Lecture 2
Simple Linear Regression

EL-GY 6143: INTRODUCTION TO MACHINE LEARNING

PROF. PEI LIU

Learning Objectives

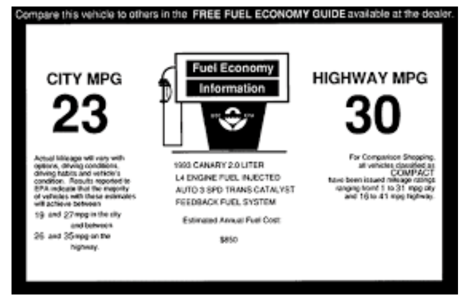
- How to load data from a text file
- How to visualize data via a scatter plot
- Describe a linear model for data
  - Identify the target variable and predictor
- Compute optimal parameters for the model using the regression formula
- Fit parameters for related models by minimizing the residual sum of 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?



Demo in Github

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.

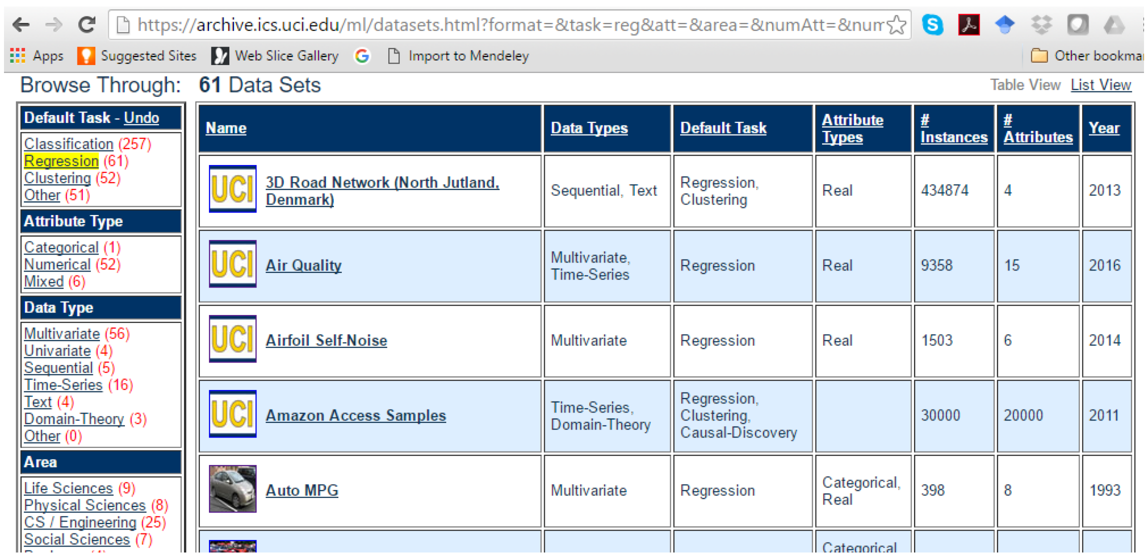
In [86]:
```
import pandas as pd
import numpy as np
```

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.php


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

Python Packages

- Python has many powerful packages
- This demo uses three key packages
- Pandas:
  - Used for reading and writing data files
  - Loads data into dataframes
- Numpy
  - Numerical operations including linear algebra
  - Data is stored in ndarray structure
  - We convert from dataframes to ndarray
- Matplotlib:
  - MATLAB-like plotting and visualization

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

```
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
```

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.
  - Ex: google “pandas.dataframe”
  - Ex. google “pandas.read”
- Dataframe has three components
  - df.columns, df.index, df.values

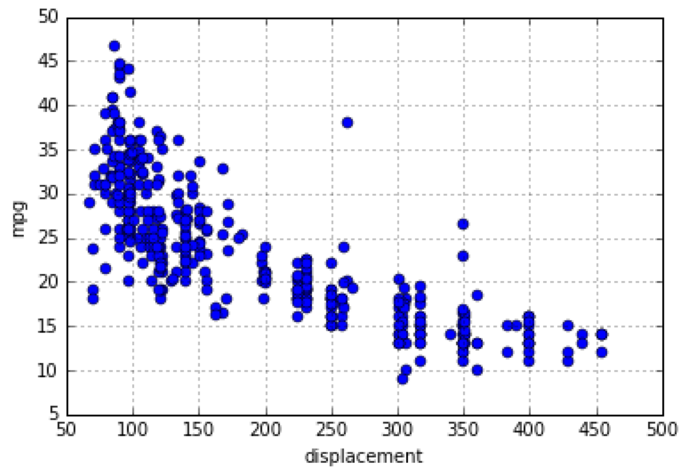
Visualizing the Data

```
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)
```

