfeld, D.L. 'Hedonic
prices and the demand for clean air', J. Environ. Economics & Management,
vol.5, 81-102, 1978.   Used in Belsley, Kuh & Welsch, 'Regression diagnostics
...', Wiley, 1980.   N.B. Various transformations are used in the table on
pages 244-261 of the latter.

The Boston house-price data has been used in many machine learning papers that
address regression problems.

.. topic:: References

   - Belsley, Kuh & Welsch, 'Regression diagnostics: Identifying Influential Data
   and Sources of Collinearity', Wiley, 1980. 244-261.
   - Quinlan,R. (1993). Combining Instance-Based and Model-Based Learning. In
   Proceedings on the Tenth International Conference of Machine Learning, 236-243,
   University of Massachusetts, Amherst. Morgan Kaufmann.
```

Let's see the first 5 examples in the dataset:

```
In [5]: boston = pd.DataFrame(boston_dataset.data,
                              columns=boston_dataset.feature_names)
        boston.head()
```

```
Out[5]:       CRIM    ZN  INDUS  CHAS    NOX     RM   AGE     DIS  RAD    TAX  \
        0  0.00632  18.0   2.31   0.0  0.538  6.575  65.2  4.0900  1.0  296.0
        1  0.02731   0.0   7.07   0.0  0.469  6.421  78.9  4.9671  2.0  242.0
        2  0.02729   0.0   7.07   0.0  0.469  7.185  61.1  4.9671  2.0  242.0
        3  0.03237   0.0   2.18   0.0  0.458  6.998  45.8  6.0622  3.0  222.0
        4  0.06905   0.0   2.18   0.0  0.458  7.147  54.2  6.0622  3.0  222.0

           PTRATIO       B  LSTAT
        0     15.3  396.90   4.98
        1     17.8  396.90   9.14
        2     17.8  392.83   4.03
        3     18.7  394.63   2.94
        4     18.7  396.90   5.33
```

In the dataset the **target feature** is missing, we can add it as follows:

```
In [6]: boston['MEDV'] = boston_dataset.target
        boston.head()
```

```
Out[6]:       CRIM    ZN  INDUS  CHAS    NOX     RM   AGE     DIS  RAD    TAX  \
        0  0.00632  18.0   2.31   0.0  0.538  6.575  65.2  4.0900  1.0  296.0
        1  0.02731   0.0   7.07   0.0  0.469  6.421  78.9  4.9671  2.0  242.0
        2  0.02729   0.0   7.07   0.0  0.469  7.185  61.1  4.9671  2.0  242.0
        3  0.03237   0.0   2.18   0.0  0.458  6.998  45.8  6.0622  3.0  222.0
        4  0.06905   0.0   2.18   0.0  0.458  7.147  54.2  6.0622  3.0  222.0

           PTRATIO       B  LSTAT  MEDV
        0     15.3  396.90   4.98  24.0
        1     17.8  396.90   9.14  21.6
        2     17.8  392.83   4.03  34.7
        3     18.7  394.63   2.94  33.4
        4     18.7  396.90   5.33  36.2
```

The data-frame has some useful utility functions too, like the one we can use to see the *spurious* examples, which count the number of null values inside the dataset:

```
In [7]: boston.isnull().sum()
```

```
Out[7]: CRIM       0
        ZN         0
        INDUS      0
        CHAS       0
        NOX        0
        RM         0
        AGE        0
        DIS        0
        RAD        0
        TAX        0
        PTRATIO    0
```

```
B           0
LSTAT       0
MEDV        0
dtype: int64
```

1.2 Plot the 'Pearson' Correlation matrix

Having a great number of features can be a problem during the training phase, especially when there are a lot of training examples. To reduce the number of features, we can ignore some of them using only the independent ones. The correlation between the features can be calculated using the **Pearson correlation index**, which is defined as follows:

$$\rho_{x,y} = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \overline{y})^2}}$$

where:

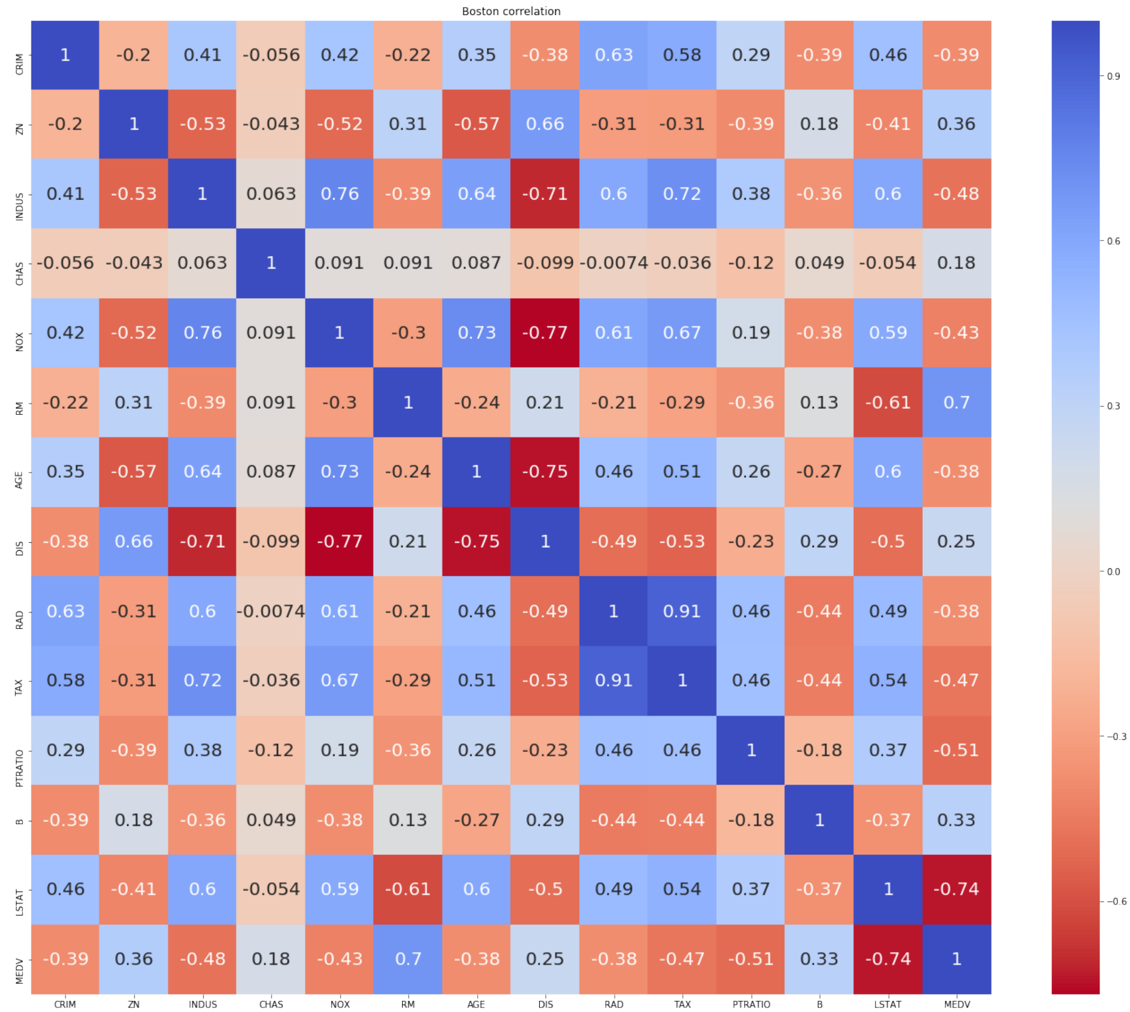
- the numerator represents the co-variance of x_i and y_i;
- the denominator represents the product of the standard deviations.

It is true that:

$$\rho_{x,y} \begin{cases} > 0 & \text{if } x \text{ and } y \text{ are positively correlated,} \\ = 0 & \text{if } x \text{ and } y \text{ are not correlated,} \\ < 0 & \text{if } x \text{ and } y \text{ are negatively correlated} \end{cases}$$

Bear in mind that this index captures the linear correlation between the two considered values, not the more complex ones like the non-linear.

