Lecture 2
Simple Linear Regression

EE-UY 4423: INTRODUCTION TO MACHINE LEARNING

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Learning Objectives

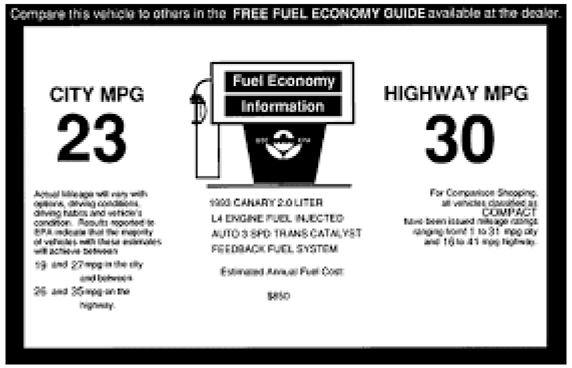
- ❑ How to load data from a text file
- ❑ How to visualize data via a scatter plot
- ❑ Describe a linear model for data
  - Identify the target variable and predictor
- ❑ Compute optimal parameters for the model using the regression formula
- ❑ Fit parameters for related models by minimizing the residual sum of squares
- ❑ Compute the R^2 measure of fit
- ❑ Visually determine goodness of fit and identify different causes for poor fit

Outline

- ❑Motivating Example: Predicting the mpg of a car
- ❑Linear Model
- ❑Least Squares Fit Problem
- ❑Sample Mean and Variance; LS Fit Solution
- ❑Assessing Goodness of Fit

Example: What Determines mpg in a Car?

- What engine characteristics determine fuel efficiency?
- Why would a data scientist be hired to answer this question?
- Not to help purchasing a specific car.
  - The mpg for a currently available car is already known.
  - (If the car company isn't lying?)
- To guide building new cars.
  - Understand what is reasonably achievable before full design
- To find cars that are outside the trend.
  - Example: What cars give great mpg for the cost or size?



Compare this vehicle to others in the **FREE FUEL ECONOMY GUIDE** available at the dealer.

CITY MPG
23

Fuel Economy Information

HIGHWAY MPG
30

Actual mileage will vary with options, driving conditions, driving habits and vehicle's condition. Results reported to EPA indicate that the majority of vehicles with these estimates will achieve between 19 and 27 mpg in the city and between 26 and 35 mpg on the highway.

1993 CANARY 2.0 LITER
L4 ENGINE FUEL INJECTED
AUTO 3 SPD TRANS CATALYST
FEEDBACK FUEL SYSTEM

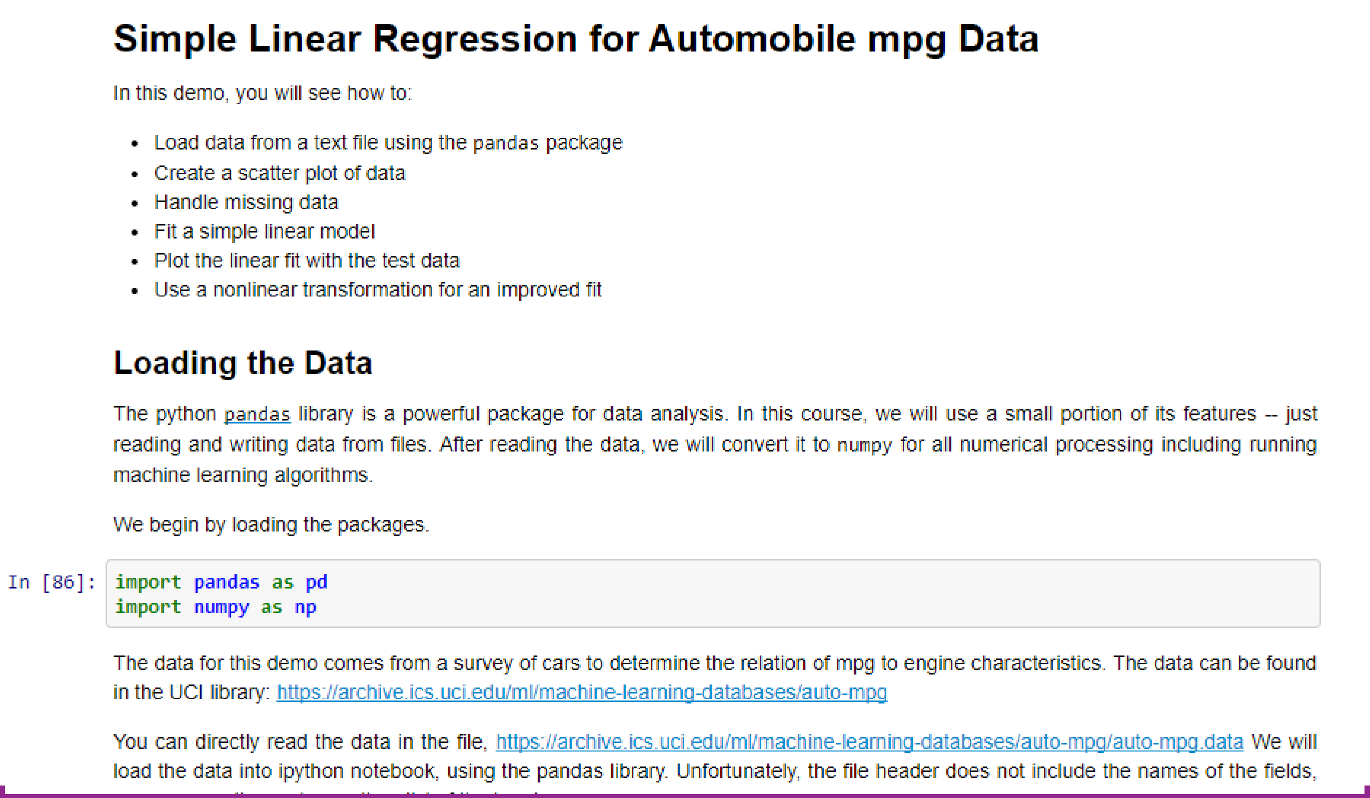
Estimated Annual Fuel Cost

$850

For Comparison Shopping, all vehicles classified as COMPACT have been issued mileage ratings ranging from 1 to 31 mpg city and 16 to 41 mpg highway.

Demo in Github

- https://github.com/sdrangan/introml/blob/master/simp_lin_reg/auto_mpg.ipynb



Simple Linear Regression for Automobile mpg Data

In this demo, you will see how to:

- Load data from a text file using the `pandas` package
- Create a scatter plot of data
- Handle missing data
- Fit a simple linear model
- Plot the linear fit with the test data
- Use a nonlinear transformation for an improved fit

Loading the Data

The python `pandas` library is a powerful package for data analysis. In this course, we will use a small portion of its features -- just reading and writing data from files. After reading the data, we will convert it to `numpy` for all numerical processing including running machine learning algorithms.

We begin by loading the packages.