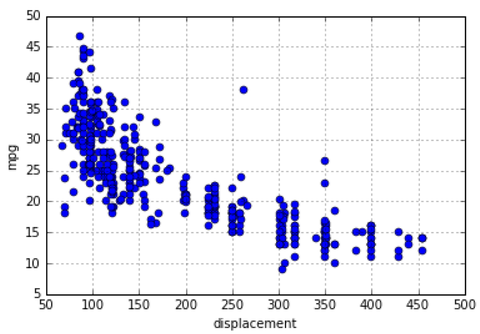
- When possible, look at data before doing anything
- Python has MATLAB-like plotting
  - Matplotlib module



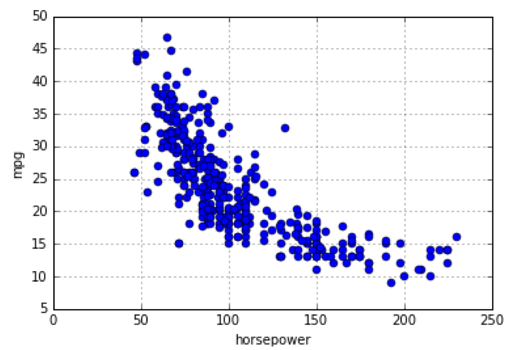
Exercise: Postulate a Model

- ❑ Try to find a mathematical to predict mpg from displacement, horsepower or acceleration
  - Make a reasonable / eyeball guess. No need for program now.
- ❑ What does your model predict when displacement = 200?
- ❑ Is the prediction reasonable? Can you improve your model?

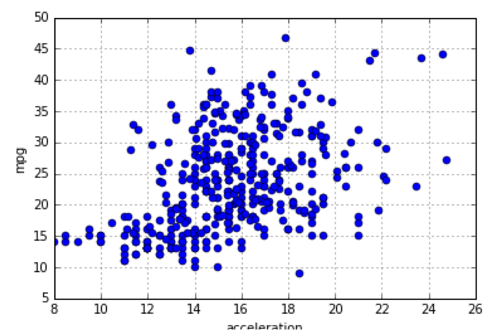
mpg



Displacement



Horsepower



Acceleration

Outline

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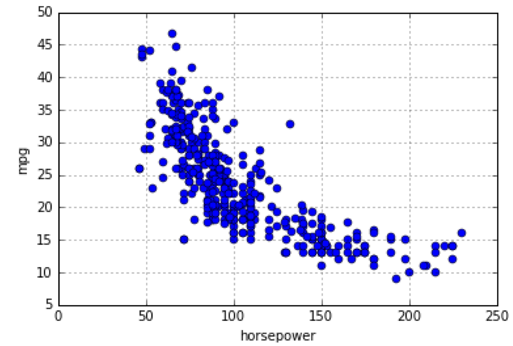
- Assessing Goodness of Fit

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, $(x_i, y_i), i = 1, \ldots, n$
  - Each data point is called a sample.
- Scatter plot

