Lecture 3
Simple Linear Regression

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

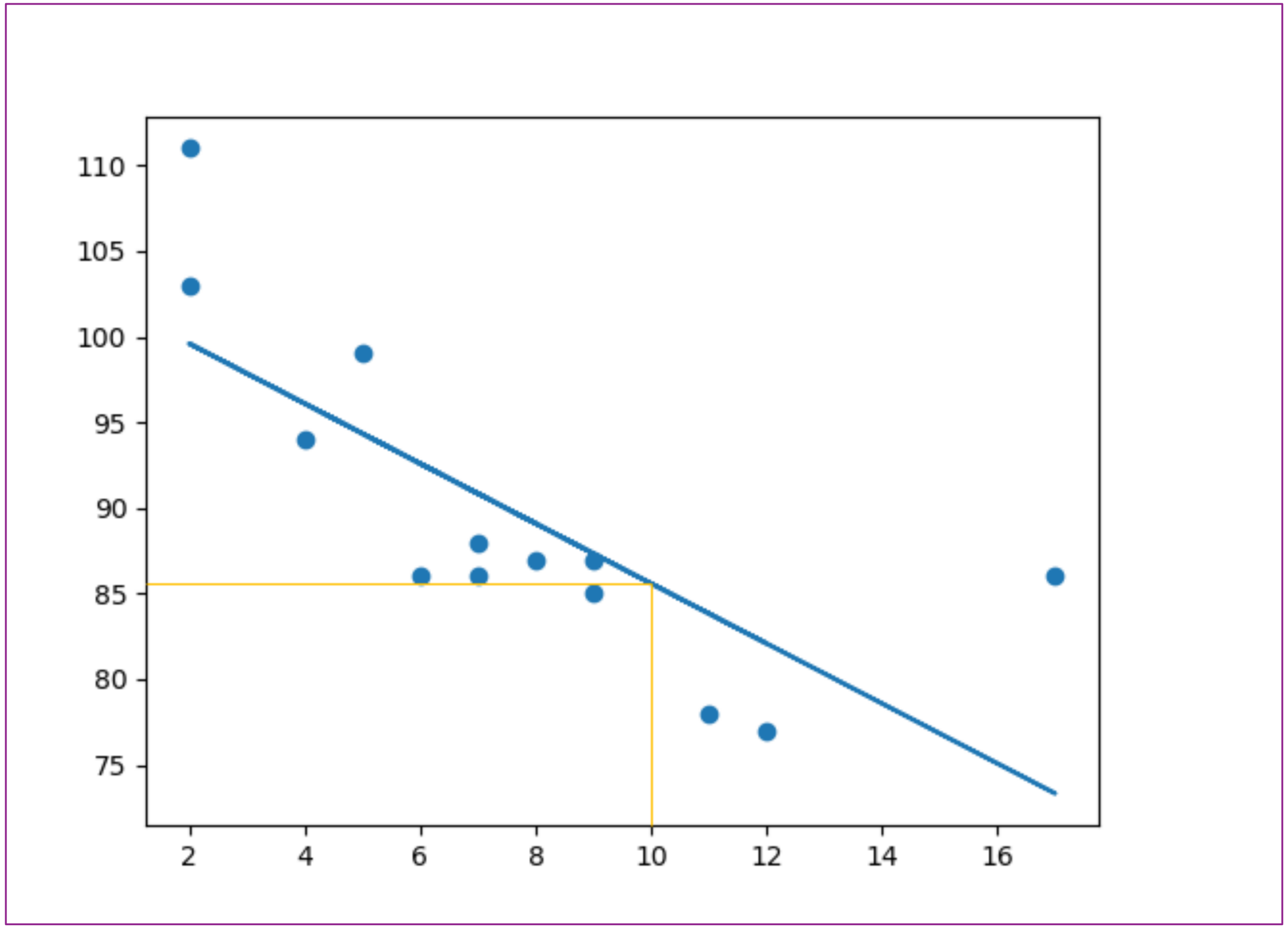
Outline

- **Motivating Example1: Predicting the prices of a house**
- Motivating Example2: Predicting the mpg of a car
- Linear Model
- Least Squares Fit Problem
- Sample Mean and Variance
- LS Fit Solution
- Assessing Goodness of Fit