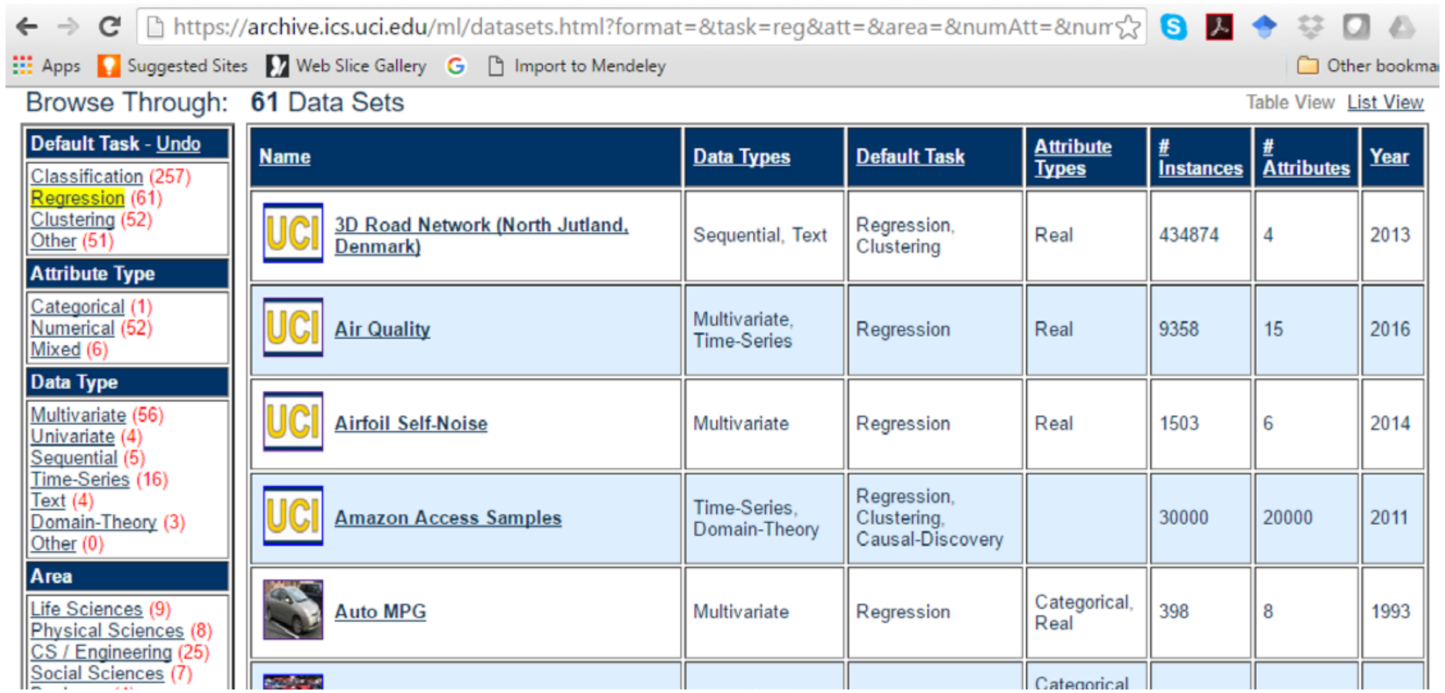
```
In [86]: import pandas as pd
         import numpy as np
```

The data for this demo comes from a survey of cars to determine the relation of mpg to engine characteristics. The data can be found in the UCI library: https://archive.ics.uci.edu/ml/machine-learning-databases/auto-mpg

You can directly read the data in the file, https://archive.ics.uci.edu/ml/machine-learning-databases/auto-mpg/auto-mpg.data We will load the data into ipython notebook, using the pandas library. Unfortunately, the file header does not include the names of the fields,

Getting Data

- ❑Data from UCI dataset library: https://archive.ics.uci.edu/ml/datasets.html



https://archive.ics.uci.edu/ml/datasets.html?format=&task=reg&att=&area=&numAtt=&num

Apps Suggested Sites Web Slice Gallery Import to Mendeley Other bookma

Browse Through: **61** Data Sets Table View List View

Default Task - Undo
Classification (257)
Regression (61)
Clustering (52)
Other (51)

Attribute Type
Categorical (1)
Numerical (52)
Mixed (6)

Data Type
Multivariate (56)
Univariate (4)
Sequential (5)
Time-Series (16)
Text (4)
Domain-Theory (3)
Other (0)

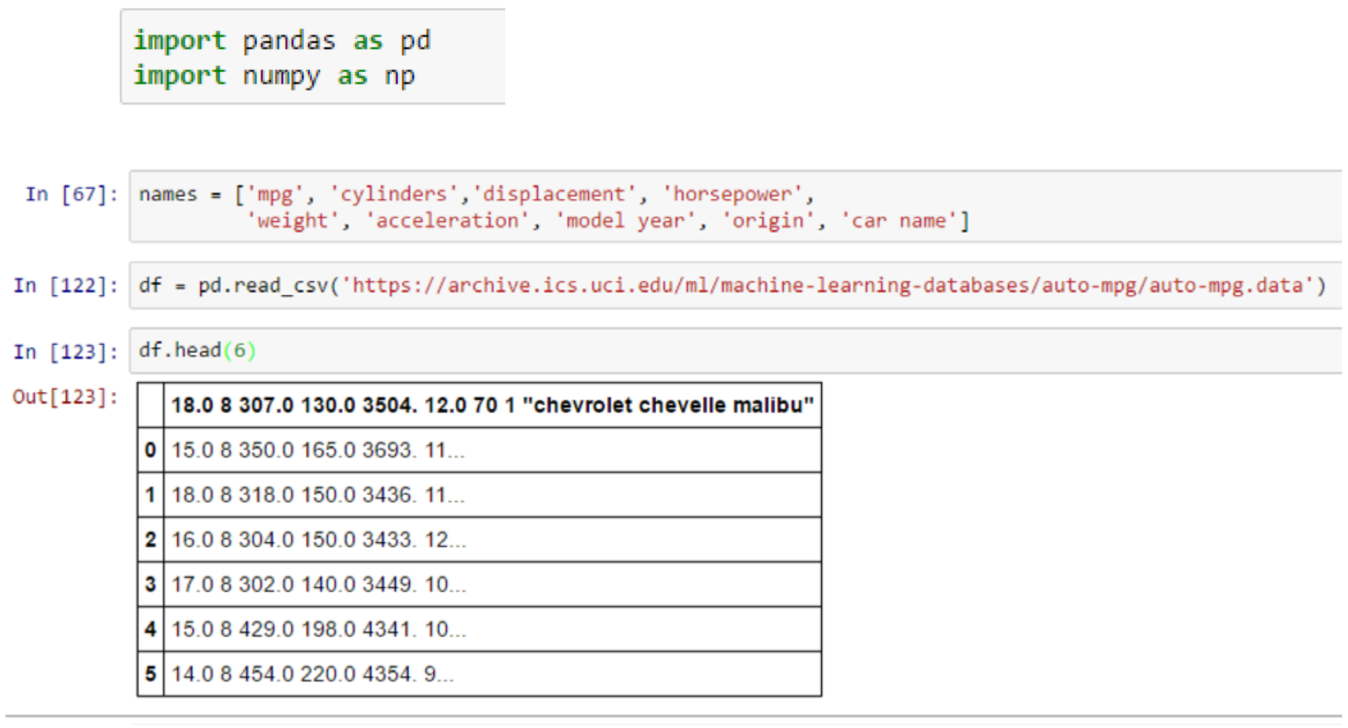
Area
Life Sciences (9)
Physical Sciences (8)
CS / Engineering (25)
Social Sciences (7)

Name	Data Types	Default Task	Attribute Types	# Instances	# Attributes	Year
3D Road Network (North Jutland, Denmark)	Sequential, Text	Regression, Clustering	Real	434874	4	2013
Air Quality	Multivariate, Time-Series	Regression	Real	9358	15	2016
Airfoil Self-Noise	Multivariate	Regression	Real	1503	6	2014
Amazon Access Samples	Time-Series, Domain-Theory	Regression, Clustering, Causal-Discovery		30000	20000	2011
Auto MPG	Multivariate	Regression	Categorical, Real	398	8	1993
			Categorical			

← Today's lecture

Loading the Data in Jupyter Notebook

Try 1: The Wrong Way!



