lab06

July 5, 2022

```
[]: # Initialize Otter
import otter
grader = otter.Notebook("lab06.ipynb")
```

1 Lab 6: Linear Regression

Due Date: Saturday, July 9, 11:59 PM PT.

1.0.1 Collaboration Policy

Data science is a collaborative activity. While you may talk to others about the labs, we ask that you write your solutions individually. If you do discuss the assignments with others, please include their names in the following cell:

Collaborators: List names here

1.1 Objectives

In this lab, you will review the details of linear regression as described in Lectures 10 and 11. In particular:

- Matrix formulation and solution to Ordinary Least Squares
- sns.lmplot as a quick visual for simple linear regression
- scikit-learn, a real world data science tool that is more robust and flexible than analytical/scipy.optimize solutions

You will also practice interpreting residual plots (vs. fitted values) and the Multiple \mathbb{R}^2 metric used in Multiple Linear Regression.

For the first part of this lab, you will predict fuel efficiency (mpg) of several models of automobiles using a single feature: engine power (horsepower). For the second part, you will perform feature engineering on multiple features to better predict fuel efficiency.

First, let's load in the data.

```
[1]: # Run this cell
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
```

%matplotlib inline

```
[2]: # Here, we load the fuel dataset, and drop any rows that have missing data
vehicle_data = sns.load_dataset('mpg').dropna()
vehicle_data = vehicle_data.sort_values('horsepower', ascending=True)
vehicle_data.head(5)
```

```
[2]:
                cylinders
                           displacement
                                         horsepower
                                                       weight
                                                               acceleration \
     19
          26.0
                                    97.0
                                                46.0
                                                         1835
                                                                       20.5
                        4
     102 26.0
                        4
                                    97.0
                                                46.0
                                                         1950
                                                                       21.0
     326 43.4
                        4
                                    90.0
                                                48.0
                                                                       23.7
                                                         2335
     325 44.3
                        4
                                    90.0
                                                 48.0
                                                         2085
                                                                       21.7
     244 43.1
                        4
                                    90.0
                                                48.0
                                                         1985
                                                                       21.5
          model_year origin
                                                           name
     19
                  70
                      europe
                                  volkswagen 1131 deluxe sedan
     102
                  73
                                       volkswagen super beetle
                      europe
     326
                  80
                      europe
                                            vw dasher (diesel)
     325
                                          vw rabbit c (diesel)
                  80
                      europe
     244
                  78
                      europe
                               volkswagen rabbit custom diesel
```

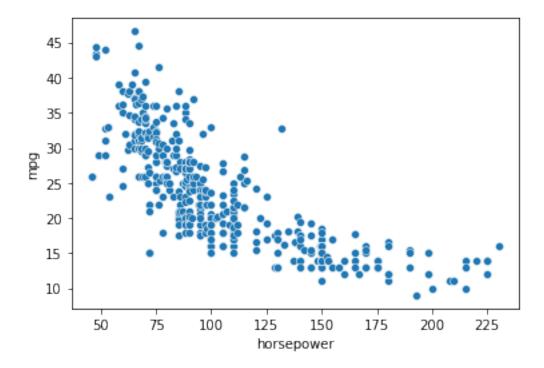
We have 392 datapoints and 8 potential features (plus our observations, mpg).

```
[3]: vehicle_data.shape
```

[3]: (392, 9)

Let us try to fit a line to the below plot, which shows mpg vs. horsepower for several models of automobiles.

```
[4]: # just run this cell
sns.scatterplot(x='horsepower', y='mpg', data=vehicle_data);
```



1.2 Question 1: Ordinary Least Squares

Instead of using the SLR formulation, in this lab we will practice linear algebra with Ordinary Least Squares. Recall that the Simple Linear Regression model is written as follows:

$$\hat{y} = \theta_0 + \theta_1 x$$

We now use $\theta=(\theta_0,\theta_1)$ so that the formulation more closely matches our multiple linear regression model:

$$\hat{y} = \theta_0 + \theta_1 x_1 + \dots + \theta_p x_p$$

We can rewrite our multiple linear regression model using matrix notation. Let \mathbb{Y} be a vector of all n observations in our sample. Then our prediction vector $\hat{\mathbb{Y}}$ is

$$\hat{\mathbb{Y}} = \mathbb{X}\theta$$

where \mathbb{X} is the **design matrix** representing the p features for all n datapoints in our sample.