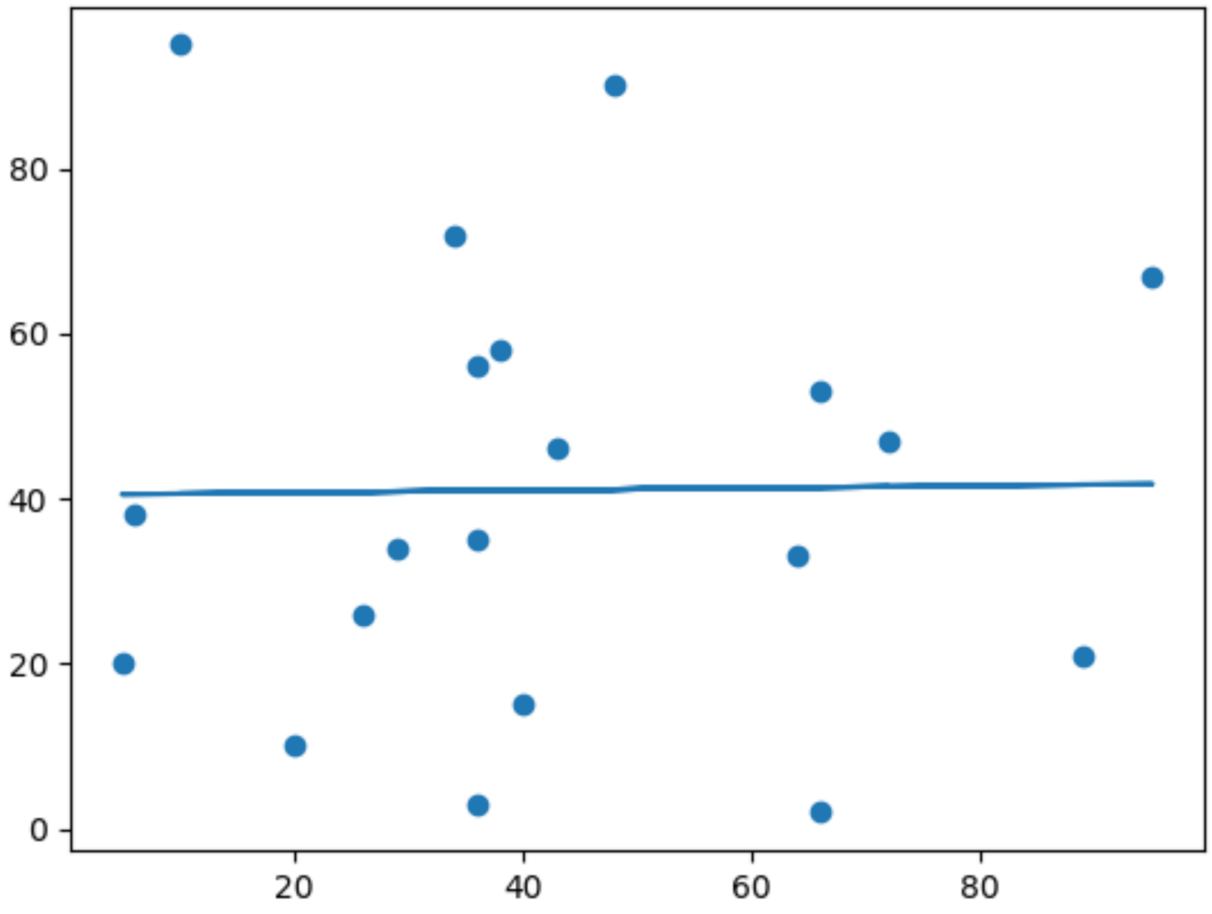
Bad Fit?

- Let us create an example where linear regression would not be the best method to predict future values.

```python
from scipy import stats

x = [5,7,8,7,2,17,2,9,4,11,12,9,6]
y = [99,86,87,88,111,86,103,87,94,78,77,85,86]

slope, intercept, r, p, std_err = stats.linregress(x, y)

def myfunc(x):
  return slope * x + intercept

speed = myfunc(10)

print(speed)
```



110
105
100
95
90
85
80
75
2
4
6
8
10
12
14
16



80
60
40
20
0
20
40
60
80

R-Squared

- It is important to know how well the relationship between the values of the x- and y-axis is, if there are no relationship the polynomial regression can not be used to predict anything.

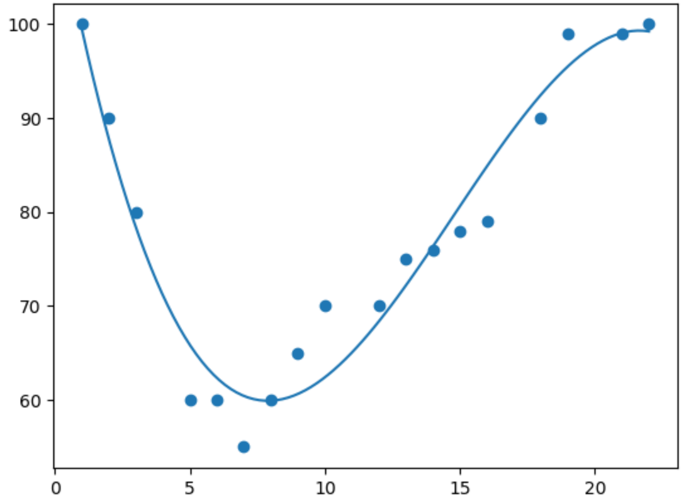
- The relationship is measured with a value called the r-squared.

- The r-squared value ranges from 0 to 1, where 0 means no relationship, and 1 means 100% related.

Polynomial Regression

- If your data points clearly will not fit a linear regression (a straight line through all data points), it might be ideal for polynomial regression.

- Polynomial regression, like linear regression, uses the relationship between the variables x and y to find the best way to draw a line through the data points.