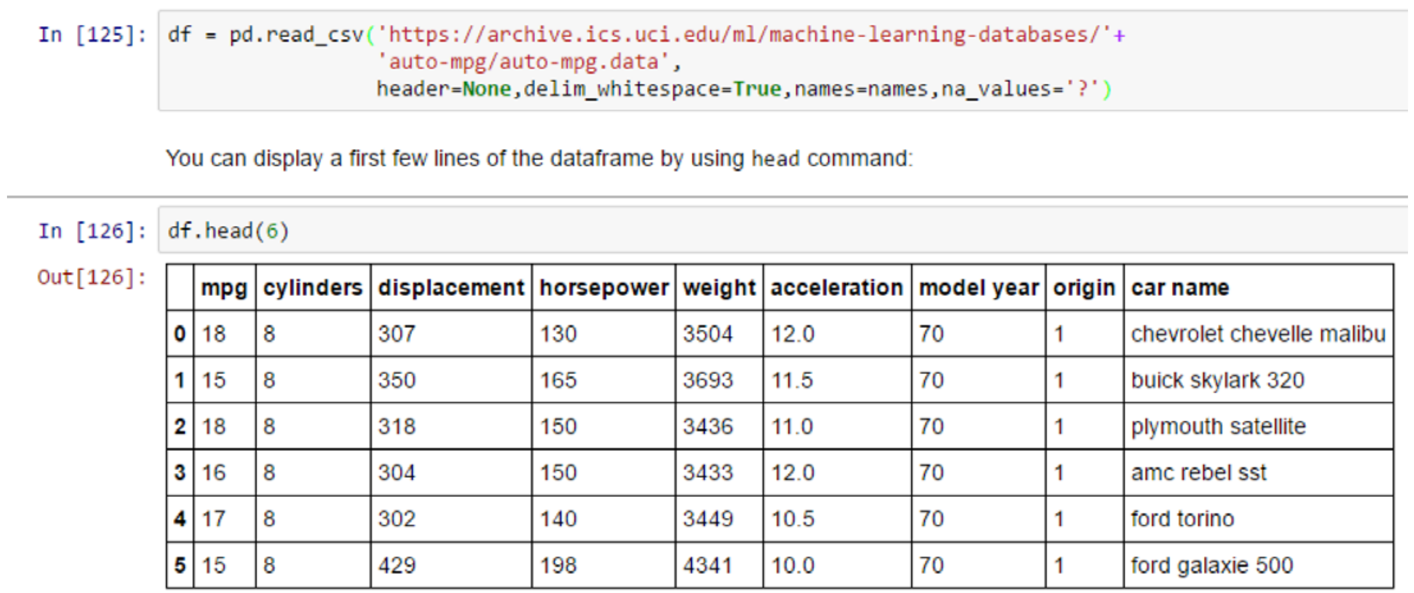
```
import pandas as pd
import numpy as np
```

```
In [67]: names = ['mpg', 'cylinders','displacement', 'horsepower',
                  'weight', 'acceleration', 'model year', 'origin', 'car name']

In [122]: df = pd.read_csv('https://archive.ics.uci.edu/ml/machine-learning-databases/auto-mpg/auto-mpg.data')

In [123]: df.head(6)

Out[123]:
```

	18.0 8 307.0 130.0 3504. 12.0 70 1 "chevrolet chevelle malibu"
0	15.0 8 350.0 165.0 3693. 11...
1	18.0 8 318.0 150.0 3436. 11...
2	16.0 8 304.0 150.0 3433. 12...
3	17.0 8 302.0 140.0 3449. 10...
4	15.0 8 429.0 198.0 4341. 10...
5	14.0 8 454.0 220.0 4354. 9...

- Python pandas library
  - Read_csv command.
  - Read URL or file location.
- Creates a dataframe object
  - http://pandas.pydata.org/pandas-docs/stable/dsintro.html#dataframe
- Problems
- Does not parse columns
  - All data in a single column
  - Read_csv assumes columns are delimited by commas
- Mistakes first line as header

Loading the Data in Jupyter
Try 2: Fixing the Errors



```
In [125]: df = pd.read_csv('https://archive.ics.uci.edu/ml/machine-learning-databases/'+
                           'auto-mpg/auto-mpg.data',
                           header=None,delim_whitespace=True,names=names,na_values='?')
```

You can display a first few lines of the dataframe by using head command:

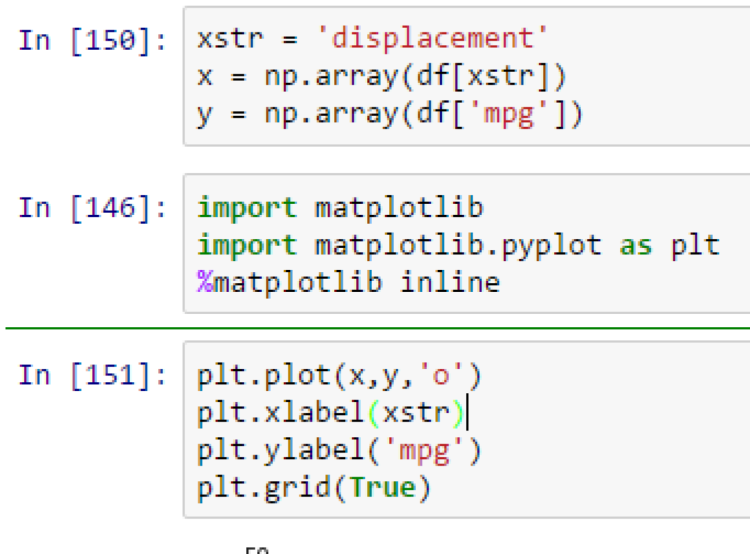
```
In [126]: df.head(6)
```

Out[126]:

	mpg	cylinders	displacement	horsepower	weight	acceleration	model year	origin	car name
0	18	8	307	130	3504	12.0	70	1	chevrolet chevelle malibu
1	15	8	350	165	3693	11.5	70	1	buick skylark 320
2	18	8	318	150	3436	11.0	70	1	plymouth satellite
3	16	8	304	150	3433	12.0	70	1	amc rebel sst
4	17	8	302	140	3449	10.5	70	1	ford torino
5	15	8	429	198	4341	10.0	70	1	ford galaxie 500

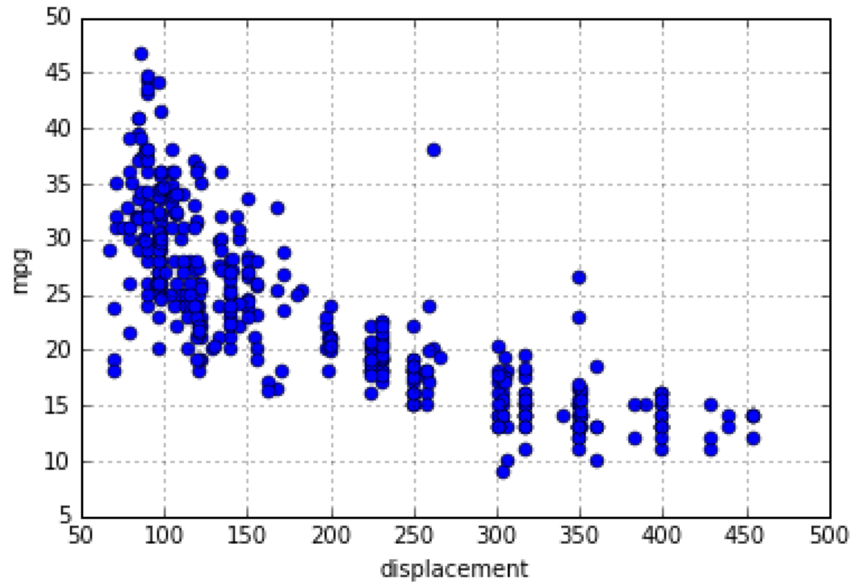
- Fix the arguments in read_csv
- Pandas routines have many options
- When you get a problem:
  - Google is your friend!
  - You are not the first to have these problems.
- Dataframe has three components
  - df.columns, df.index, df.values
- More in recitation

Visualizing the Data



```
In [150]: xstr = 'displacement'
          x = np.array(df[xstr])
          y = np.array(df['mpg'])

In [146]: import matplotlib
          import matplotlib.pyplot as plt
          %matplotlib inline

In [151]: plt.plot(x,y,'o')
          plt.xlabel(xstr)
          plt.ylabel('mpg')
          plt.grid(True)
```