Note that for our SLR model, p = 1 and therefore the matrix notation seems rather silly. Nevertheless it is valuable to start small and build on our intuition.

1.2.1 Question 1a: Construct X with an intercept term

Because we have an intercept term θ_0 in our parameter vector θ , our design matrix \mathbb{X} for p features actually has dimension

```
\mathbb{X} \in \mathbb{R}^{n \times (p+1)}
```

Therefore, the resulting matrix expression $\hat{\mathbb{Y}} = \mathbb{X}\theta$ represents n linear equations, where equation i is $\hat{y_i} = \theta_0 \cdot 1 + \theta_1 \cdot x_1 + \dots + \theta_p x_p$. The constant all-ones column of \mathbb{X} is sometimes called the bias feature; θ_0 is frequently called the **bias or intercept term**.

Below, implement add_intercept, which computes a design matrix such that the first (left-most) column is all ones. The function has two lines: you are responsible for constructing the all-ones column bias_feature using the np.ones function (NumPy documentation). This is then piped into a call to np.concatenate (documentation), which we've implemented for you.

Note: bias_feature should be a matrix of dimension (n,1), not a vector of dimension (n,).

[5]: (392, 2)

```
[]: grader.check("q1a")
```

1.2.2 Question 1b: Define the OLS Model

The predictions for all n points in our data are (note $\theta = (\theta_0, \theta_1, \dots, \theta_p)$):

$$\hat{\mathbb{Y}} = \mathbb{X}\theta$$

Below, implement the linear_model function to evaluate this product.

Hint: You can use np.dot, pd.DataFrame.dot, or the @ operator to multiply matrices/vectors. However, while the @ operator can be used to multiply numpy arrays, it generally will not work between two pandas objects, so keep that in mind when computing matrix-vector products!

```
[10]: def linear_model(thetas, X):

"""

Return the linear combination of thetas and features as defined above.

Parameters

------

thetas: a 1D vector representing the parameters of our model ([theta1, | theta2, | ... ])

X: a 2D dataframe of numeric features (may also be a 2D numpy array)

Returns

------

A 1D vector representing the linear combination of thetas and features as | defined above.

"""

# BEGIN SOLUTION

return X.dot(thetas)

# END SOLUTION
```

[]: grader.check("q1b")

1.2.3 Question 1c: Least Squares Estimate, Analytically

Recall from lecture that Ordinary Least Squares is when we fit a linear model with mean squared error, which is equivalent to the following optimization problem:

$$\min_{\theta} ||\mathbb{X}\theta - \mathbb{Y}||^2$$

We showed in Lecture that the optimal estimate $\hat{\theta}$ when X^TX is invertible is given by the equation:

$$\hat{\theta} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbb{Y}$$

Below, implement the analytic solution to $\hat{\theta}$ using np.linalg.inv (link) to compute the inverse of $\mathbb{X}^T\mathbb{X}$.

Reminder: To compute the transpose of a matrix, you can use X.T or X.transpose() (link).

Note: You can also consider using np.linalg.solve (link) instead of np.linalg.inv because it is more robust (more on StackOverflow here).

```
[14]: def get_analytical_sol(X, y):
          Computes the analytical solution to our
          least squares problem
          Parameters
          X: a 2D dataframe (or numpy array) of numeric features
          y: a 1D vector of tip amounts
          Returns
          The estimate for theta (a 1D vector) computed using the
          equation mentioned above.
          # BEGIN SOLUTION
          xTx = X.T.dot(X)
          xTy = X.T.dot(y)
            return np.linalq.solve(xTx, xTy) # this is better than inverse
          return np.linalg.inv(xTx).dot(xTy)
          # END SOLUTION
      Y = vehicle_data['mpg']
      analytical_thetas = get_analytical_sol(X, Y)
      analytical_thetas
```

```
[14]: array([39.93586102, -0.15784473])
```

```
[]: grader.check("q1c")
```