```
In [8]: f, (ax1) = plt.subplots(1, 1, figsize = (24, 20))
        corr = boston.corr(method = "pearson")
        sns.heatmap(corr, cmap = 'coolwarm_r', annot = True,
                    annot_kws = {'size': 20}, ax = ax1)
        ax1.set_title('Boston correlation')
        plt.show()
```



The table shows all the correlation indices between every couple of features. In the last row, we have all the correlation indices between every feature in the dataset and the target feature.

Only two features are highly correlated to the target feature:

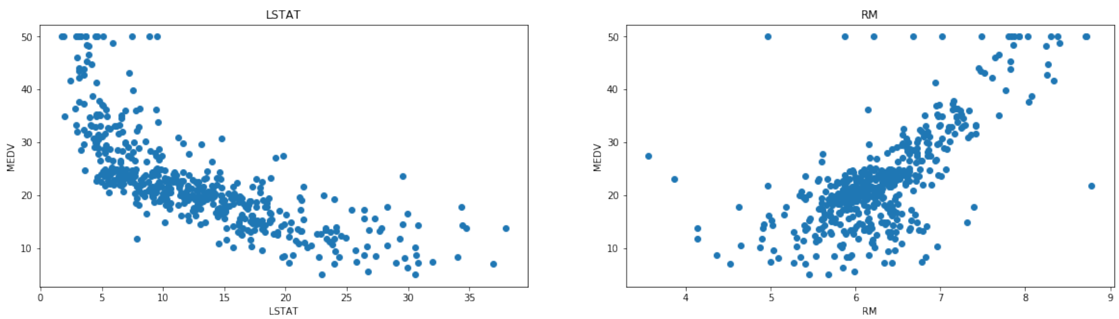
- **RM**, which has a correlation index of **0.7**
- **LSTAT**, which has a correlation index of **-0.74**

Because of the high degree of correlation between these features, we should not use both of them in the training phase, since using both of them could potentially bring numerical instability in the solution.

Let's plot the target feature with respect to the two considered features:

```
In [9]: plt.figure(figsize=(20, 5))

        features = ['LSTAT', 'RM']
        target = boston['MEDV']
```

```
for i, col in enumerate(features):
    plt.subplot(1, len(features) , i+1)
    x = boston[col]
    y = target
    plt.scatter(x, y, marker='o')
    plt.title(col)
    plt.xlabel(col)
    plt.ylabel('MEDV')
```



1.3 Linear regression with one variable

The linear regression model isn't always the best fit to analyze data, even if it adapts well to data. Hence, the model can fail to generalize on unseen events, giving a poor performance on the validation or test set.

Let's build our custom dataset using only the feature we will consider:

```
In [10]: VARIABLE = 'LSTAT' #'RM'

         x = pd.DataFrame(np.c_[boston[VARIABLE]], columns = [VARIABLE])
         x.head()
         y = boston['MEDV'].values.reshape((y.shape[0], 1))

         x = np.concatenate([np.ones((x.shape[0], 1)), x], axis = 1)

         m = x.shape[0]
         n = x.shape[1]

         print('# Training examples: ', m)
         print('# Features : ', n)
```

```
# Training examples:  506
# Features :  2
```

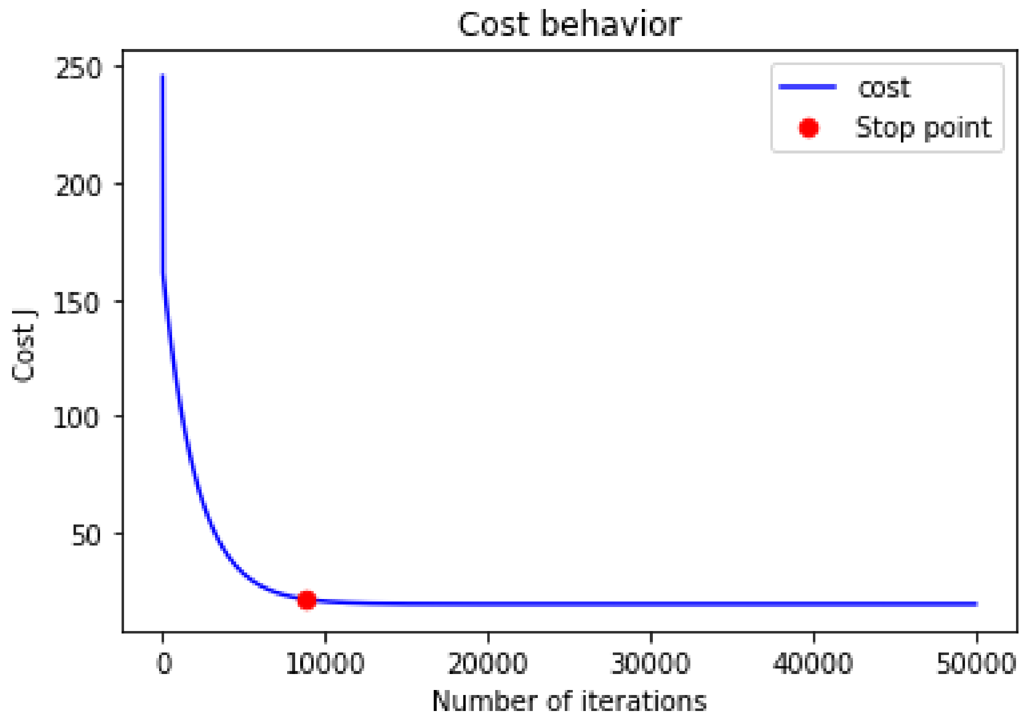
We can now train the model using the gradient descent method:

```
In [11]: theta = np.zeros((2,1))
         num_iters = 50000
         alpha = 0.001
         theta, J_history = gradient_descent_vectorized(x, y,
                                                       theta, alpha, num_iters)

         stop_point = find_flat(J_history)

         print(theta)
         print("Early stop at step: {}".format(stop_point))
         print("Cost at early stop: {}".format(J_history[stop_point]))
```