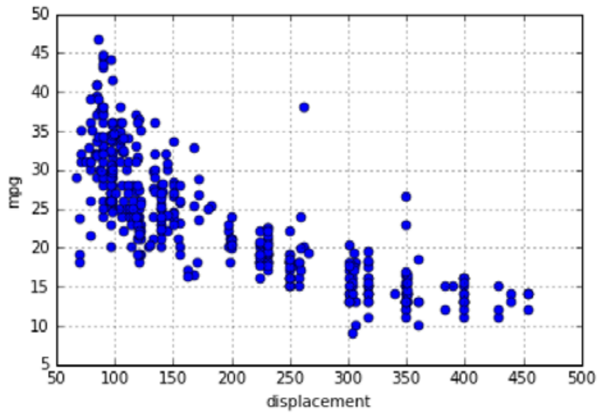
- ❑When possible, look at data before doing anything
- ❑Python has MATLAB-like plotting
  - Matplotlib module

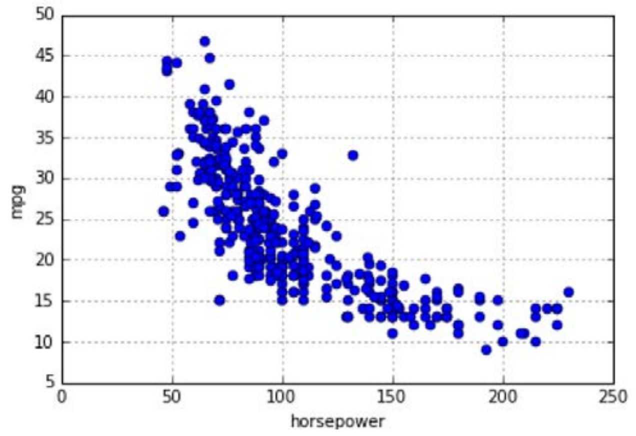


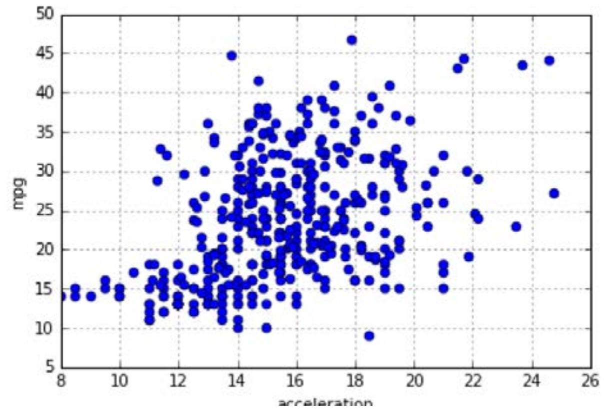
Postulating a Model

- ❑What relationships do you see?
- ❑Is there a mathematical model relating the variables?
- ❑How well can you predict mpg from these variables?

mpg







Displacement

Horsepower

Acceleration

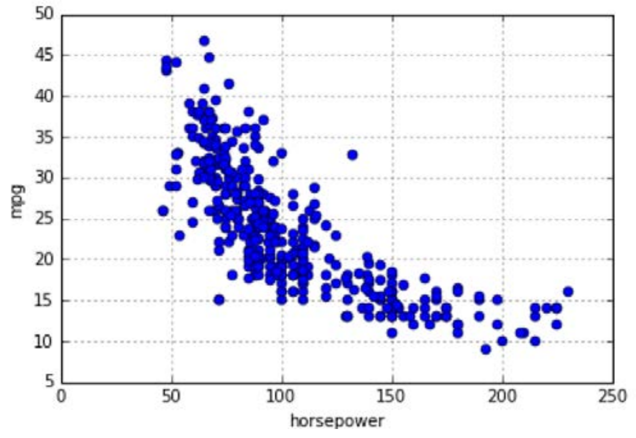
Outline

- ❑ Motivating Example: Predicting the mpg of a car
- ❑ Linear Model
- ❑ Least Squares Fit Problem
- ❑ Sample Mean and Variance; LS Fit Solution
- ❑ Assessing Goodness of Fit

Data

- y = variable you are trying to predict.
  - Called many names: Dependent variable, response variable, target, regressand, …
- x = what you are using to predict:
  - Predictor, attribute, covariate, regressor, …
- Data: Set of points, $(x_i, y_i), i = 1, \dots, n$
  - Each data point is called a sample.
- Scatter plot

y = mpg



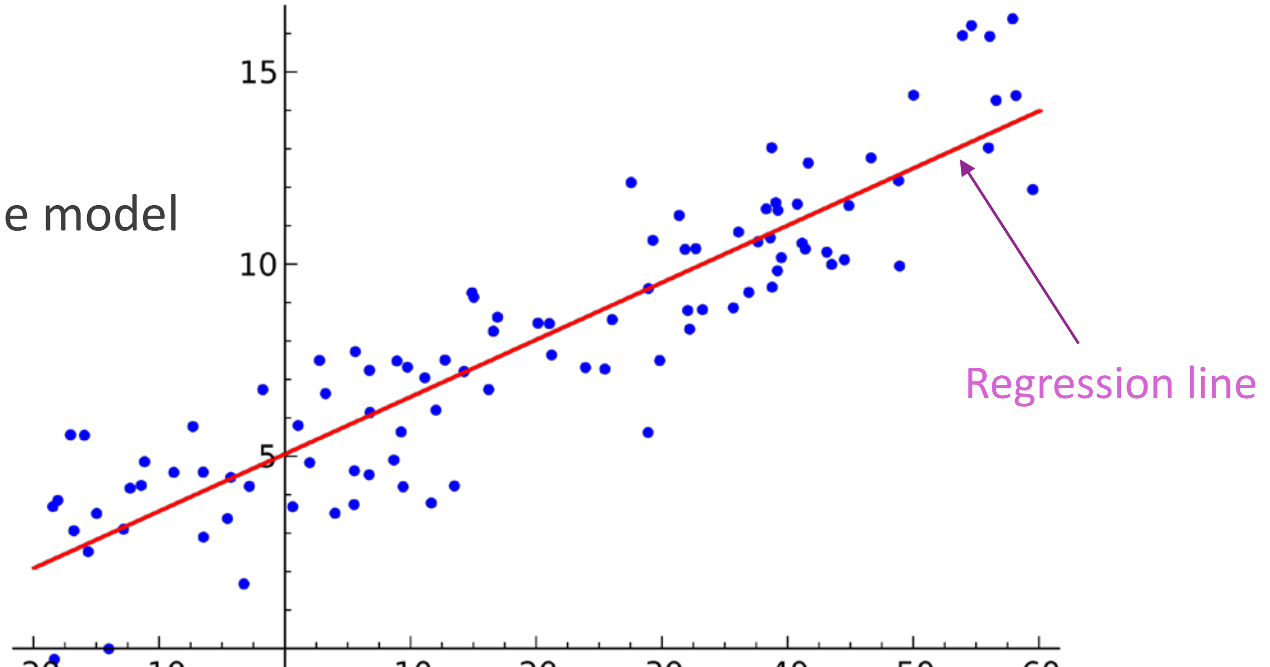
x = horsepower

Linear Model

- Assume a linear relation

$$y \approx \beta_0 + \beta_1 x$$

  - β_0 = intercept
  - β_1 = slope
- $\beta = (\beta_0, \beta_1)$ are the parameters of the model
- What are the units of β_0, β_1?
- When is this model good?



Why Use a Linear Model?