$$x = [1,2,3,4,5]$$

$$y = [5,7,9,11,13]$$

$$y = 2x + 3$$

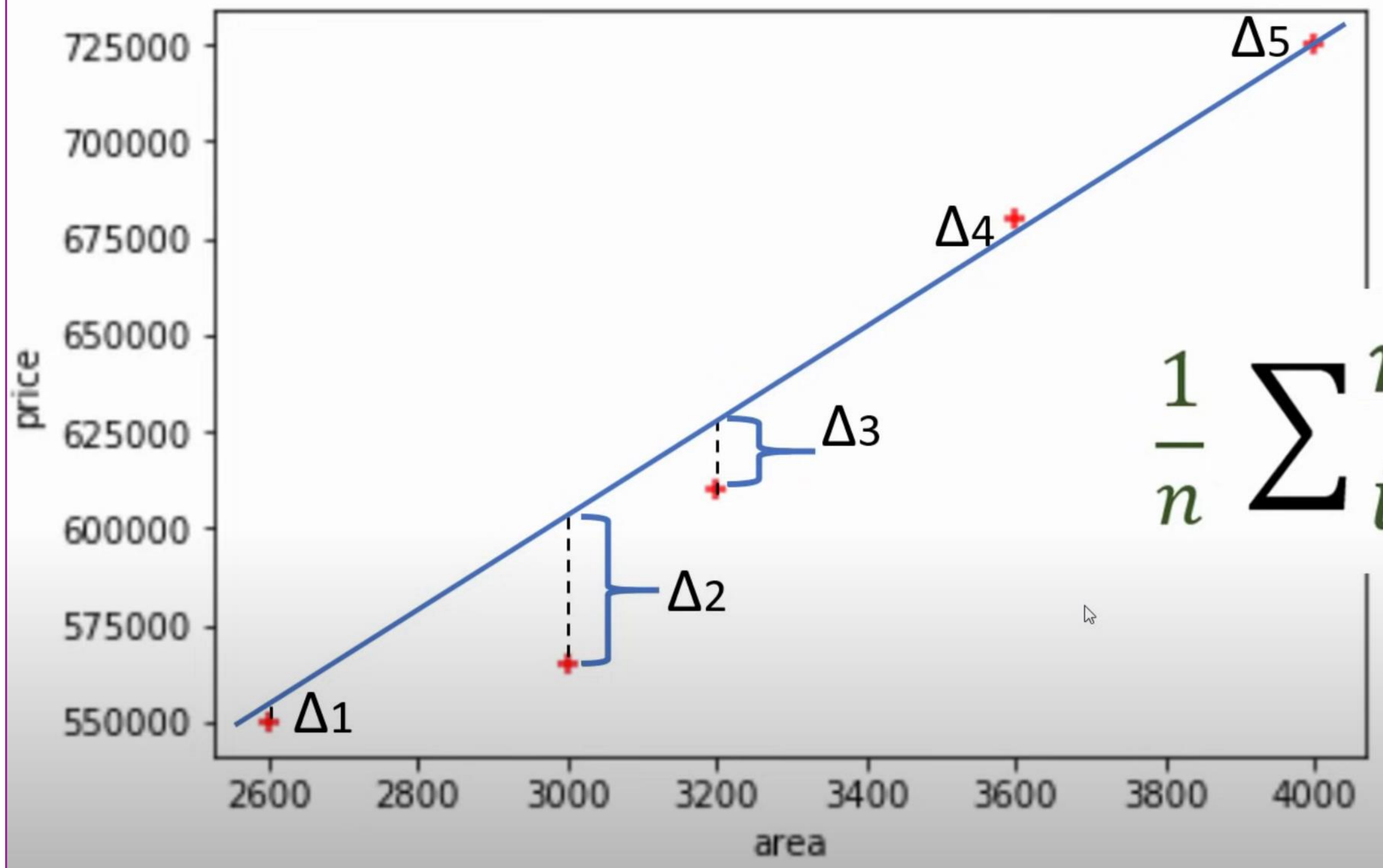
area = [2600,3000,3200,3600,4000]

price = [550k,565k,610k,680k,725k]

area = [2600,3000,3200,3600,4000]

price = [550k,565k,610k,680k,725k]

price = 135.78 * area + 180616.43



$$\frac{1}{n}\sum_{i=1}^{n}(\Delta i)^2$$

Mean Squared Error

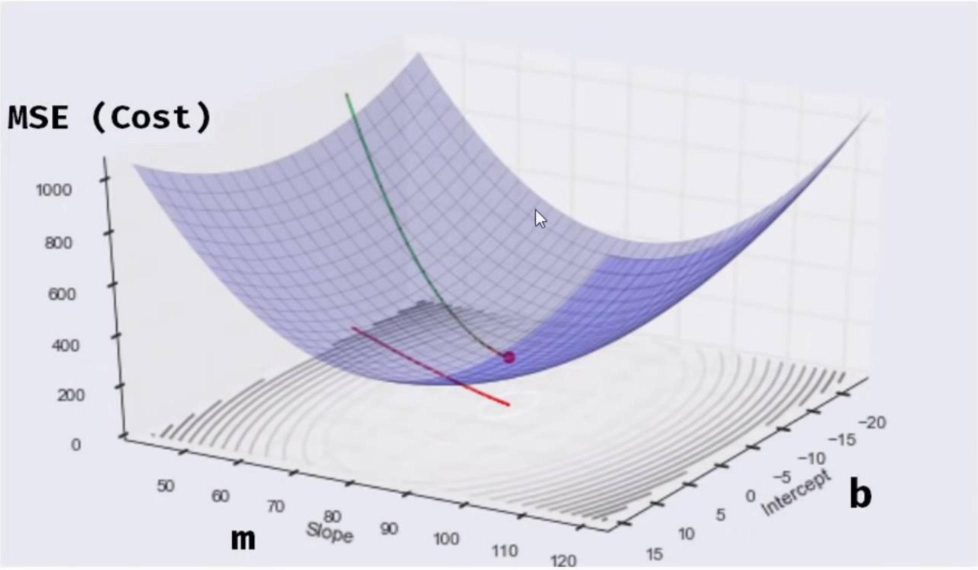
$$ms\varepsilon = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - y_{predicted}\right)^2$$