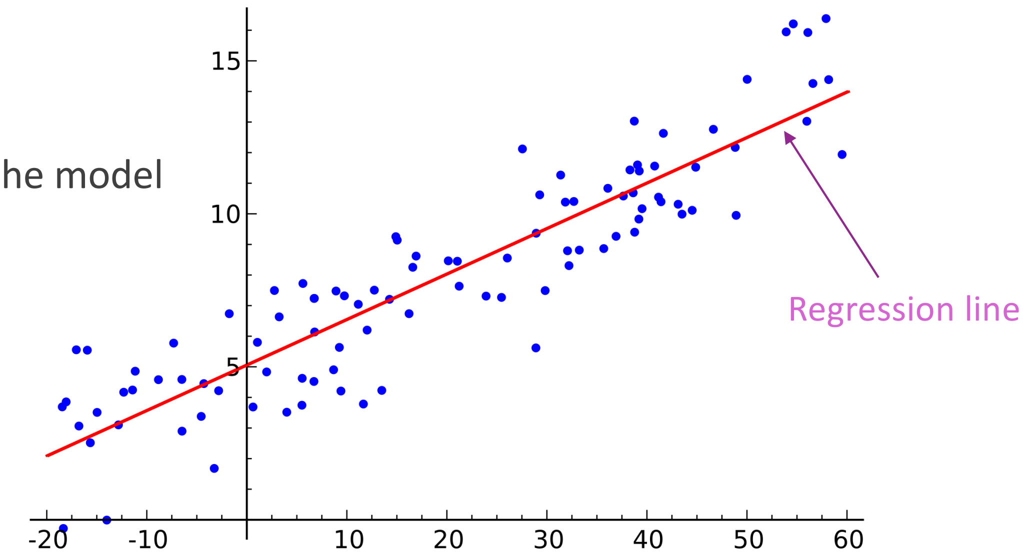
y = mpg



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

$$y \approx f(x_0) + f'(x_0)(x - x_0) = \beta_0 + \beta_1 x,$$

$$\beta_0 = f(x_0) - f'(x_0)x_0, \qquad \beta_1 = f'(x_0)$$

- Simple to compute
- Easy to interpret relation
- Gaussian random variables: If x and y were Gaussian, optimal estimator of y is linear in x

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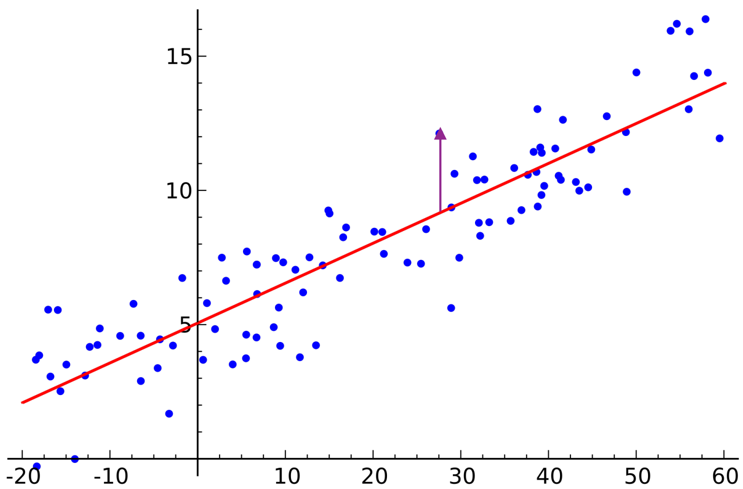
Linear Model Residual

- Knowing x does not exactly predict y
  - Variation in y due to factors other than x
- 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:

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

  - 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	Linear model: $\hat{y} = \beta_0 + \beta_1 x$
❑ Get data	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	Loss function: $RSS(\beta_0, \beta_1) \coloneqq \sum (y_i - \beta_0 + \beta_1 x_i)^2$
❑ Find parameters that minimizes loss	Select β_0, β_1 to minimize $RSS(\beta_0, \beta_1)$

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Sample Mean and Standard Deviations

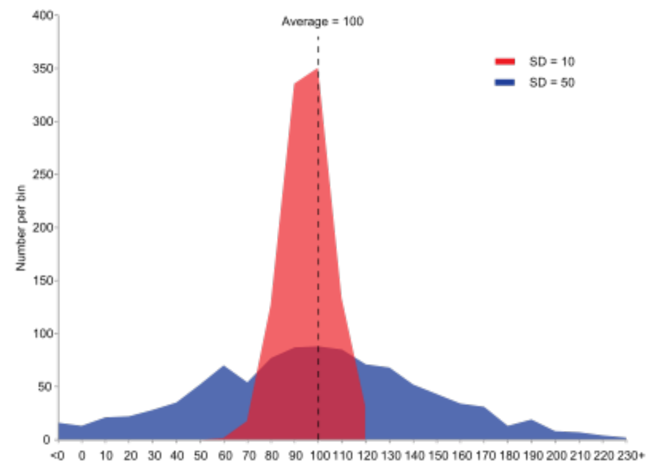
- Given data $(x_i, y_i), i = 1, \dots, N$
- Sample mean

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

- 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
  - For technical reasons, above formulae are called the biased variances.
- Sample standard deviation
  - s_x, s_y
  - Square root of variances