- ❑Many natural phenomena have linear relationship
- ❑Predictor has small variation
  - Suppose $y = f(x)$
  - If variation of x is small around some value x_0, then $y \approx f'(x_0)(x - x_0)$
- ❑Gaussian random variables (See Lecture 3)
- ❑Simple to compute
- ❑Easy to interpret relation

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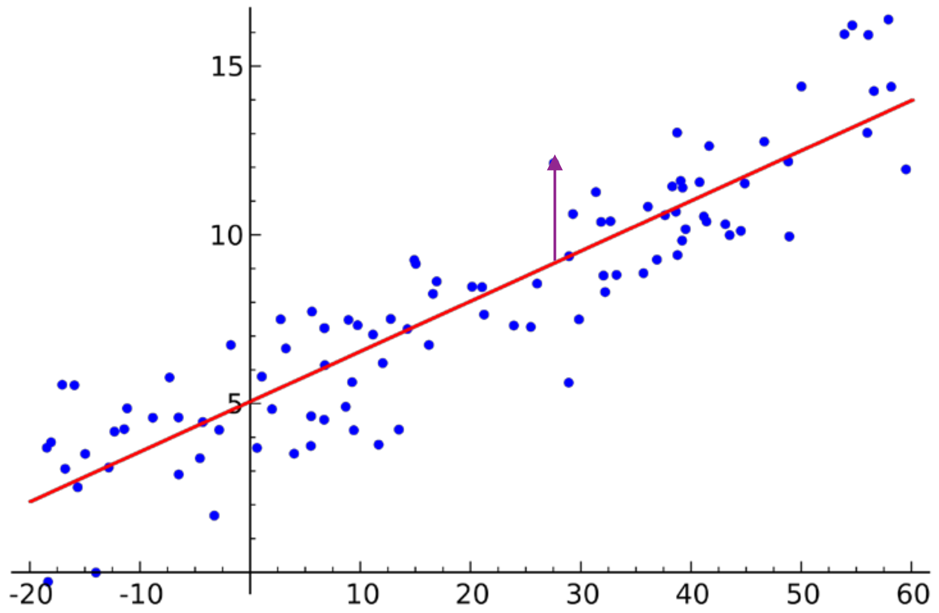
Linear Model Residual

- Knowing x does not exactly predict y
- Add a residual term

$$y = \beta_0 + \beta_1 x + \epsilon$$

- Residual = component the model does not explain
  - Predicted value: $\hat{y}_i = \beta_1 x_i + \beta_0$
  - Residual: $\epsilon_i = y_i - \hat{y}_i$
- Vertical deviation from the regression line



Least Squares Model Fitting

- How do we select parameters $\beta = (\beta_0, \beta_1)$?
- Define $\hat{y}_i = \beta_1 x_i + \beta_0$
  - Predicted value on sample i for parameters $\beta = (\beta_0, \beta_1)$
- Define average residual sum of squares:

$$\text{RSS}(\beta_0, \beta_1) := \sum_{I=1}^{n} (y_i - \hat{y}_i)^2$$

  - Note that $\hat{y}_i$ is implicitly a function of $\beta = (\beta_0, \beta_1)$
  - Also called the sum of squared residuals (SSR) and sum of squared errors (SSE)
- Least squares solution: Find (β_0, β_1) to minimize RSS.
  - Geometrically, minimizes squared distances of samples to regression line

Finding Parameters via Optimization
A general ML recipe

General ML problem		Simple linear regression
❑ Find a model with parameters	$\rightarrow$	Linear model: $\hat{y} = \beta_0 + \beta_1 x$
❑ Get data	$\rightarrow$	Data: $(x_i, y_i), i = 1,2,\ldots,N$
❑ Pick a loss function ◦ Measures goodness of fit model to data ◦ Function of the parameters	$\rightarrow$	Loss function: $RSS(\beta_0, \beta_1) \coloneqq \sum(y_i - \beta_0 + \beta_1 x_i)^2$
❑ Find parameters that minimizes loss	$\rightarrow$	Select β_0, β_1 to minimize $RSS(\beta_0, \beta_1)$

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Sample Mean and Standard Deviations

- Sample mean

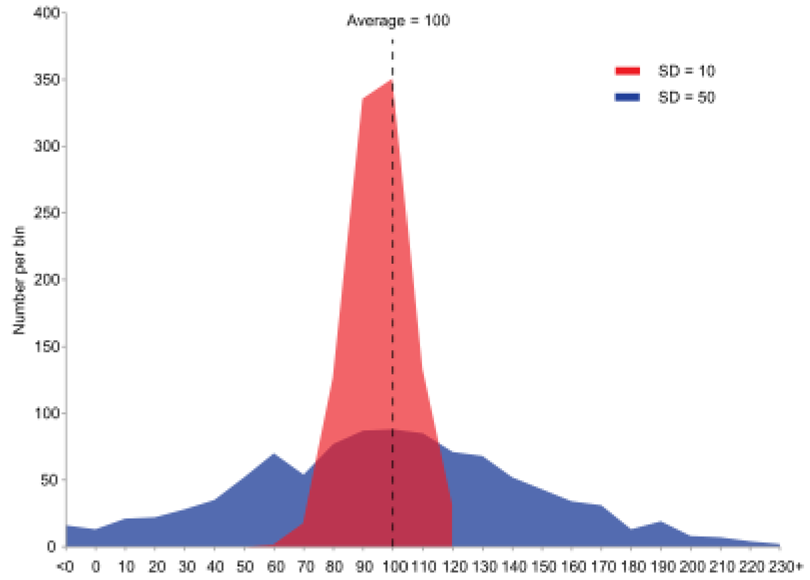
$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i\,, \qquad \bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i$$

- Sample variances

$$s_x^2 = \frac{1}{N}\sum_{i=1}^{N} (x_i - \bar{x})^2\,, \qquad s_y^2 = \frac{1}{N}\sum_{i=1}^{N} (y_i - \bar{y})^2$$

  - Some formulae have a $N-1$ on denominator
  - Creates an unbiased estimate. More on this later.

- Sample standard deviation
  - s_x, s_y
  - Square root of variances



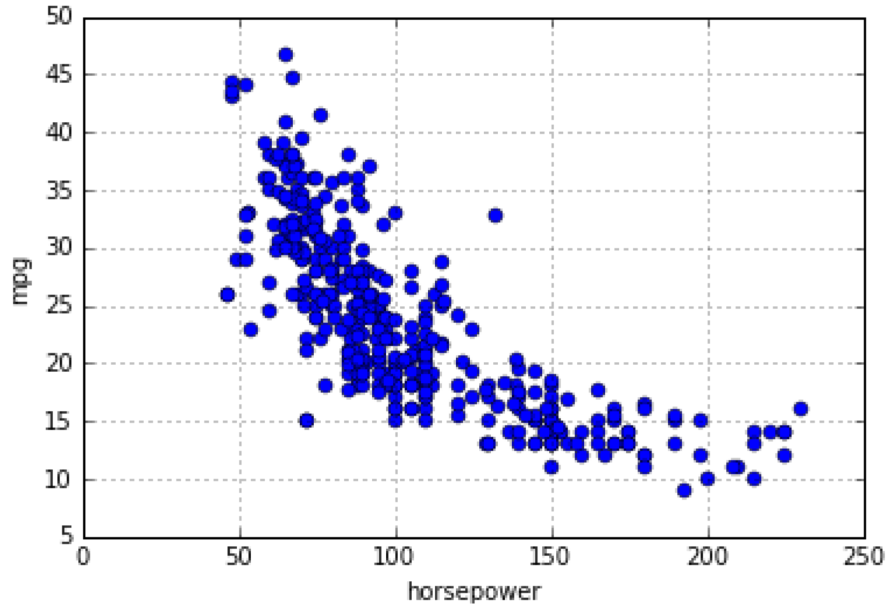
Visualizing standard deviation
https://en.wikipedia.org/wiki/Standard_deviation

Visualizing Mean and SD on Scatter Plot
Question

Using the picture only (no calculators), estimate the following (roughly):