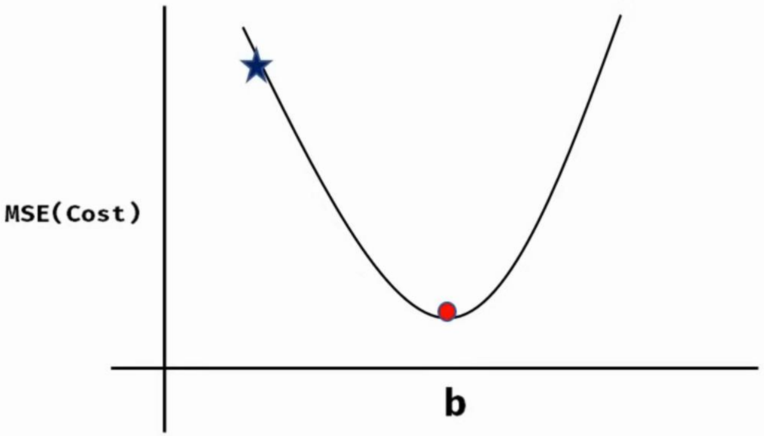
Mean Squared Error

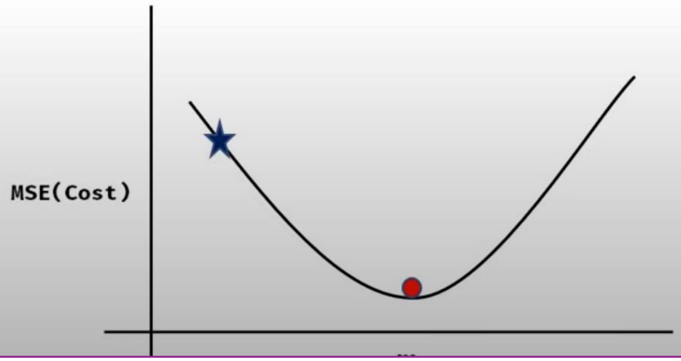
$$ms\varepsilon = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (mx_i + b)\right)^2$$

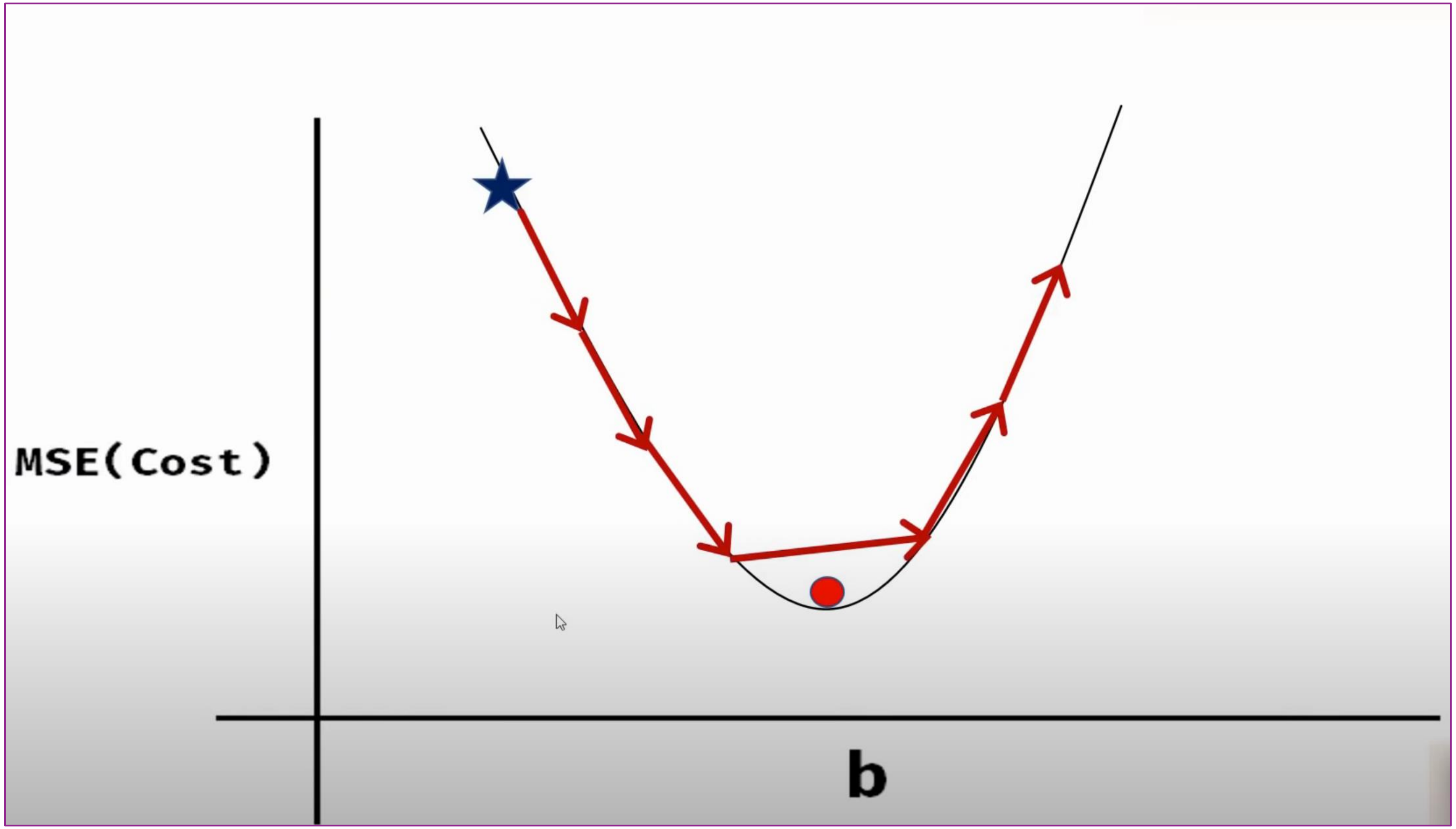
Cost Function

Gradient descent is an algorithm that finds best fit line for given training data set