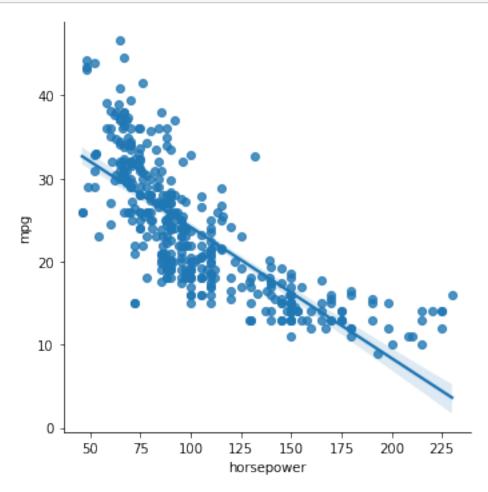
Now, let's analyze our model's performance. Your task will be to interpret the model's performance using the two visualizations and one performance metric we've implemented below.

First, we run **sns.lmplot**, which will both provide a scatterplot of **mpg** vs **horsepower** and display the least-squares line of best fit. (If you'd like to verify the OLS fit you found above is the same line found through Seaborn, change **include_OLS** to True.)

```
[17]: include_OLS = False # change this flag to visualize OLS fit

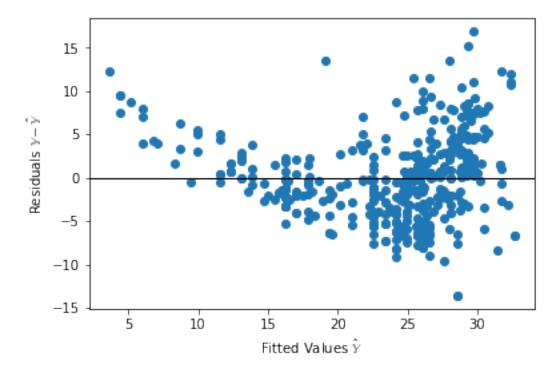
sns.lmplot(x='horsepower', y='mpg', data=vehicle_data);
predicted_mpg_hp_only = linear_model(analytical_thetas, X)
```

```
if include_OLS:
    # if flag is on, add OLS fit as a dotted red line
    plt.plot(vehicle_data['horsepower'], predicted_mpg_hp_only, 'r--')
```



Next, we **plot the residuals.** While in Simple Linear Regression we have the option to plot residuals vs. the single input feature, in Multiple Linear Regression we often plot residuals vs fitted values $\hat{\mathbb{Y}}$. In this lab, we opt for the latter.

```
[18]: plt.scatter(predicted_mpg_hp_only, Y - predicted_mpg_hp_only)
    plt.axhline(0, c='black', linewidth=1)
    plt.xlabel(r'Fitted Values $\hat{\mathbb{Y}}$')
    plt.ylabel(r'Residuals $\mathbb{Y} - \hat{\mathbb{Y}}$');
```



Finally, we compute the **Multiple** R^2 metric. As described in Lecture 11 (link),

$$R^2 = \frac{\text{variance of fitted values}}{\text{variance of true } y} = \frac{\sigma_{\hat{y}}^2}{\sigma_y^2}$$

 \mathbb{R}^2 can be used in the multiple regression setting, whereas r (the correlation coefficient) is restricted to SLR since it depends on a single input feature. In SLR, r^2 and Multiple \mathbb{R}^2 are equivalent; the proof is left to you.

```
[19]: r2_hp_only = np.var(predicted_mpg_hp_only) / np.var(Y)
print('Multiple R^2 using only horsepower: ', r2_hp_only)
```

Multiple R^2 using only horsepower: 0.605948257889435

1.2.4 Question 1d

In the cell below, comment on the above visualization and performance metrics, and whether horsepower and mpg have a good linear fit.

Type your answer here, replacing this text.

SOLUTION The r value of -0.778 suggests a medium strong negative correlation since it is within the middle range of [-1, 0]. Both the scatterplot and the residual plot show a clear skew to the residuals, suggesting this linear model is not the best fit for our data.

1.3 Question 2: Transform a Single Feature

The Tukey-Mosteller Bulge Diagram tells us to transform our \mathbb{X} or \mathbb{Y} to find a linear fit.