```
[[34.55363291]
 [-0.95003687]]
Early stop at step: 8806
Cost at early stop: 21.320640024786734
```

Let's show how the cost varies with respect to the iteration number:

```
In [12]: plt.plot([i for i in range(num_iters)],
                  J_history, 'b', label = 'cost')
         if (stop_point != -1):
             plt.plot(stop_point, J_history[stop_point],
                      '.r', label = 'Stop point',  markersize=13)
         plt.xlabel('Number of iterations')
         plt.ylabel('Cost J')
         plt.title('Cost behavior')
         plt.legend()
         plt.show()
```



As can be seen in the graph, the cost function decreases smoothly. The red point represents the point where the cost flattens out: after that point, the cost function decrease of less than *0.1%* at each iteration.

Let's calculate the θ parameter applying a closed-form solution by using the **normal equation** method:

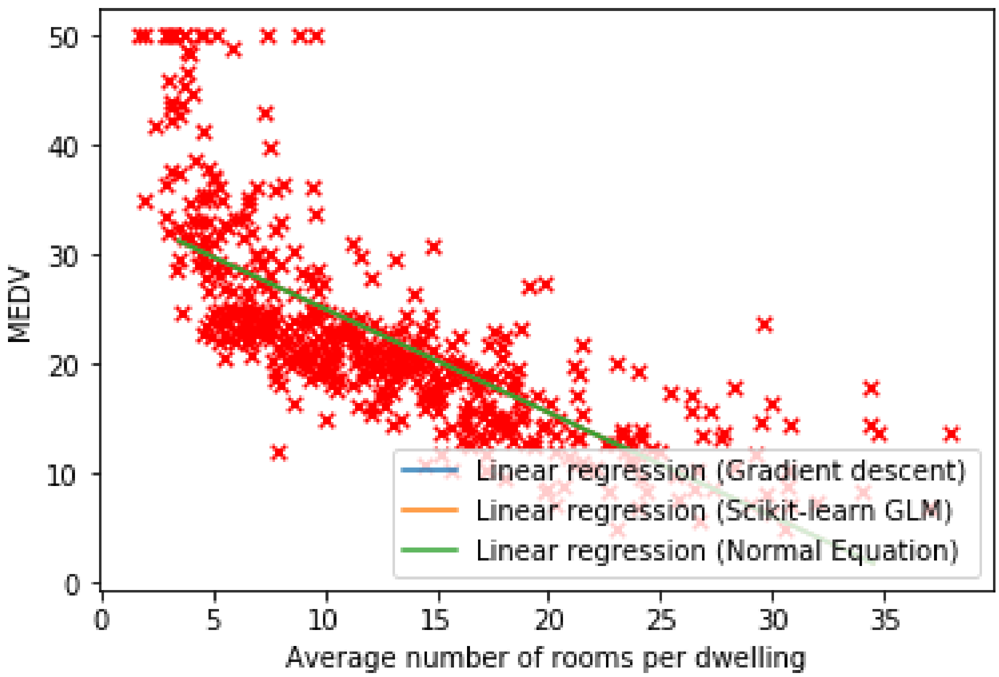
```
In [13]: theta_ne = normal_equations(x, y)
         print("The parametes (using the normal equations) are:\n{}"
               .format(theta_ne))
         cost = compute_cost_vectorized(x, y, theta_ne)
```

```
The parametes (using the normal equations) are:
[[34.55384088]
 [-0.95004935]]
```

We can now show how the different parameters are represented on the training set:

```
In [14]: xx = np.arange(3.5,35)
         yy = theta[0] + theta[1] * xx

         # Plot gradient descent
         plt.scatter(x[:,1], y, s=30, c='r', marker='x', linewidths=1)
         plt.plot(xx,yy, label='Linear regression (Gradient descent)')

         # Compare with Scikit-learn Linear regression
```

```
regr = LinearRegression()
regr.fit(x[:,1].reshape(-1,1), y.ravel())
plt.plot(xx, regr.intercept_ + regr.coef_ * xx,
         label='Linear regression (Scikit-learn GLM)')

# Compare with Normal Equations
plt.plot(xx, theta_ne[0] + theta_ne[1] * xx,
         label='Linear regression (Normal Equation)')


plt.xlabel('Average number of rooms per dwelling')
plt.ylabel('MEDV')
plt.legend(loc=4);
```



The three lines in the graph coincide, and for this reason, we can see only the green one. Let's now calculate the error committed using the *root mean square error*:

```
In [15]: y_pred = np.zeros((x.shape[0], 1))
         y_pred = x.dot(theta)

         result = np.sqrt(mean_squared_error(y, y_pred))
         print("The error done by the model is: {}".format(result))
```

```
The error done by the model is: 6.2034641322672694
```

2 Polynomial regression

We have seen simple models like the linear ones, but we can use some more complex models as the non-linear ones.

In [16]:
```
dataframe = pd.DataFrame(x[:, 1], columns = [VARIABLE])
new_data = polynomial_features(dataframe, 1)
new_data.head()
```

Out[16]:

	LSTAT
0	4.98
1	9.14
2	4.03
3	2.94
4	5.33

2.1 Comparing higher order hypothesis function

In this section, we'll use a polynomial hypothesis function as the following:

$$h_\theta(x) = \theta_0 + \sum_{i=1}^{k} \theta_i x^i$$

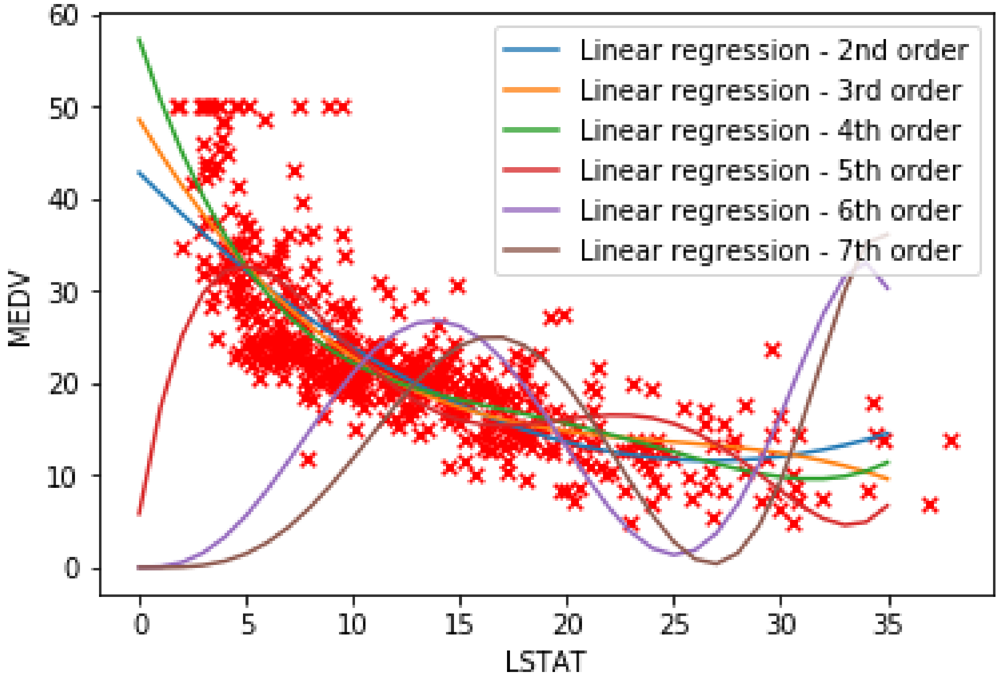
Below we will calculate the parameters for each model from the 2^{nd} to the 7^{th} degree:

In [17]:
```
new_data = polynomial_features(dataframe, 2)
x_2 = np.concatenate([x,
        new_data.iloc[:,1].values.reshape((y.shape[0], 1))], axis = 1)
theta_ne_2 = normal_equations(x_2, y)