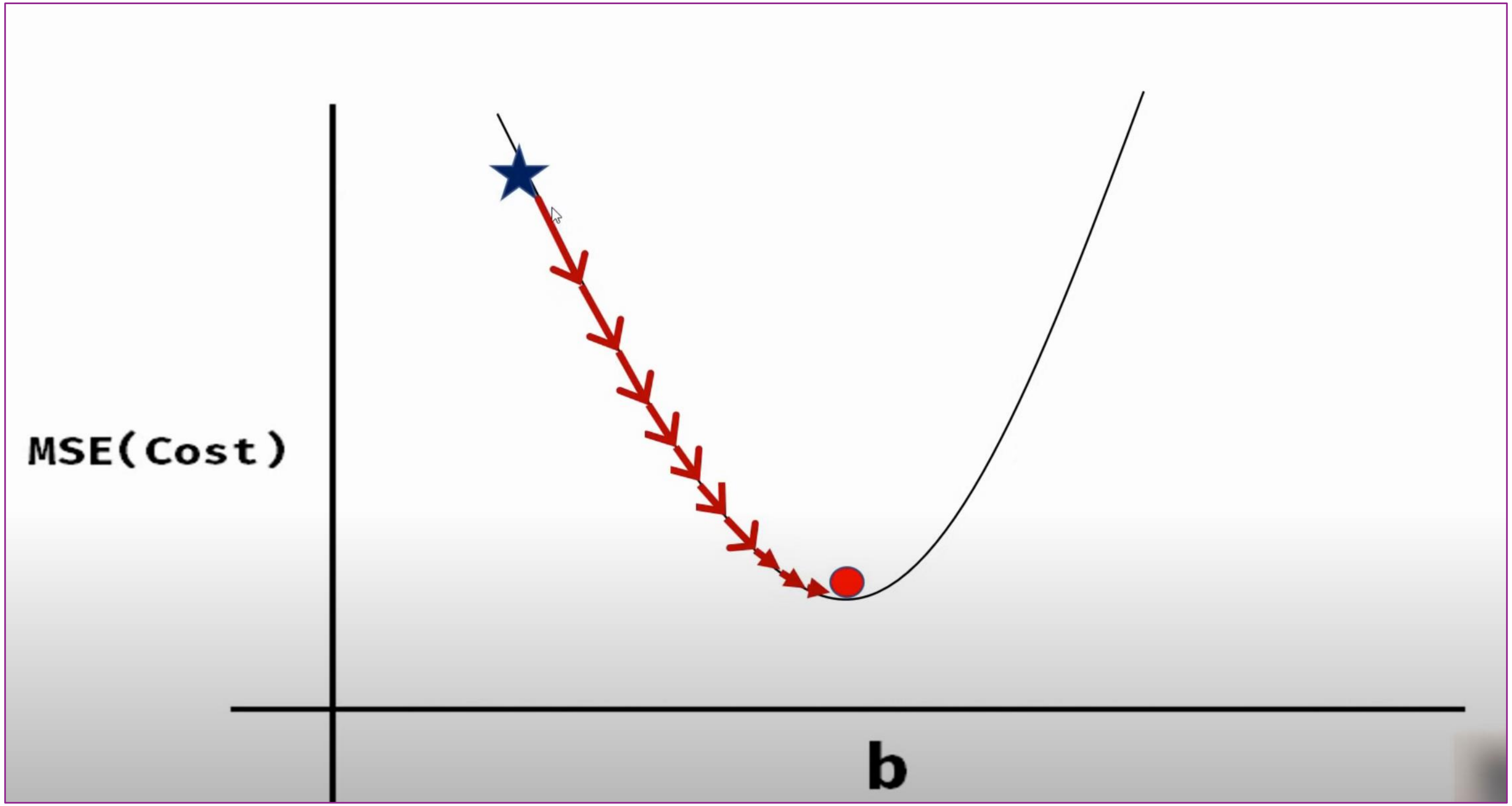

MSE (Cost)
1000
800
600
400
200
0
50
60
70
80
90
100
110
120
Slope
m
-20
-15
-10
-5
0
5
10
15
Intercept
b