Let's consider the following linear model:

predicted mpg =
$$\theta_0 + \theta_1 \sqrt{\text{horsepower}}$$

1.3.1 Question 2a

In the cell below, explain why we use the term "linear" to describe the model above, even though it incorporates a square-root of horsepower as a feature.

Type your answer here, replacing this text.

SOLUTION:

The model is linear in the parameters we are learning. It is a linear combination of θ_0 and θ_1 .

1.3.2 Introduction to sklearn

Yet another way to fit a linear regression model is to use **scikit learn**, an industry standard package for machine learning applications. Because it is application-specific, **sklearn** is often faster and more robust than the analytical/**scipy**-based computation methods we've used thus far.

To use sklearn:

- 1. Create an sklearn object
- 2. fit the object to data
- 3. Analyze fit or call predict.
- 1. Create object. We first create a LinearRegression object. Here's the sklearn documentation. Note that by default, the object will include an intercept term when fitting.

Here, model is like a "blank slate" for a linear model.

```
[20]: # 1. just run this cell
from sklearn.linear_model import LinearRegression
model = LinearRegression(fit_intercept=True)
```

2. fit the object to data. Now, we need to tell model to "fit" itself to the data. Essentially, this is doing exactly what you did in the previous part of this lab (creating a risk function and finding the parameters that minimize that risk).

Note: X needs to be a matrix (or DataFrame), as opposed to a single array (or Series). This is because sklearn.linear_model is robust enough to be used for multiple regression, which we will look at later this lab.

```
[21]: # 2. run this cell to add sqrt(hp) column for each car in the dataset
  vehicle_data['sqrt(hp)'] = np.sqrt(vehicle_data['horsepower'])
  vehicle_data.head()
```

```
[21]:
                 cylinders
                             displacement
                                           horsepower
                                                        weight
                                                                acceleration \
            mpg
      19
           26.0
                          4
                                      97.0
                                                  46.0
                                                           1835
                                                                          20.5
      102 26.0
                          4
                                      97.0
                                                  46.0
                                                           1950
                                                                          21.0
      326
           43.4
                          4
                                      90.0
                                                  48.0
                                                           2335
                                                                          23.7
      325
           44.3
                          4
                                      90.0
                                                  48.0
                                                           2085
                                                                          21.7
      244
           43.1
                                      90.0
                                                  48.0
                                                           1985
                                                                          21.5
           model_year
                       origin
                                                             name
                                                                   sqrt(hp)
      19
                                                                   6.782330
                   70
                       europe
                                   volkswagen 1131 deluxe sedan
      102
                   73
                        europe
                                         volkswagen super beetle
                                                                   6.782330
      326
                                              vw dasher (diesel)
                   80
                        europe
                                                                   6.928203
      325
                   80
                        europe
                                            vw rabbit c (diesel)
                                                                   6.928203
      244
                    78
                        europe
                                volkswagen rabbit custom diesel
                                                                   6.928203
```

```
[22]: # 2. run this cell
      model.fit(X = vehicle_data[['sqrt(hp)']], y= vehicle_data['mpg'])
```

- [22]: LinearRegression()
 - 3. Analyze fit. Now that the model exists, we can look at the $\hat{\theta_0}$ and $\hat{\theta_1}$ values it found, which are given in the attributes intercept and coef, respectively.
- [23]: model.intercept_
- [23]: 58.70517203721748
- [24]: model.coef_
- [24]: array([-3.50352375])
 - 3 (continued). Call predict. To use the scikit-learn linear regression model to make predictions, you can use the model.predict method.

Below, we find the estimated mpg for a single datapoint with a sqrt(hp) of 6.78 (i.e., horsepower 46).

Note that unlike the linear algebra approach, we do not need to manually add an intercept term, because our model (which was created with fit_intercept=True) will auto-add one.