new_data = polynomial_features(dataframe, 3)
x_3 = np.concatenate([x_2,
        new_data.iloc[:,2].values.reshape((y.shape[0], 1))], axis = 1)
theta_ne_3 = normal_equations(x_3, y)

new_data = polynomial_features(dataframe, 4)
x_4 = np.concatenate([x_3,
        new_data.iloc[:,3].values.reshape((y.shape[0], 1))], axis = 1)
theta_ne_4 = normal_equations(x_4, y)

new_data = polynomial_features(dataframe, 5)
x_5 = np.concatenate([x_4,
        new_data.iloc[:,4].values.reshape((y.shape[0], 1))], axis = 1)
theta_ne_5 = normal_equations(x_5, y)

new_data = polynomial_features(dataframe, 6)
x_6 = np.concatenate([x_5,
        new_data.iloc[:,5].values.reshape((y.shape[0], 1))], axis = 1)
theta_ne_6 = normal_equations(x_6, y)
```

```
new_data = polynomial_features(dataframe, 7)
x_7 = np.concatenate([x_6,
        new_data.iloc[:,6].values.reshape((y.shape[0], 1))], axis = 1)
theta_ne_7 = normal_equations(x_7, y)
```

We can now fit the lines using the parameters just found so we can draw them on a graph. In this way, we can make a visual comparison of the different models.

In [18]:
```
xx = np.arange(0,36)

yy_2 = theta_ne_2[0] + theta_ne_2[1] * xx + theta_ne_2[2] * xx**2

yy_3 = theta_ne_3[0] + theta_ne_3[1] * xx + theta_ne_3[2] * xx**2 \
        + theta_ne_3[3] * xx**3

yy_4 = theta_ne_4[0] + theta_ne_4[1] * xx + theta_ne_4[2] * xx**2 \
        + theta_ne_4[3] * xx**3 + theta_ne_4[4] * xx**4

yy_5 = theta_ne_5[0] + theta_ne_5[1] * xx + theta_ne_5[2] * xx**2 \
        + theta_ne_5[3] * xx**3 + theta_ne_5[4] * xx**4 \
        + theta_ne_5[5] * xx**5

yy_6 = theta_ne_6[0] + theta_ne_6[1] * xx + theta_ne_6[2] * xx**2 \
        + theta_ne_6[3] * xx**3 + theta_ne_6[4] * xx**4 \
        + theta_ne_6[5] * xx**5 + theta_ne_6[6] * xx**6

yy_7 = theta_ne_7[0] + theta_ne_7[1] * xx + theta_ne_7[2] * xx**2 \
        + theta_ne_7[3] * xx**3 + theta_ne_7[4] * xx**4 \
        + theta_ne_7[5] * xx**5 + theta_ne_7[6] * xx**6 \
        + theta_ne_7[7] * xx**7


# Plot gradient descent
plt.scatter(x[:,1], y, s=30, c='r', marker='x', linewidths=1)
plt.plot(xx,yy_2, label='Linear regression - 2nd order')
plt.plot(xx,yy_3, label='Linear regression - 3rd order')
plt.plot(xx,yy_4, label='Linear regression - 4th order')
plt.plot(xx,yy_5, label='Linear regression - 5th order')
plt.plot(xx,yy_6, label='Linear regression - 6th order')
plt.plot(xx,yy_7, label='Linear regression - 7th order')


#plt.ylim(-2,55)
#plt.xlim(-2,13)
plt.xlabel('LSTAT')
plt.ylabel('MEDV')
plt.legend(loc=1);
```



When we want to choose the right model, we need to compare the features in the training set and their relation with the target features. After that, we find the models that are correct from a conceptual point of view. We can finally choose the better among them by using metrics like the *root mean squared error*.

2.2 Calculating root mean squared error and comparison

The definition of the **RMSE** is:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=0}^{N}(\hat{y}_i - y_i)^2}{N}}$$

In order to calculate this:

- we can iterate over the data-set taking the target feature;
- do a prediction step using θ_{ne} found;
- apply the formula for RMSE introduced above.

This will be done on the training set, even if it should be done on a test set for better comparisons.

Let's calculate the predictions for each of the hypothesis function used:

```
In [19]: pred_2 = theta_ne_2[0] + theta_ne_2[1] * x[:,1] \
                  + theta_ne_2[2] * x[:,1]**2
```

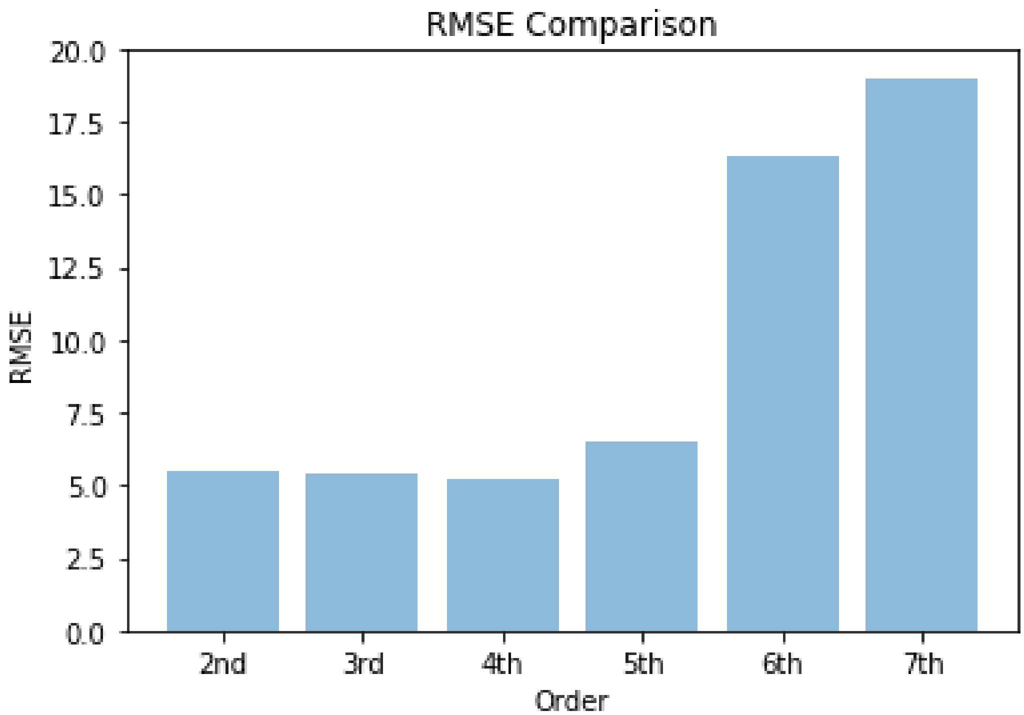
```
pred_3 = theta_ne_3[0] + theta_ne_3[1] * x[:,1] \
        + theta_ne_3[2] * x[:,1]**2 + theta_ne_3[3] * x[:,1]**3