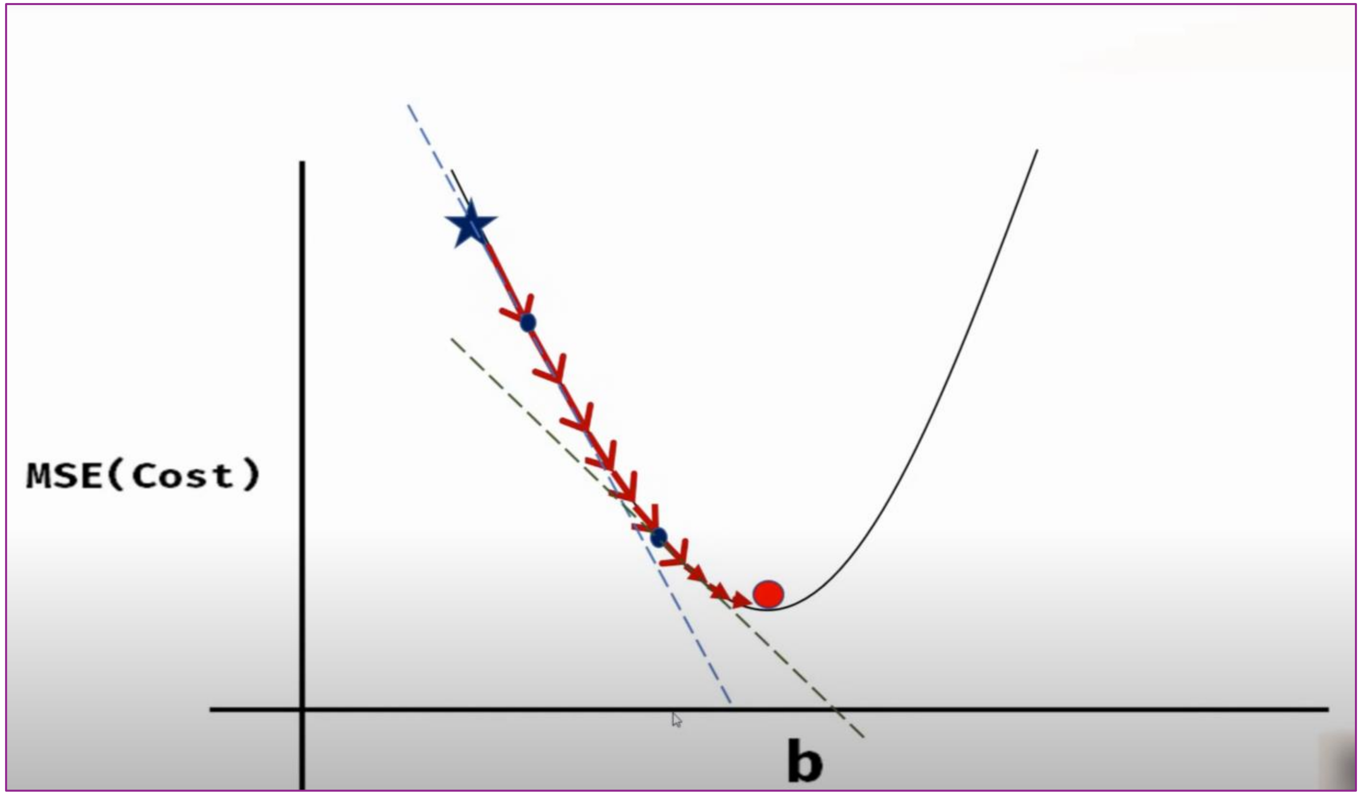

MSE(Cost)
b


MSE(Cost)



MSE(Cost)
b


MSE(Cost)
b


MSE(Cost)
b

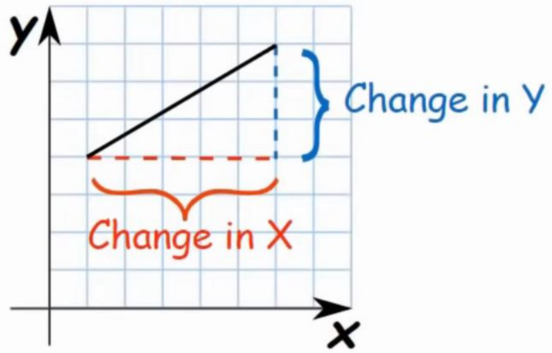
https://www.mathsisfun.com/equation_of_line.html

https://www.mathsisfun.com/calculus/derivatives-introduction.html

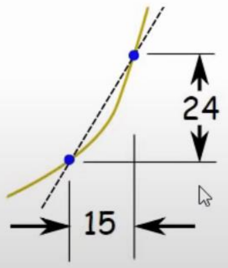
https://www.mathsisfun.com/calculus/derivatives-partial.html

It is all about slope!

$$\text{Slope} = \frac{\text{Change in Y}}{\text{Change in X}}$$



We can find an **average** slope between two points.



$$\text{average slope} = \frac{24}{15}$$

$$mse = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (mx_i + b)\right)^2$$

$$\partial/_{\partial m} = \frac{2}{\mathrm{n}}\sum_{i=1}^{n} -x_i\left(y_i - (mx_i + b)\right)$$

$$\partial/_{\partial b} = \frac{2}{\mathrm{n}}\sum_{i=1}^{n} -\left(y_i - (mx_i + b)\right)$$

$$m = m - \text{learning rate} * \partial/_{\partial m}$$

$$b = b - \text{learning rate} * \partial/_{\partial b}$$

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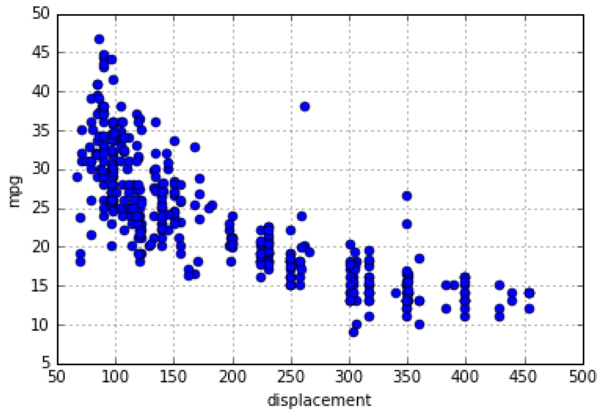
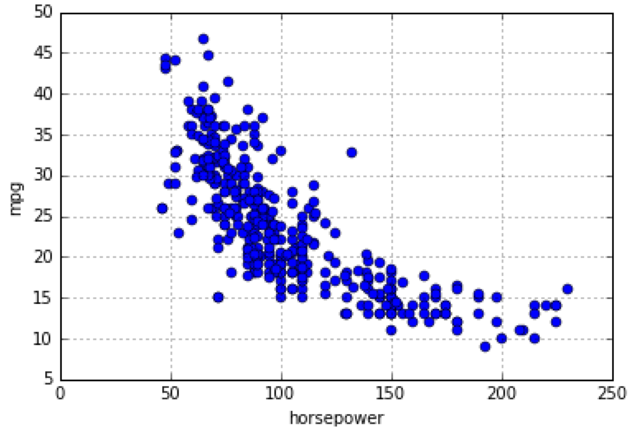
Exercise: Postulate a Model

- ❑Break into small groups
- ❑Try to find a mathematical model 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?