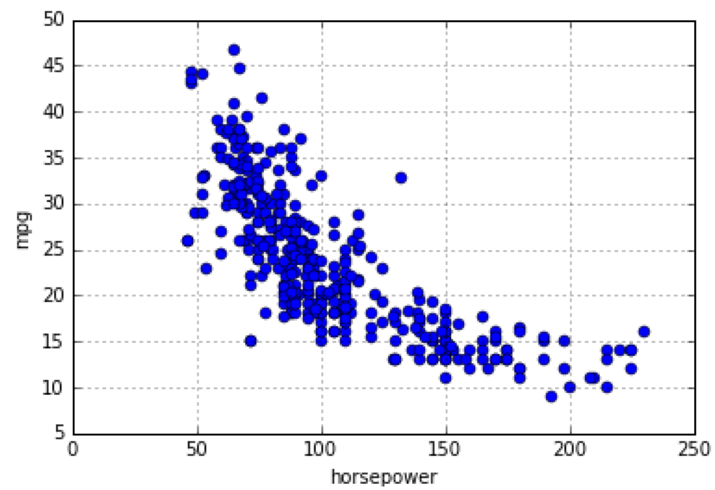
Visualizing standard deviation
https://en.wikipedia.org/wiki/Standard_deviation

Visualizing Mean and SD on Scatter Plot
Question

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

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

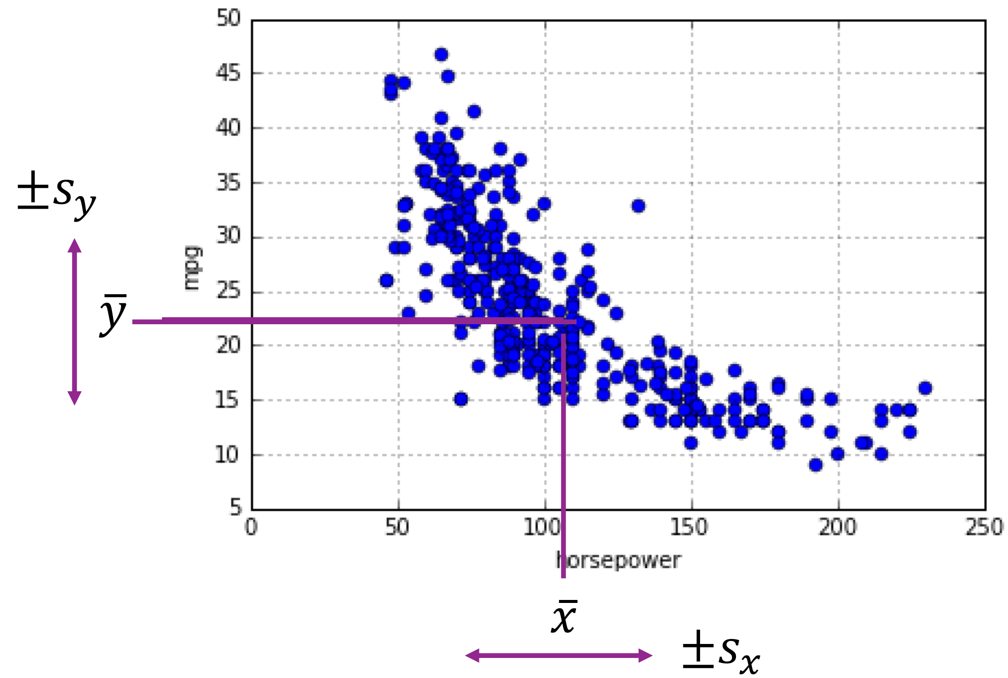
- ❑The sample std deviations: s_x, s_y



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:
    0.27% of points are 3 SDs from mean