pred_4 = theta_ne_4[0] + theta_ne_4[1] * x[:,1] \
        + theta_ne_4[2] * x[:,1]**2 + theta_ne_4[3] * x[:,1]**3 \
        + theta_ne_4[4] * x[:,1]**4

pred_5 = theta_ne_5[0] + theta_ne_5[1] * x[:,1] \
        + theta_ne_5[2] * x[:,1]**2 + theta_ne_5[3] * x[:,1]**3 \
        + theta_ne_5[4] * x[:,1]**4 + theta_ne_5[5] * x[:,1]**5

pred_6 = theta_ne_6[0] + theta_ne_6[1] * x[:,1] \
        + theta_ne_6[2] * x[:,1]**2 + theta_ne_6[3] * x[:,1]**3 \
        + theta_ne_6[4] * x[:,1]**4 + theta_ne_6[5] * x[:,1]**5 \
        + theta_ne_6[6] * x[:,1]**6

pred_7 = theta_ne_7[0] + theta_ne_7[1] * x[:,1] \
        + theta_ne_7[2] * x[:,1]**2 + theta_ne_7[3] * x[:,1]**3 \
        + theta_ne_7[4] * x[:,1]**4 + theta_ne_7[5] * x[:,1]**5 \
        + theta_ne_7[6] * x[:,1]**6 + theta_ne_7[7] * x[:,1]**7
```

Let's calculate the RMSE metrics on each prediction vector:

```
In [20]: rmse_2 = np.sqrt(mean_squared_error(y, pred_2))
         rmse_3 = np.sqrt(mean_squared_error(y, pred_3))
         rmse_4 = np.sqrt(mean_squared_error(y, pred_4))
         rmse_5 = np.sqrt(mean_squared_error(y, pred_5))
         rmse_6 = np.sqrt(mean_squared_error(y, pred_6))
         rmse_7 = np.sqrt(mean_squared_error(y, pred_7))
```

Let's now plot a bar chart to see how the different degrees for the hypothesis functions behave by comparing the errors done by each one of them:

```
In [21]: objects = ('2nd', '3rd', '4th', '5th', '6th', '7th')
         y_pos = np.arange(len(objects))
         performance = [rmse_2, rmse_3, rmse_4, rmse_5, rmse_6, rmse_7]

         plt.bar(y_pos, performance, align='center', alpha=0.5)
         plt.xticks(y_pos, objects)
         plt.ylabel('RMSE')
         plt.xlabel('Order')
         plt.title('RMSE Comparison')

         plt.show()
```



Here we can see that the lower error comes with a polynomial of 4^{th} degree, basing our considerations only on the training set. The right thing to do would be to see which polynomial hypothesis function works better on a validation dataset.

The problem here is that the model can overfit the data, giving us low error on the training set, but higher errors on test or validation set.

3 Let's take an interpolation of LSTAT and RM

The new hypothesis function will be:

$$h_\theta(x) = \theta_0 + \theta_1 x_{\mathrm{LSTAT}} + \theta_2 x_{\mathrm{RM}}$$

We will use it to apply a multivariate regression.

In [22]:
```
VARIABLE_1 = 'LSTAT'
VARIABLE_2 = 'RM'

x = pd.DataFrame(np.c_[boston[VARIABLE_1], boston[VARIABLE_2]],
                 columns = [VARIABLE_1, VARIABLE_2])
x.head()
```

Out[22]:

	LSTAT	RM
0	4.98	6.575
1	9.14	6.421
2	4.03	7.185

```
3   2.94  6.998
4   5.33  7.147
```

```
In [23]: # Concatenate the 1s to deal with theta_0
         dataset_as_matrix = np.concatenate([np.ones((x.shape[0], 1)),
                                  x.LSTAT.values.reshape((y.shape[0], 1)),
                                  x.RM.values.reshape((y.shape[0], 1))], axis = 1)

         theta_ne_int = normal_equations(dataset_as_matrix, y)

         print(theta_ne_int)
```

```
[[-1.35827281]
 [-0.64235833]
 [ 5.09478798]]
```

4 Using validation and test datasets

We'll divide the data-set into three parts:

- **Training set**, used to train the model (60% of the original data-set);
- **Validation set**, used to test the trained model to get the right hyper-parameters and to see how the trained model performs when these parameters vary (20% of the original data-set);
- **Test set**, used to test the model and to get the performance metrics on unseen events (the remaining 20% of the orginal data-set).

```
In [24]: training_dimension = int(m * 0.6)
         validation_dimension = int(m * 0.2)
         test_dimension = m - training_dimension - validation_dimension

         print("Dimension of the training set: {}".format(training_dimension))
         print("Dimension of the validation set: {}".format(validation_dimension))
         print("Dimension of the test set: {}".format(test_dimension))
```

```
Dimension of the training set: 303
Dimension of the validation set: 101
Dimension of the test set: 102
```

Let's show the first five example rows in the training set:

```
In [25]: # Training set
         df_training = boston.loc[0:training_dimension-1]
         df_training.head()
```

```
Out[25]:       CRIM    ZN  INDUS  CHAS    NOX     RM   AGE     DIS  RAD    TAX  \
         0  0.00632  18.0   2.31   0.0  0.538  6.575  65.2  4.0900  1.0  296.0
         1  0.02731   0.0   7.07   0.0  0.469  6.421  78.9  4.9671  2.0  242.0
         2  0.02729   0.0   7.07   0.0  0.469  7.185  61.1  4.9671  2.0  242.0
         3  0.03237   0.0   2.18   0.0  0.458  6.998  45.8  6.0622  3.0  222.0
         4  0.06905   0.0   2.18   0.0  0.458  7.147  54.2  6.0622  3.0  222.0

            PTRATIO       B  LSTAT  MEDV
         0     15.3  396.90   4.98  24.0
         1     17.8  396.90   9.14  21.6
         2     17.8  392.83   4.03  34.7
         3     18.7  394.63   2.94  33.4
         4     18.7  396.90   5.33  36.2
```

Let's show the first five example rows in the validation set:

```
In [26]: # Validation set
         df_validation = boston.loc[
             training_dimension:training_dimension+test_dimension-1]
         df_validation.head()
```