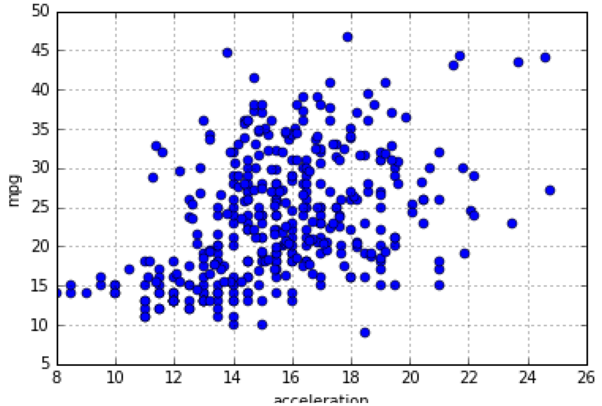
mpg



Displacement



Horsepower

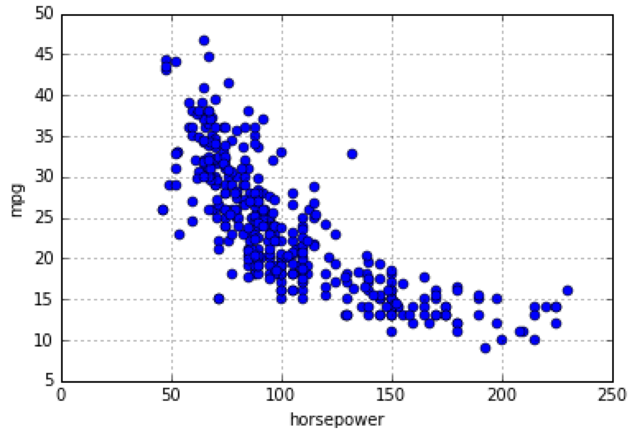


Acceleration

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

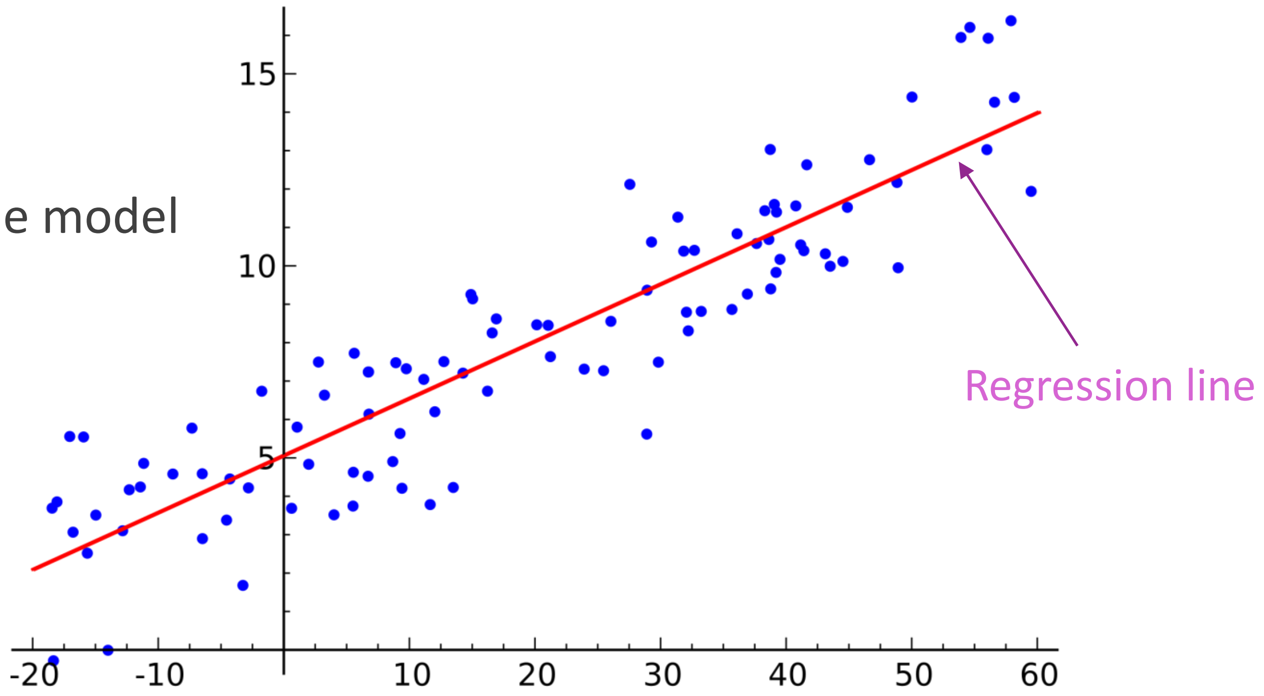
$$y \approx \beta_0 + \beta_1 x$$

  - 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

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

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

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


ANY
QUESTIONS?