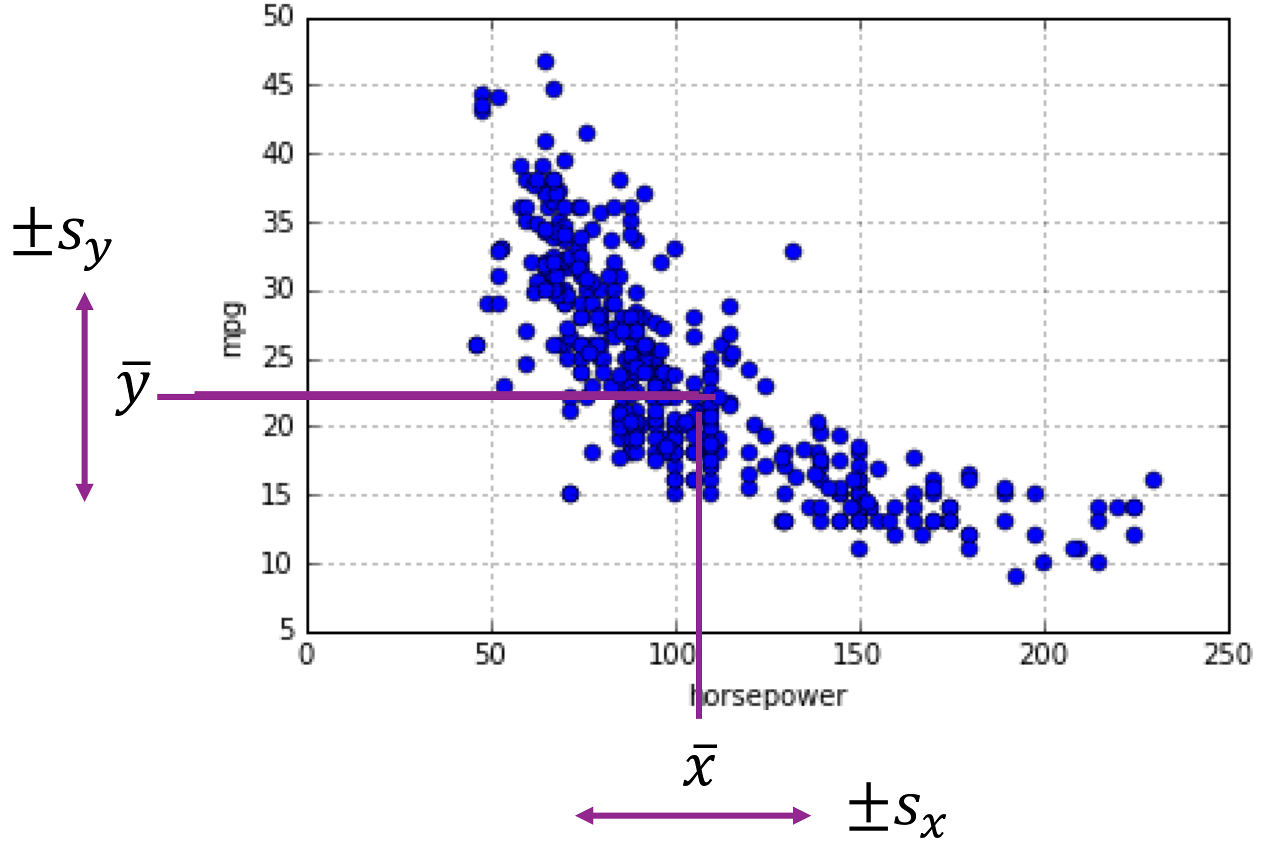
- ❑The sample mean mpg and horsepower: $\bar{x}, \bar{y}$

- ❑The sample std deviations: s_x, s_y



Visualizing Mean and SD on Scatter Plot
Approximate answer

- ❑Means: $\bar{x}$ and $\bar{y}$
  - Weighted center of the points in each axis
- ❑Standard deviations: s_x and s_y
  - Represents "variation" in each axis from mean
  - With Gaussian distributions:
    1% of points are 3 SDs from mean

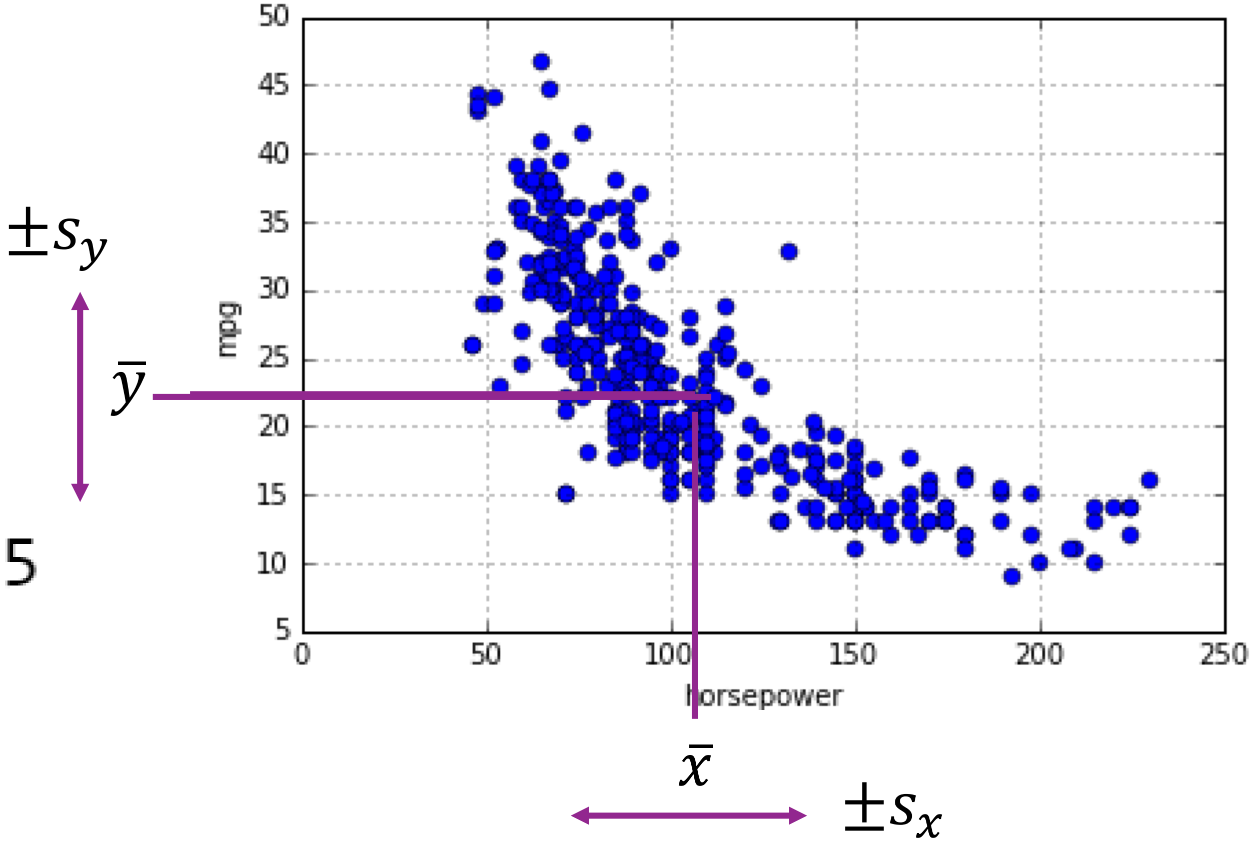


Computing Means and SD in Python

- Exact answer can be computed in python

```
xm = np.mean(x)
ym = np.mean(y)
syy = np.mean((y-ym)**2)
syx = np.mean((y-ym)*(x-xm))
sxx = np.mean((x-xm)**2)
beta1 = syx/sxx
beta0 = ym - beta1*xm
```

```
xbar= 104.47, ybar=  23.45
sxx=  38.44,  syy=   7.80
```



Sample Covariance

- ❑Sample covariance:

$$s_{xy} = \frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})$$

- ❑Will interpret this momentarily
- ❑Cauchy-Schartz Law: $|s_{xy}| < s_x s_y$
- ❑Sample correlation coefficient

$$r_{xy} = \frac{s_{xy}}{s_x s_y} \in [-1,1]$$

Alternate Equation for Variance

- Recall sample variance: $s_x^2 = \frac{1}{N}\sum(x_i - \bar{x})^2$
  - Alternate formula:

$$s_x^2 = \frac{1}{N}\sum x_i^2 - \left(\frac{1}{N}\sum x_i\right)^2 = \frac{1}{N}\sum x_i^2 - \bar{x}^2$$