```
Out[26]:         CRIM    ZN  INDUS  CHAS    NOX     RM   AGE     DIS  RAD    TAX  \
         303  0.10000  34.0   6.09   0.0  0.433  6.982  17.7  5.4917  7.0  329.0
         304  0.05515  33.0   2.18   0.0  0.472  7.236  41.1  4.0220  7.0  222.0
         305  0.05479  33.0   2.18   0.0  0.472  6.616  58.1  3.3700  7.0  222.0
         306  0.07503  33.0   2.18   0.0  0.472  7.420  71.9  3.0992  7.0  222.0
         307  0.04932  33.0   2.18   0.0  0.472  6.849  70.3  3.1827  7.0  222.0

              PTRATIO       B  LSTAT  MEDV
         303     16.1  390.43   4.86  33.1
         304     18.4  393.68   6.93  36.1
         305     18.4  393.36   8.93  28.4
         306     18.4  396.90   6.47  33.4
         307     18.4  396.90   7.53  28.2
```

Let's show the first five example rows in the test set:

```
In [27]: # Test set
         df_test = boston.loc[training_dimension+test_dimension: m-1]
         df_test.head()
```

```
Out[27]:          CRIM   ZN  INDUS  CHAS    NOX     RM    AGE     DIS   RAD    TAX  \
         405  67.92080  0.0   18.1   0.0  0.693  5.683  100.0  1.4254  24.0  666.0
         406  20.71620  0.0   18.1   0.0  0.659  4.138  100.0  1.1781  24.0  666.0
         407  11.95110  0.0   18.1   0.0  0.659  5.608  100.0  1.2852  24.0  666.0
         408   7.40389  0.0   18.1   0.0  0.597  5.617   97.9  1.4547  24.0  666.0
         409  14.43830  0.0   18.1   0.0  0.597  6.852  100.0  1.4655  24.0  666.0

              PTRATIO       B  LSTAT  MEDV
```

```
405      20.2  384.97  22.98   5.0
406      20.2  370.22  23.34  11.9
407      20.2  332.09  12.13  27.9
408      20.2  314.64  26.40  17.2
409      20.2  179.36  19.78  27.5
```

4.1 Let's train the model using the training set

We'll train the model using a combination of two features. We will use the following hypothesis functions:

$$h_\theta(x) = \theta_0 + \theta_1 x_{\text{LSTAT}}\ x^2_{\text{RM}}$$
$$h_\theta(x) = \theta_0 + \theta_1 x^2_{\text{LSTAT}}\ x_{\text{RM}}$$

In [28]:
```python
TRAINING_VARIABLES = ['LSTAT', 'RM']


x_rm = pd.DataFrame(np.c_[df_training[TRAINING_VARIABLES]],
                    columns = TRAINING_VARIABLES)
x_lstat = pd.DataFrame(np.c_[df_training[TRAINING_VARIABLES]],
                       columns = TRAINING_VARIABLES)

y_training = df_training['MEDV'].values.reshape((df_training.shape[0], 1))

# Combine the columns obtaining a new column having the wanted features
x_rm['VAR'] = x_rm['LSTAT'] * x_rm['RM']**2
x_lstat['VAR'] = x_lstat['LSTAT']**2 * x_lstat['RM']
```

Let's now see the training set having the $x_{LSTAT}x^2_{RM}$ in the VAR column:

In [29]:
```python
# Dataset having RM squared
x_rm.head()
```

Out[29]:

	LSTAT	RM	VAR
0	4.98	6.575	215.288513
1	9.14	6.421	376.835263
2	4.03	7.185	208.045627
3	2.94	6.998	143.977692
4	5.33	7.147	272.254316

Let's see the training set having the $x^2_{LSTAT}x_{RM}$ in the VAR column:

In [30]:
```python
# Dataset having LSTAT squared
x_lstat.head()
```

Out[30]:

	LSTAT	RM	VAR
0	4.98	6.575	163.062630
1	9.14	6.421	536.407772
2	4.03	7.185	116.690867
3	2.94	6.998	60.487913
4	5.33	7.147	203.038408

We will now delete the useless column in the data-sets created, like the *LSTAT* and the *RM* columns, as we will use only the *VAR* columns.

```
In [31]: # Discard the first two columns as we will use only the "VAR" column
         adapted_training_set_rm =  pd.DataFrame(np.c_[x_rm["VAR"]], columns = ["VAR"])
          # Add a columns of 1s to the training set
         x_rm = np.concatenate([np.ones((x_rm.shape[0], 1)),
                                adapted_training_set_rm], axis = 1)

         # Convert in dataframe and display it
         dataframe_rm = pd.DataFrame(x_rm[:], columns = ["CONST", "VAR"])
         dataframe_rm.head()
```

```
Out[31]:    CONST         VAR
         0    1.0  215.288513
         1    1.0  376.835263
         2    1.0  208.045627
         3    1.0  143.977692
         4    1.0  272.254316
```

```
In [32]: # Discard the first two columns as we will use only the "VAR" column
         adapted_training_set_lstat =  pd.DataFrame(
             np.c_[x_lstat["VAR"]], columns = ["VAR"])
         # Add a columns of 1s
         x_lstat = np.concatenate([np.ones((x_lstat.shape[0], 1)),
                                   adapted_training_set_lstat], axis = 1)

         # Convert in dataframe and display it
         dataframe_lstat = pd.DataFrame(x_lstat[:], columns = ["CONST", "VAR"])
         dataframe_lstat.head()
```

```
Out[32]:    CONST         VAR
         0    1.0  163.062630
         1    1.0  536.407772
         2    1.0  116.690867
         3    1.0   60.487913
         4    1.0  203.038408
```

Let's train the two models on the newly created data-set:

```
In [33]: # Let's train the model and get the cost
         x_rm = np.concatenate([dataframe_rm], axis = 1)
         x_lstat = np.concatenate([dataframe_lstat], axis = 1)

         theta_ne_rm = normal_equations(x_rm, y_training)
         cost_rm = compute_cost_vectorized(x_rm, y_training, theta_ne_rm)
         print("The trained model having RM squared has parameters:\n{}\n \
                It has a cost of {}\n\n".format(theta_ne_rm, cost_rm))
```

```
theta_ne_lstat = normal_equations(x_lstat, y_training)
cost_lstat = compute_cost_vectorized(x_lstat, y_training, theta_ne_lstat)
print("The trained model having LSTAT squared has parameters:\n{}\n\
        It has a cost of {}".format(theta_ne_lstat, cost_lstat))
```

```
The trained model having RM squared has parameters:
[[ 3.76188776e+01]
 [-2.98815284e-02]]
         It has a cost of [[14.84208928]]