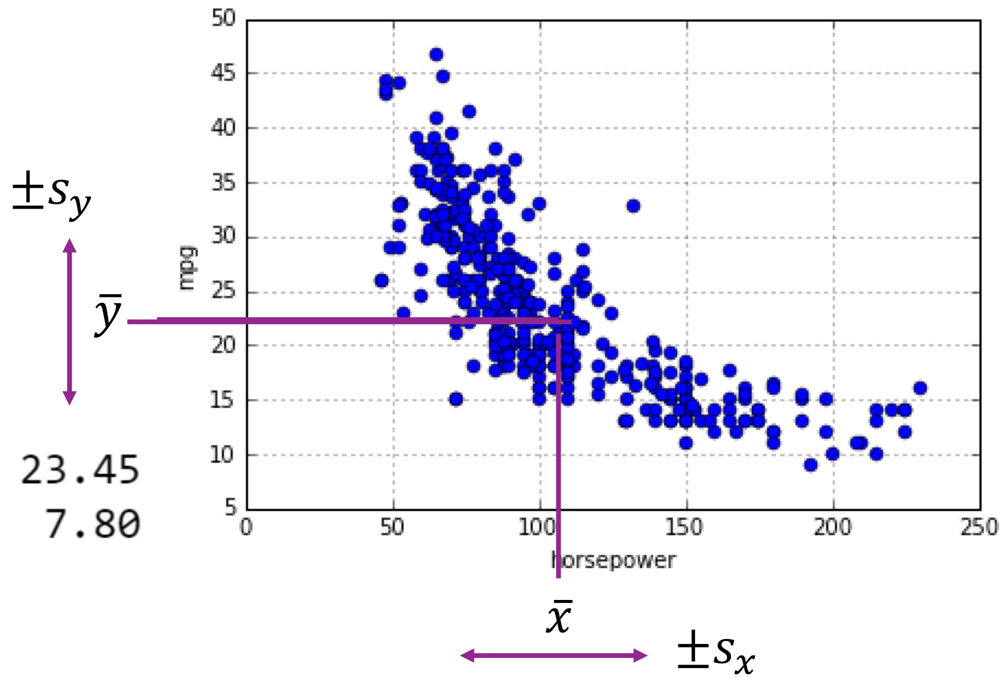


Computing Means and SD in Python

- 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
sqrt(sxx)=  38.44,   sqrt(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-schwarz inequality : $|s_{xy}| \leq s_x s_y$
- Sample correlation coefficient

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

Statistics

- Often need to compute averages of other functions of data
- Definition: The sample mean of a function $g(x, y)$ is:

$$\langle g(x_i, y_i)\rangle := \frac{1}{N}\sum_{i=1}^{N} g(x_i, y_i)$$

  - Represents the average of $g(x, y)$ on the data
  - Function $g(x, y)$ is called a statistic
- With this notation:
  - $\bar{x} = \langle x_i \rangle, \quad \bar{y} = \langle y_i \rangle$
  - $s_{xx} = \langle (x_i - \bar{x})^2 \rangle, \; s_{yy} = \langle (y_i - \bar{y})^2 \rangle$

Alternate Equation for Variance

- Alternate equations for variance and sample co-variance:
  - Sample variances $s_{xx} = \langle x_i^2 \rangle - \langle x_i \rangle^2$, $s_{yy} = \langle y_i^2 \rangle - \langle y_i \rangle^2$
  - Sample co-variance $s_{xy} = \langle x_i y_i \rangle - \langle x_i \rangle \langle y_i \rangle$

- Proof:
  - $s_{xx} = \frac{1}{N} \sum (x_i - \bar{x})^2 = \frac{1}{N} \sum (x_i^2 - 2x_i\bar{x} + \bar{x}^2) = \langle x_i^2 \rangle - 2\bar{x}\langle x_i \rangle + \bar{x}^2$
  - Recall $\bar{x} = \langle x_i \rangle$
  - Therefore, $s_{xx} = \langle x_i^2 \rangle - \langle x_i \rangle^2$
  - Other relations $s_{yy} = \langle y_i^2 \rangle - \langle y_i \rangle^2$ and $s_{xy} = \langle x_i y_i \rangle - \langle x_i \rangle \langle y_i \rangle$ proved similarly

Notation

- This class will use the following notation
- We will try to be consistent
- Note: Other texts use different notations

Statistic	Notation	Formula	Python
Sample mean	$\bar{x}$	$\frac{1}{n}\sum_{i=1}^{n} x_i$	`xm`
Sample variance	$s_x^2 = s_{xx}$	$\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$	`sxx`
Sample standard deviation	$s_x = \sqrt{s_{xx}}$	$s_x = \sqrt{s_{xx}}$	`sx`
Sample covariance	s_{xy}	$\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$	`sxy`

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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.