- Similarly, for covariance:

$$s_{xy} = \frac{1}{N}\sum x_i y_i - \overline{xy}$$

Minimizing RSS

- To minimize $\mathrm{RSS}(\beta_0, \beta_1)$ take partial derivatives:

$$\frac{\partial \mathrm{RSS}}{\partial \beta_0} = 0, \qquad \frac{\partial \mathrm{RSS}}{\partial \beta_1} = 0$$

- Taking derivatives we get two conditions (proof on board):

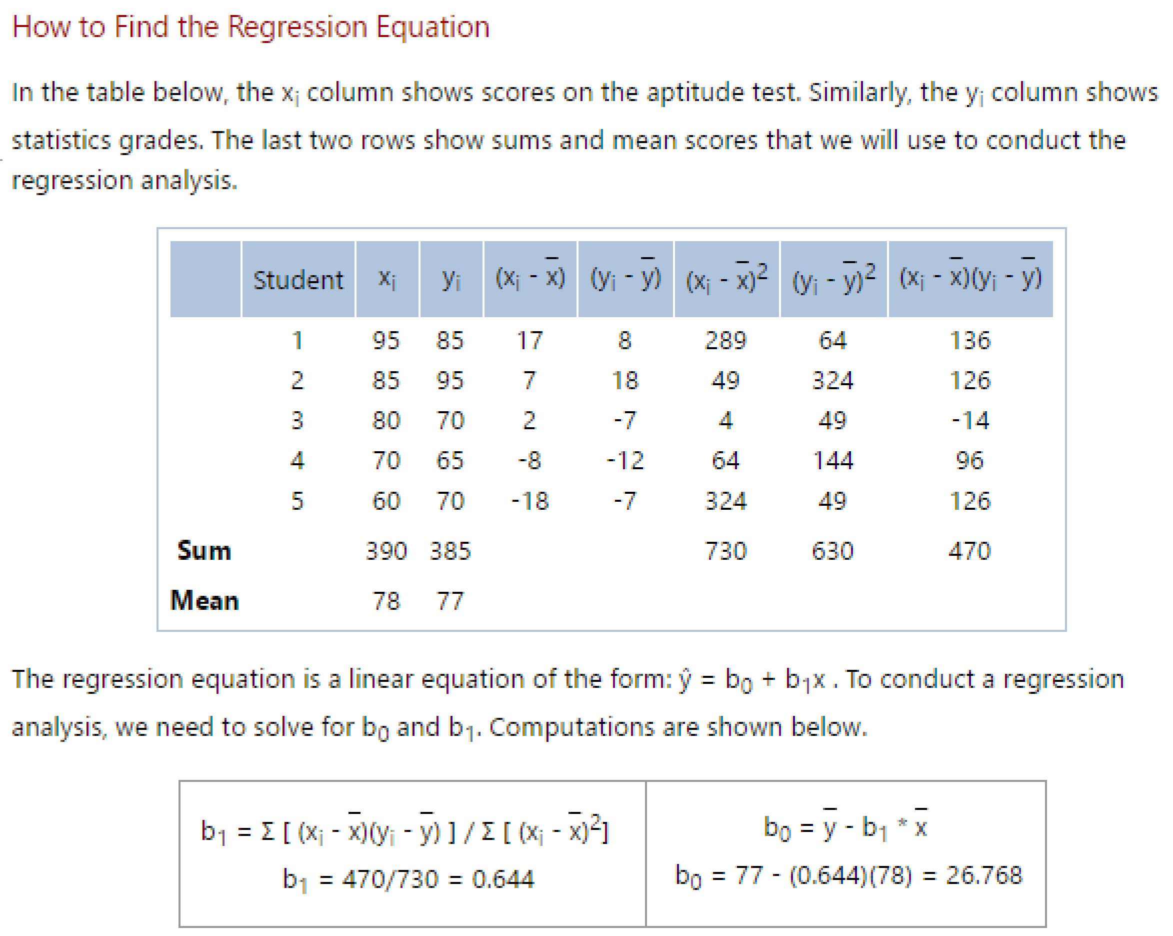
$$\sum_{i=1}^{N} \epsilon_i = 0, \qquad \sum_{i=1}^{N} x_i \epsilon_i = 0 \quad \text{where } \epsilon_i = y_i - \beta_0 - \beta_1 x_i$$

- Regression equation:
  - After some manipulation, (proof on board), solution to optimal slope and intercept:

$$\beta_1 = \frac{s_{xy}}{s_x^2} = \frac{r_{xy} s_y}{s_x}, \qquad \beta_0 = \bar{y} - \beta_1 \bar{x}$$

Simple Example

- From: http://stattrek.com/regression/regression-example.aspx?Tutorial=AP
  - Very nice simple problems
- Predict aptitude on one test from an earlier test
- Draw a scatter plot and regression line



How to Find the Regression Equation

In the table below, the x_i column shows scores on the aptitude test. Similarly, the y_i column shows statistics grades. The last two rows show sums and mean scores that we will use to conduct the regression analysis.

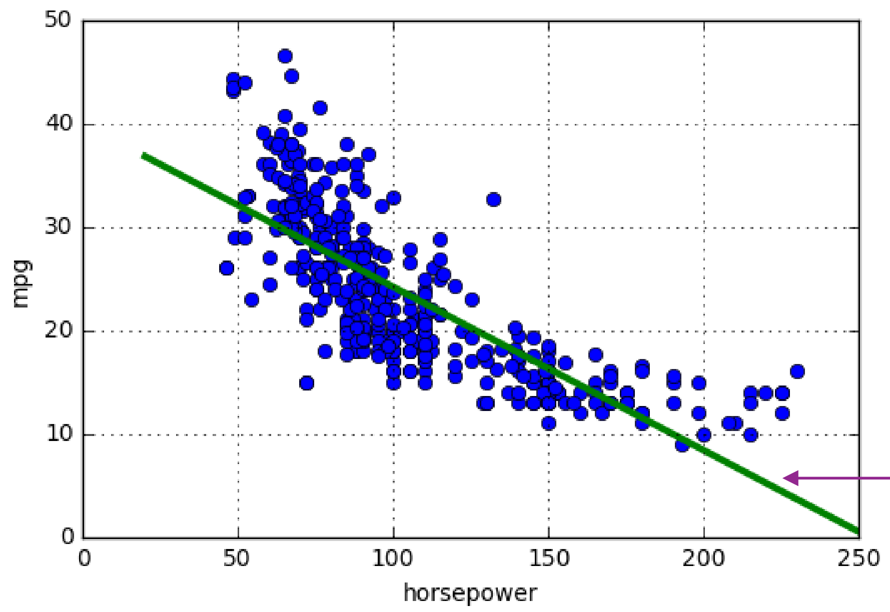
	Student	x_i	y_i	$(x_i - \bar{x})$	$(y_i - \bar{y})$	$(x_i - \bar{x})^2$	$(y_i - \bar{y})^2$	$(x_i - \bar{x})(y_i - \bar{y})$
	1	95	85	17	8	289	64	136
	2	85	95	7	18	49	324	126
	3	80	70	2	-7	4	49	-14
	4	70	65	-8	-12	64	144	96
	5	60	70	-18	-7	324	49	126
Sum		390	385			730	630	470
Mean		78	77					

The regression equation is a linear equation of the form: $\hat{y} = b_0 + b_1 x$. To conduct a regression analysis, we need to solve for b_0 and b_1. Computations are shown below.