The trained model having LSTAT squared has parameters:
[[ 2.99835436e+01]
 [-5.00082409e-03]]
        It has a cost of [[15.71867252]]
```

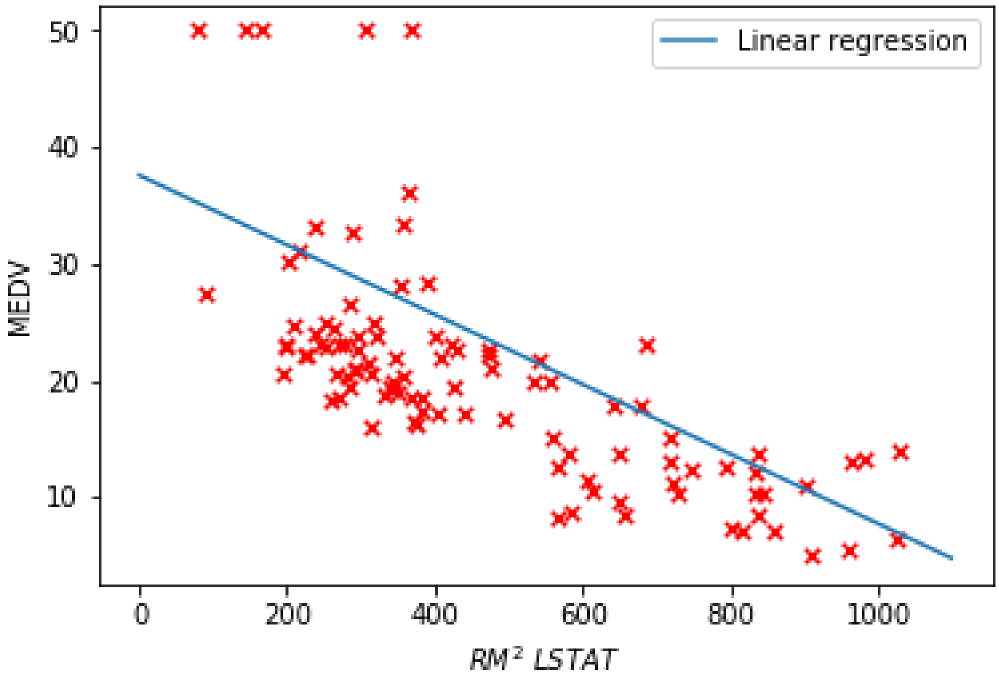
4.2 Let's use the validation set to see how the models perform

Let's convert the validation set into a matrix so we can use it to make predictions and let's take the target feature out of the validation set.

```
In [34]: # Let's adapt the validation set
         x = pd.DataFrame(np.c_[df_validation[TRAINING_VARIABLES]],
                          columns = TRAINING_VARIABLES)
         y_validation = df_validation['MEDV'].values \
             .reshape((df_validation.shape[0], 1))

         # Add a columns of 1s
         x = np.concatenate([np.ones((x.shape[0], 1)), x],
                            axis = 1)
```

Let's now create an array that goes from 0 to 1100, so we can use it to make forecasts. At this point, we can plot the predictions to see the training line on the validation examples. We will now consider the first hypothesis function (the one having the combination $x_{LSTAT}x_{RM}^2$).

```
In [35]: xx = np.arange(0,1100)
         yy = theta_ne_rm[0] + theta_ne_rm[1] * xx

         # Plot gradient descent
         plt.scatter(x[:,1] * x[:,2]**2, y_validation, s=30,
                     c='r', marker='x', linewidths=1)
         plt.plot(xx,yy, label='Linear regression')

         plt.xlabel('$RM^2\ LSTAT$')
         plt.ylabel('MEDV')
         plt.legend(loc=1);
```



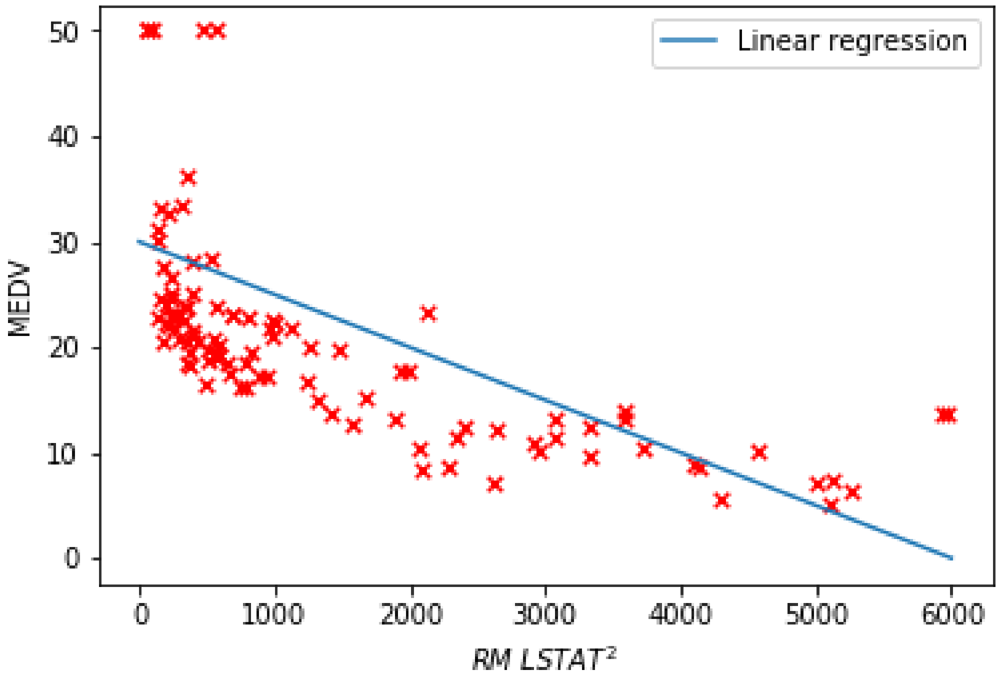
We can now calculate the RMSE committed by the model on the validation set:

```
In [36]: # Let's see the RMSE for the validation set
         predictions = theta_ne_rm[0] + theta_ne_rm[1] * x[:,1] * x[:,2]**2
         rmse_rm = np.sqrt(mean_squared_error(y_validation, predictions))

         print("The RMSE value for the validation set using RM squared is: {}".format(rmse_rm))
```

```
The RMSE value for the validation set using RM squared is: 7.620990352107873
```

Let's do the same thing considering the other hypothesis function:

```
In [37]: xx = np.arange(0,6000)
         yy = theta_ne_lstat[0] + theta_ne_lstat[1] * xx

         # Plot gradient descent
         plt.scatter(x[:,1]**2 * x[:,2], y_validation, s=30, c='r', marker='x', linewidths=1)
         plt.plot(xx,yy, label='Linear regression')