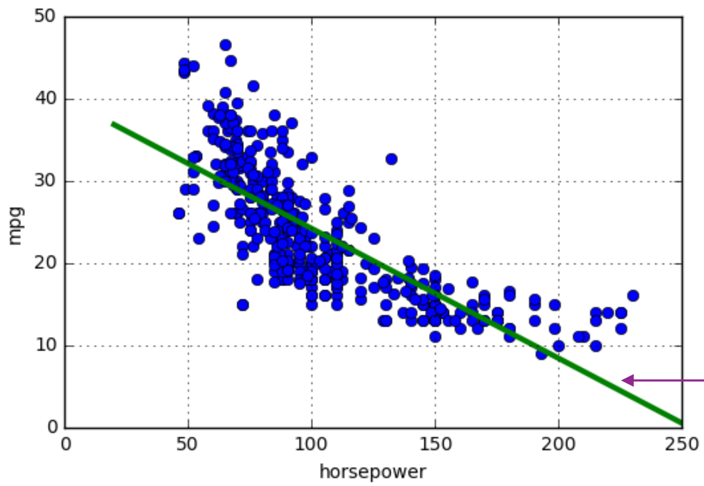
	Student	x_i	y_i	$(x_i - \bar{x})$	$(y_i - \bar{y})$	$(x_i - \bar{x})^2$	$(y_i - \bar{y})^2$	$(x_i - \bar{x})(y_i - \bar{y})$
	1	95	85	17	8	289	64	136
	2	85	95	7	18	49	324	126
	3	80	70	2	-7	4	49	-14
	4	70	65	-8	-12	64	144	96
	5	60	70	-18	-7	324	49	126
Sum		390	385			730	630	470
Mean		78	77					

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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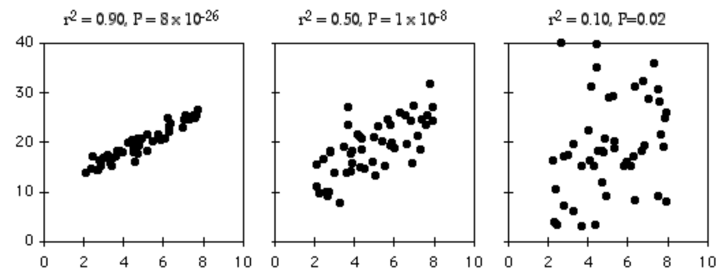
Minimum RSS

- Minimum RSS (Proof on board)

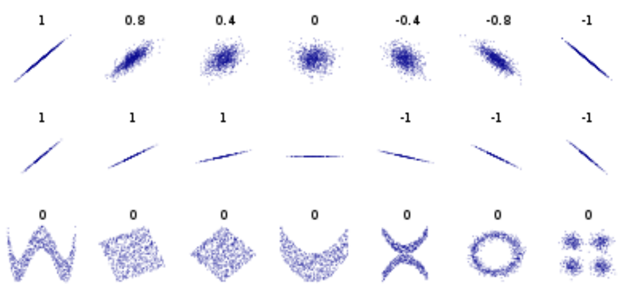
$$\min_{\beta_0,\beta_1} \text{RSS}(\beta_0,\beta_1) = N\left(1 - r_{xy}^2\right)s_y^2$$



- 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})

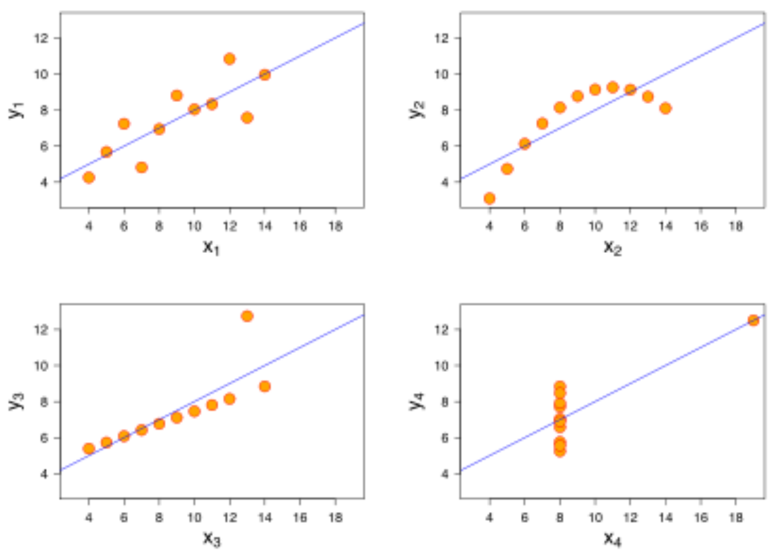


Linear models with varying levels of r_{xy}

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 visually 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