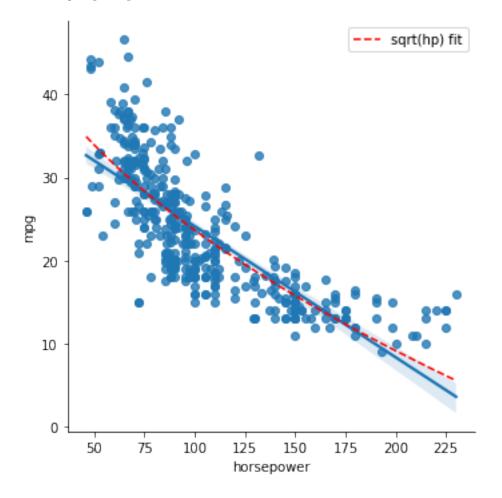
```
[25]: single_datapoint = [[6.78]] # needs to be a 2D array since the X in step 2 was
       →a 2D array.
      model.predict(single_datapoint)
```

[25]: array([34.95128104])

1.3.3 Question 2b

Using the model defined above, set $predicted_mpg$ to the predicted mpg for the data below. Running the cell will then compute the multiple R^2 value and create a linear regression plot for this new square root feature, overlaid on the original least squares estimate (used in Question 1c).

Multiple R^2 using sqrt(hp): 0.6437035832706473



The visualization shows a slight improvement, but note that the underlying pattern is parabolic—suggesting that perhaps we should try a quadratic feature. Next, we use the power of multiple linear regression to add an additional feature.

1.4 Add an Additional Feature

For the second part of this lab, we move from SLR to multiple linear regression.

Until now, we have established relationships between one independent explanatory variable and one response variable. However, with real-world problems you will often want to use **multiple features** to model and predict a response variable. Multiple linear regression attempts to model the relationship between two or more explanatory variables and a response variable by fitting a linear equation to the observed data.

We can consider including functions of existing features as **new features** to help improve the predictive power of our model. (This is something we will discuss in further detail in the Feature Engineering lecture.)

The cell below adds a column which contains the square of the horsepower for each car in the dataset.

```
[27]: # just run this cell
      vehicle_data['hp^2'] = vehicle_data['horsepower'] ** 2
      vehicle data.head()
[27]:
                  cylinders
                             displacement
                                            horsepower
                                                          weight
                                                                  acceleration
      19
           26.0
                           4
                                      97.0
                                                   46.0
                                                            1835
                                                                           20.5
      102 26.0
                           4
                                      97.0
                                                   46.0
                                                            1950
                                                                           21.0
      326
           43.4
                           4
                                      90.0
                                                   48.0
                                                                           23.7
                                                            2335
      325
           44.3
                           4
                                      90.0
                                                   48.0
                                                                           21.7
                                                            2085
      244
           43.1
                           4
                                      90.0
                                                   48.0
                                                            1985
                                                                           21.5
                                                                     sqrt(hp)
           model_year
                        origin
                                                                                  hp<sup>2</sup>
                                                              name
      19
                                                                     6.782330
                    70
                        europe
                                    volkswagen 1131 deluxe sedan
                                                                               2116.0
      102
                    73
                        europe
                                         volkswagen super beetle
                                                                     6.782330
                                                                               2116.0
      326
                    80
                        europe
                                               vw dasher (diesel)
                                                                     6.928203
                                                                               2304.0
      325
                    80
                        europe
                                             vw rabbit c (diesel)
                                                                     6.928203
                                                                               2304.0
      244
                                 volkswagen rabbit custom diesel
                    78
                        europe
                                                                     6.928203
                                                                               2304.0
```

1.5 Question 3

1.5.1 Question 3a

Using scikit learn's LinearRegression, create and fit a model that tries to predict mpg from horsepower AND hp^2 using the DataFrame vehicle_data. Name your model model_multi.

Hint: We did something very similar in Question 2.

```
[28]: model_multi = LinearRegression() # by default, fit_intercept=True model_multi.fit(X = vehicle_data[['horsepower', 'hp^2']], y=⊔ 

→vehicle_data['mpg']) # SOLUTION
```

[28]: LinearRegression()

```
[]: grader.check("q3a")
```

After fitting, we can see the coefficients and intercept. Note, there are now two elements in model_multi.coef_, since there are two features.

```
[31]: model_multi.intercept_

[31]: 56.90009970211295

[32]: model_multi.coef_

[32]: array([-0.46618963, 0.00123054])
```

1.5.2 Question 3b

Using the above values, in LaTeX, write out the function that the model is using to predict mpg from horsepower and hp^2.