         plt.xlabel('$RM\ LSTAT^2$')
         plt.ylabel('MEDV')
         plt.legend(loc=1);
```

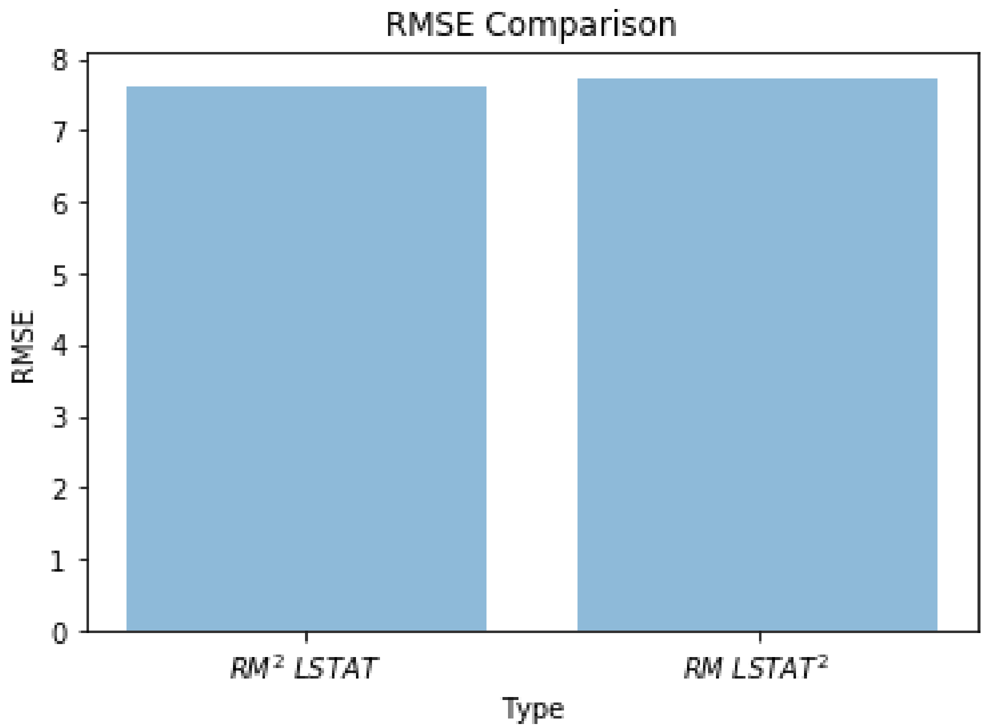



```
In [38]: # Let's see the RMSE for the validation set
         predictions = theta_ne_lstat[0] + theta_ne_lstat[1] * x[:,1]**2 * x[:,2]
         rmse_lstat = np.sqrt(mean_squared_error(y_validation, predictions))

         print("The RMSE value for the validation set using \
                LSTAT squared is: {}".format(rmse_lstat))
```

```
The RMSE value for the validation set using LSTAT squared is: 7.730818593681602
```

We can plot the differences of the error committed by our two models and compare the errors:

```
In [39]: objects = ('$RM^2\ LSTAT$', '$RM\ LSTAT^2$')
         y_pos = np.arange(len(objects))
         performance = [rmse_rm, rmse_lstat]

         plt.bar(y_pos, performance, align='center', alpha=0.5)
         plt.xticks(y_pos, objects)
         plt.ylabel('RMSE')
         plt.xlabel('Type')
         plt.title('RMSE Comparison')

         plt.show()
```



Using the two values obtained for the root mean squared error, we can see that the model implementing the hypothesis function

$$h_\theta(x) = \theta_0 + \theta_1 x_{\mathrm{LSTAT}}\ x^2_{\mathrm{RM}}$$

works better, having a lower RMSE value. The validation set is used for doing these types of choices and reasonings. It is for this reason that the chosen model used for testing purposes will be the one implementing the formula written above.

4.3 Let's use the test set to see how the model performs

Let's convert a matrix from the test set and let's take the target feature out of it:

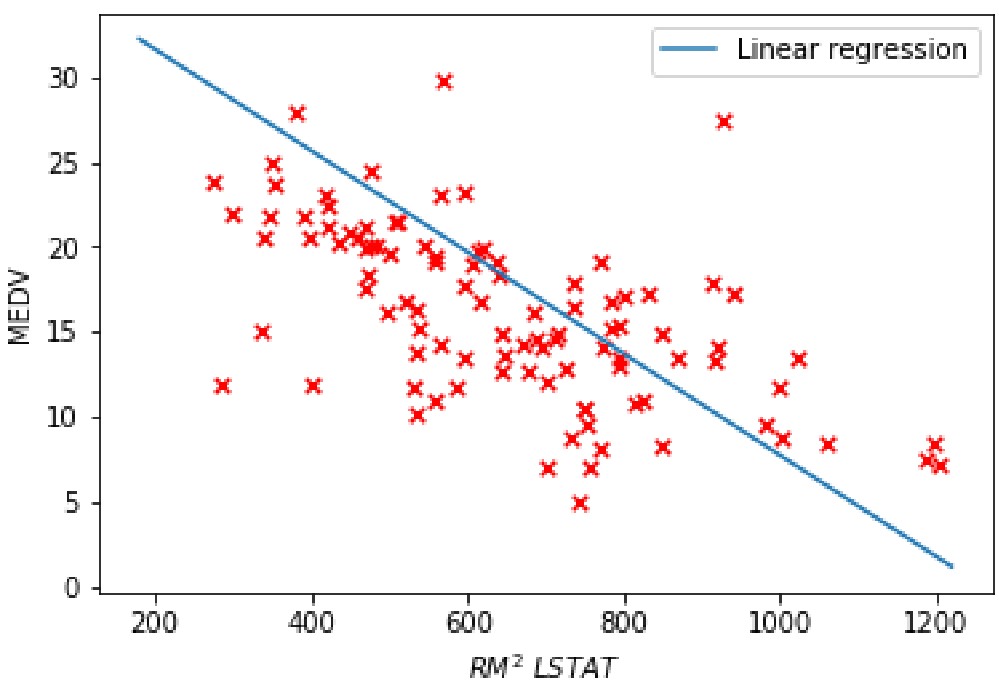
```
In [40]: # Let's adapt the test set
         x = pd.DataFrame(np.c_[df_test[TRAINING_VARIABLES]], columns = TRAINING_VARIABLES)
         y = df_test['MEDV'].values.reshape((df_test.shape[0], 1))

         x = np.concatenate([np.ones((x.shape[0], 1)), x], axis = 1) # Add a columns of 1

         # Convert in dataframe and display it
         dataframe = pd.DataFrame(x[:], columns = ["CONST", "LSTAT", "RM"])
         dataframe.head()
```

```
Out[40]:    CONST  LSTAT     RM
         0    1.0  22.98  5.683
```

```
1    1.0  23.34  4.138
2    1.0  12.13  5.608
3    1.0  26.40  5.617
4    1.0  19.78  6.852
```

Let's do the same operations done before and let's calculate the error done by the model on the test set:

In [41]:
```
x = np.concatenate([dataframe], axis = 1)

xx = np.arange(180,1220)
yy = theta_ne_rm[0] + theta_ne_rm[1] * xx

# Plot gradient descent
plt.scatter(x[:,1] * x[:,2]**2, y, s=30, c='r', marker='x', linewidths=1)
plt.plot(xx,yy, label='Linear regression')

#plt.ylim(-2,55)
#plt.xlim(-2,13)
plt.xlabel('$RM^2\ LSTAT$')
plt.ylabel('MEDV')
plt.legend(loc=1);
```



In [42]:
```
# Let's see the RMSE for the validation set
predictions = theta_ne_rm[0] + theta_ne_rm[1] * x[:,1] * x[:,2]**2
```

```python
rmse = np.sqrt(mean_squared_error(y, predictions))

print("The RMSE value for the test set is: {}".format(rmse))
```

```
The RMSE value for the test set is: 5.591531084890972
```