$b_1 = \Sigma [(x_i - \bar{x})(y_i - \bar{y})] / \Sigma [(x_i - \bar{x})^2]$ $b_1 = 470/730 = 0.644$	$b_0 = \bar{y} - b_1 * \bar{x}$ $b_0 = 77 - (0.644)(78) = 26.768$

Auto Example

- Python code



```
xm = np.mean(x)
ym = np.mean(y)
syy = np.mean((y-ym)**2)
syx = np.mean((y-ym)*(x-xm))
sxx = np.mean((x-xm)**2)
beta1 = syx/sxx
beta0 = ym - beta1*xm
```

```
beta0=  39.94, beta1=  -0.16
```

Regression line:

$$\text{mpg} = \beta_0 + \beta_1 \text{ horsepower}$$

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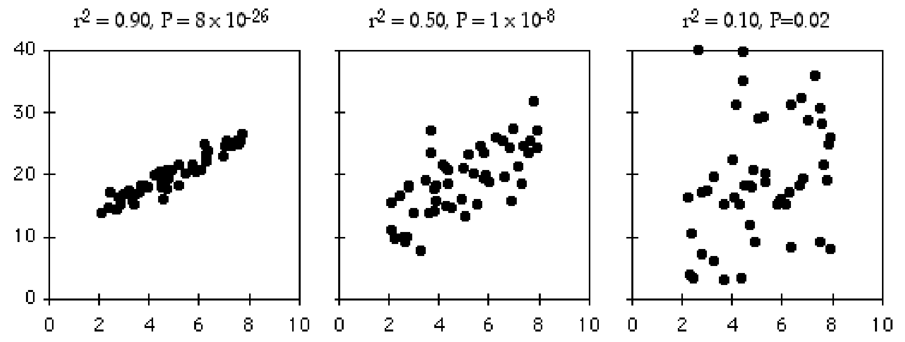
Mimimum RSS

- Minimum RSS (Proof on board)

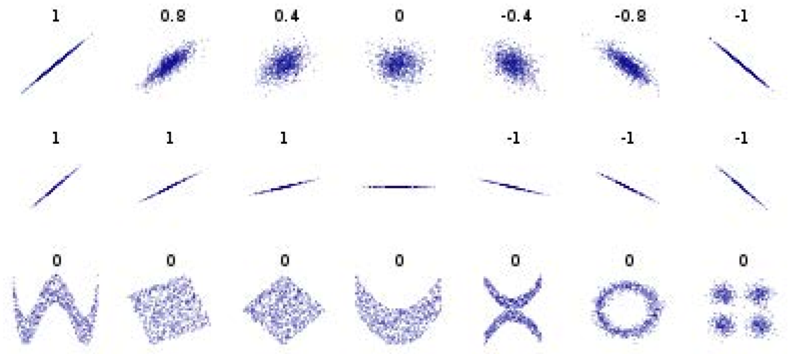
$$\min_{\beta_0,\beta_1} \text{RSS}(\beta_0,\beta_1) = N\left(1 - r_{xy}^2\right)s_y^2$$



- Coefficient of Determination: $R^2 = r_{xy}^2$
  - Explains portion of variance in y explained by x
  - s_y^2=variance in target y
  - $(1 - R^2)s_y^2$=residual sum of squares after accounting for x

Visually seeing correlation

- $R^2 = r_{xy}^2 \approx 1$: Linear model is a very good fit
- $R^2 = r_{xy}^2 \approx 0$: Linear model is a poor fit.
- $\beta_1 = \frac{r_{xy} s_y}{s_x} \Rightarrow$ Sign(β_1) = Sign(r_{xy})

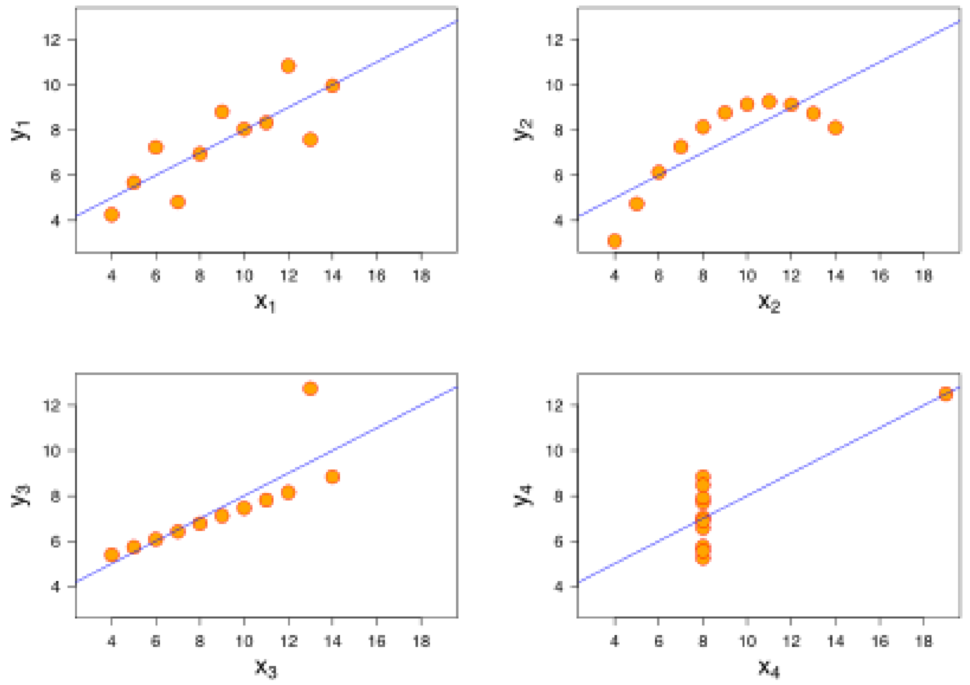


Linear models with varying levels of r_{xy}

Very good fit

No linear relationship
But, may be other relationships

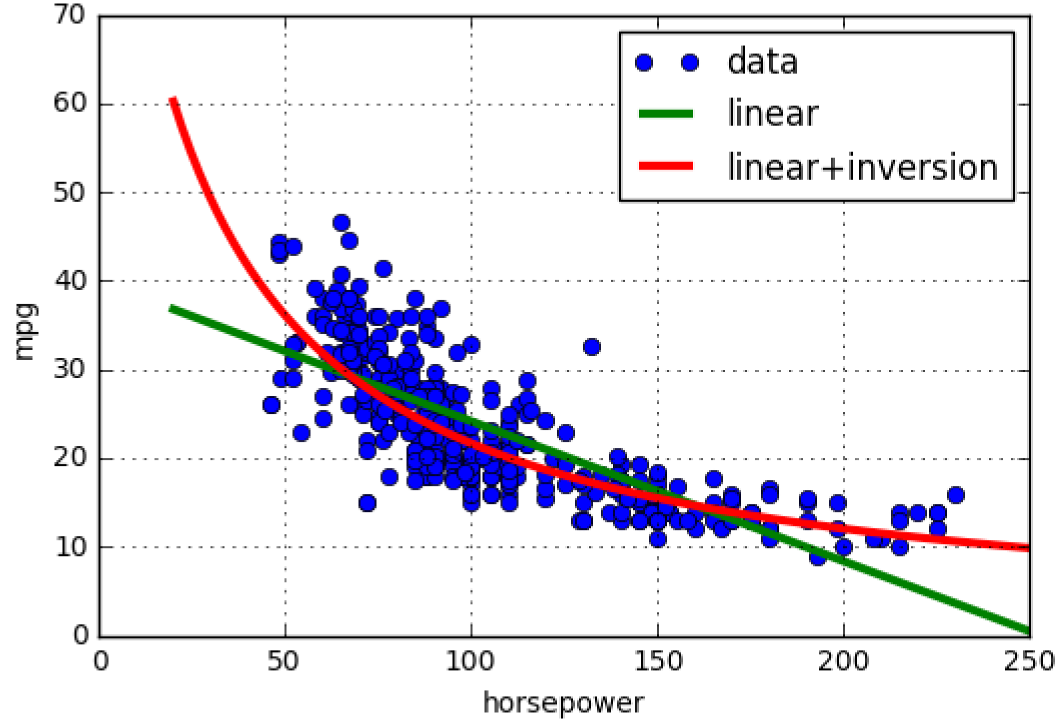
When the Error is Large…



- Many sources of error for a linear model
- Always good to visual inspect the scatter plot
  - Look for trends
- Example to the left
  - All four data sets have same regression line
  - But, errors and their reasons are different
- How would you describe these errors?

A Better Model for the Auto Example

- Fit the inverse: $\frac{1}{\text{mpg}} = \beta_0 + \beta_1 \text{horsepower}$
- Uses a nonlinear transformation
- Will cover this idea later


data
linear
linear+inversion
mpg
horsepower