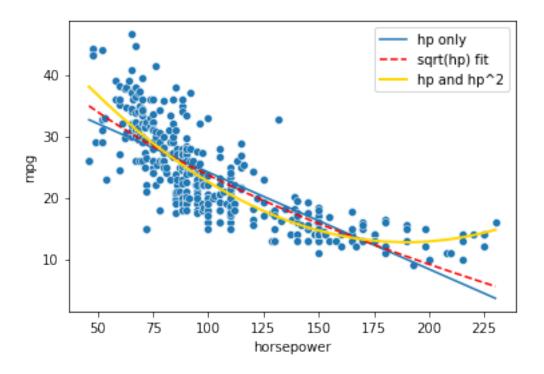
Type your answer here, replacing this text.

SOLUTION:

```
mpg = 56.9 - 0.466 \cdot horsepower + 0.00123 \cdot horsepower^2
```

The plot below shows the prediction of our model. It's much better!

Multiple R^2 using both horsepower and horsepower squared: 0.6875590305127517



1.5.3 Question 3c

grader.check("q3c")

In the cell below, we assign the mean of the mpg column of the vehicle data dataframe to mean_mpg. Given this information, what is the mean of the mean_predicted_mpg_hp_only, predicted_mpg_hp_sqrt, and predicted_mpg_multi arrays?

Hint: You should not have to call np.mean in your code.

```
[34]: mean_mpg = np.mean(vehicle_data['mpg'])
mean_predicted_mpg_hp_only = mean_mpg # SOLUTION
mean_predicted_mpg_hp_sqrt = mean_mpg # SOLUTION
mean_predicted_mpg_multi = mean_mpg # SOLUTION
```

1.6 Faulty Feature Engineering: Redundant Features

Suppose we used the following linear model:

$$mpg = \theta_0 + \theta_1 \cdot horsepower + \tag{1}$$

$$\theta_2 \cdot \text{horsepower}^2 + \theta_3 \cdot \text{horsepower}$$
 (2)

Notice that horsepower appears twice in our model!! We will explore how this redundant feature affects our modeling.

1.7 Question 4

1.7.1 Question 4a: Linear Algebra

Construct a matrix X_redundant that uses the vehicle data DataFrame to encode the "three" features above, as well as a bias feature.

Hint: Use the add_intercept term you implemented in Question 1a.

```
[38]: X_redundant = add_intercept(vehicle_data[['horsepower', 'hp^2', 'horsepower']])__ 
# SOLUTION
X_redundant.shape
```

[38]: (392, 4)

```
[]: grader.check("q4a")
```

Now, run the cell below to find the analytical OLS Estimate using the get_analytical_sol function you wrote in Question 1c.

Depending on the machine that you run your code on, you should either see a singular matrix error or end up with thetas that are nonsensical (magnitudes greater than 10^15). This is not good!

```
[40]: # just run this cell
    # the try-except block suppresses errors during submission
    import traceback
    try:
        analytical_thetas = get_analytical_sol(X_redundant, vehicle_data['mpg'])
        analytical_thetas
    except Exception as e:
        print(traceback.format_exc())
```

```
Traceback (most recent call last):
    File "/tmp/ipykernel_7526/1270488367.py", line 5, in <cell line: 4>
        analytical_thetas = get_analytical_sol(X_redundant, vehicle_data['mpg'])
    File "/tmp/ipykernel_7526/1214822988.py", line 20, in get_analytical_sol
        return np.linalg.inv(xTx).dot(xTy)
    File "<_array_function__ internals>", line 5, in inv
    File "/opt/conda/lib/python3.9/site-packages/numpy/linalg/linalg.py", line
545, in inv
        ainv = _umath_linalg.inv(a, signature=signature, extobj=extobj)
    File "/opt/conda/lib/python3.9/site-packages/numpy/linalg/linalg.py", line 88,
in _raise_linalgerror_singular
        raise_linalgerror("Singular matrix")
```

```
numpy.linalg.LinAlgError: Singular matrix
```

1.7.2 Question 4b

In the cell below, explain why we got the error above when trying to calculate the analytical solution to predict mpg.

Type your answer here, replacing this text.

SOLUTION: After adding the redundant feature, our data became non-invertible/singular because it has linearly dependent columns.

Note: While we encountered errors when using the linear algebra approach, a model fitted with sklearn will not encounter matrix singularity errors since it uses numerical methods to find optimums (to be covered in Gradient Descent lecture).

[41]: array([5.69000997e+01, -2.33094815e-01, 1.23053610e-03, -2.33094815e-01])

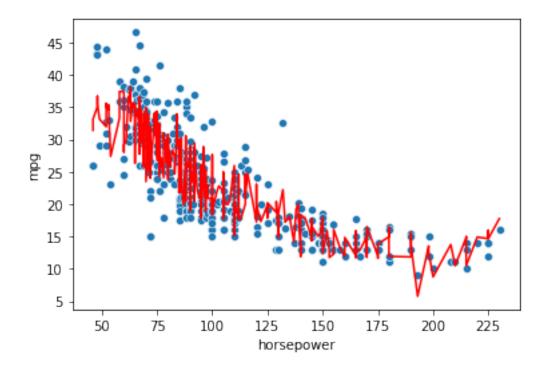
1.8 Overfitting with Too Many Features

Let's take what we've learned so far and go one step further: introduce even more features.

Again, using scikit learn's LinearRegression, we fit a model that tries to predict mpg using each of the following as features: - horsepower - hp^2 - model_year - acceleration

The plot below shows the prediction of our more sophisticated model. Note we arbitrarily plot against horsepower for the ease of keeping our plots 2-dimensional.

```
[43]: # just run this cell
sns.scatterplot(x='horsepower', y='mpg', data=vehicle_data)
plt.plot(vehicle_data['horsepower'], predicted_mpg_overfit, color = 'r');
```



Think about what you see in the above plot. Why is the shape of our prediction curve so jagged? Do you think this is a good model to predict the mpg of some car we don't already have information on?

This idea –the bias-variance tradeoff– is an idea we will explore in the coming weeks.

1.9 Question 5: Comparing R^2

Lastly, set r2_overfit to be the multiple R^2 coefficient obtained by using model_overfit.

• Hint: This is very similar to several pre-computed cells in Questions 1c, 2b, and 3b.

```
[44]: r2_overfit = np.var(predicted_mpg_overfit) / np.var(vehicle_data['mpg']) #__

$\times SOLUTION$

r2_overfit
```

[44]: 0.8163086433998623

```
[]: grader.check("q5")
```

Comparing this model with previous models:

```
[46]: # just run this cell
# compares q1, q2, q3, and overfit models (ignores redundant model)
print('Multiple R^2 using only horsepower: ', r2_hp_only)
```

```
print('Multiple R^2 using sqrt(hp): ', r2_hp_sqrt)
print('Multiple R^2 using both hp and hp^2: ', r2_multi)
print('Multiple R^2 using hp, hp^2, model year, and acceleration: ', r2_overfit)
```

```
Multiple R^2 using only horsepower: 0.605948257889435

Multiple R^2 using sqrt(hp): 0.6437035832706473

Multiple R^2 using both hp and hp^2: 0.6875590305127517

Multiple R^2 using hp, hp^2, model year, and acceleration: 0.8163086433998623
```

If everything was done correctly, the multiple R^2 of our latest model should be substantially higher than that of the previous models. This is because multiple R^2 increases with the number of covariates (i.e., features) we add to our model.

A Word on Overfitting: We might not always want to use models with large multiple R^2 values because these models could be **overfitting** to our specific sample data, and won't generalize well to unseen data from the population. Again, this is an idea we will explore in future lectures and assignments.

2 Congratulations! You finished the lab!

To double-check your work, the cell below will rerun all of the autograder tests.

```
[]: grader.check_all()
```

2.1 Submission

Make sure you have run all cells in your notebook in order before running the cell below, so that all images/graphs appear in the output. The cell below will generate a zip file for you to submit. Please save before exporting!

```
[]: # Save your notebook first, then run this cell to export your submission. grader.export(pdf=False)
```