Outline

- ❑Motivating Example: Predicting the mpg of a car
- ❑Linear Model
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- ❑Sample Mean and Variance
- ❑LS Fit Solution
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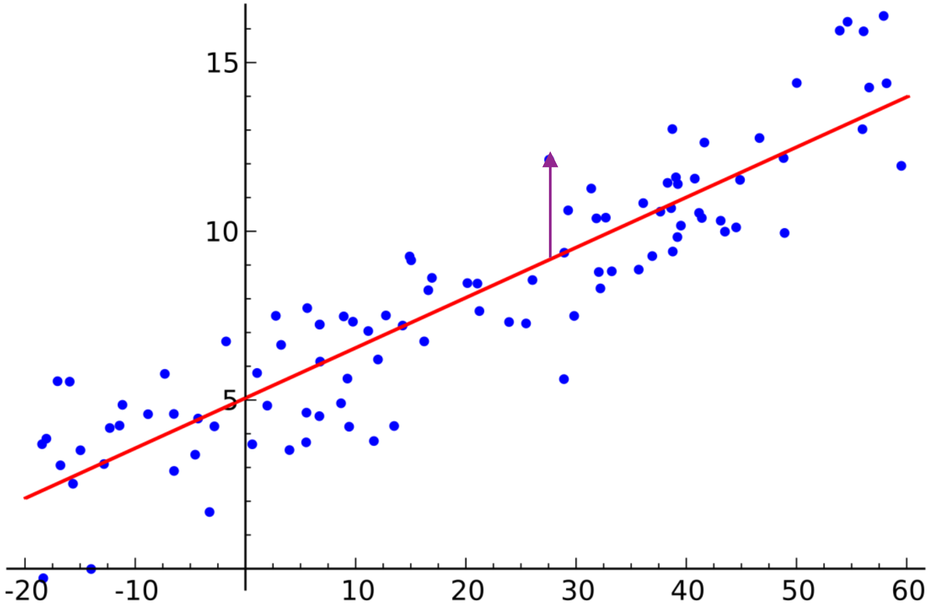
Linear Model Residual

- ❑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

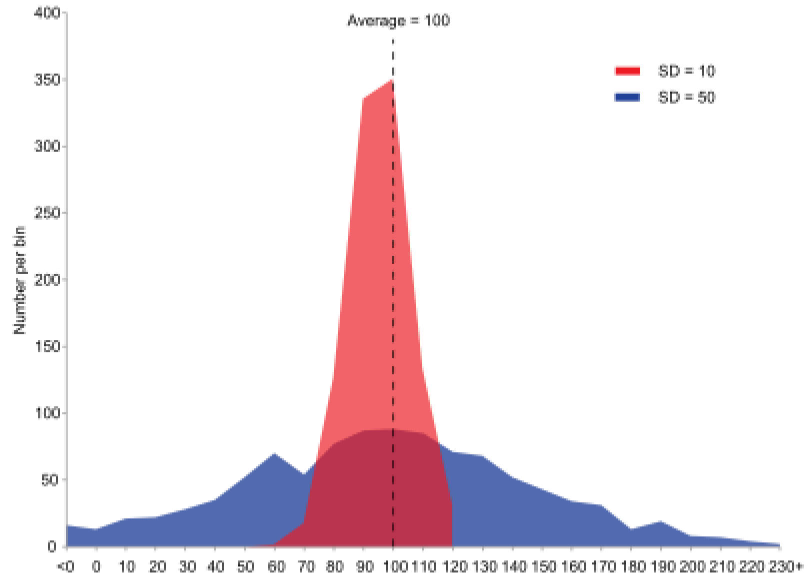
- Given data $(x_i, y_i), i = 1, \dots, N$
- Sample mean

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

- 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

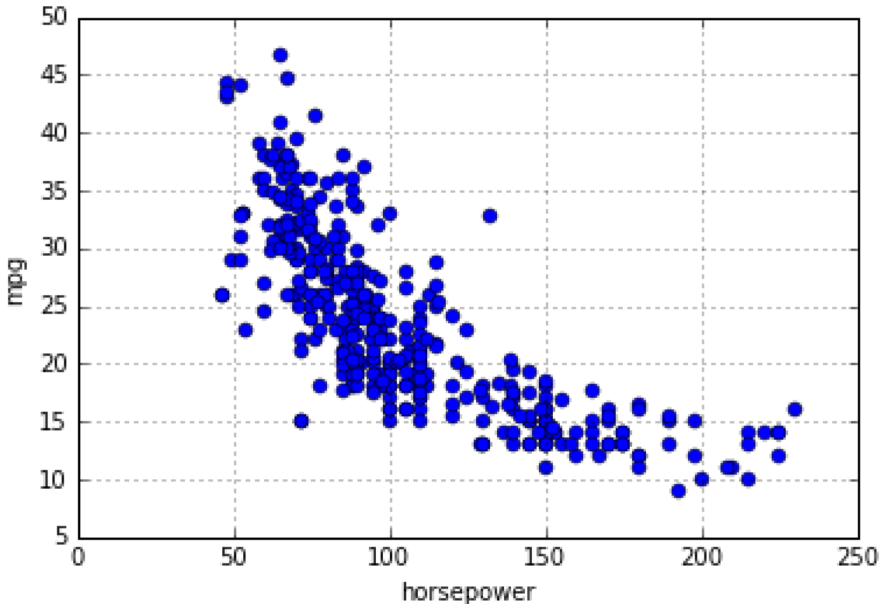


Visualizing Mean and SD on Scatter Plot
Question

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

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

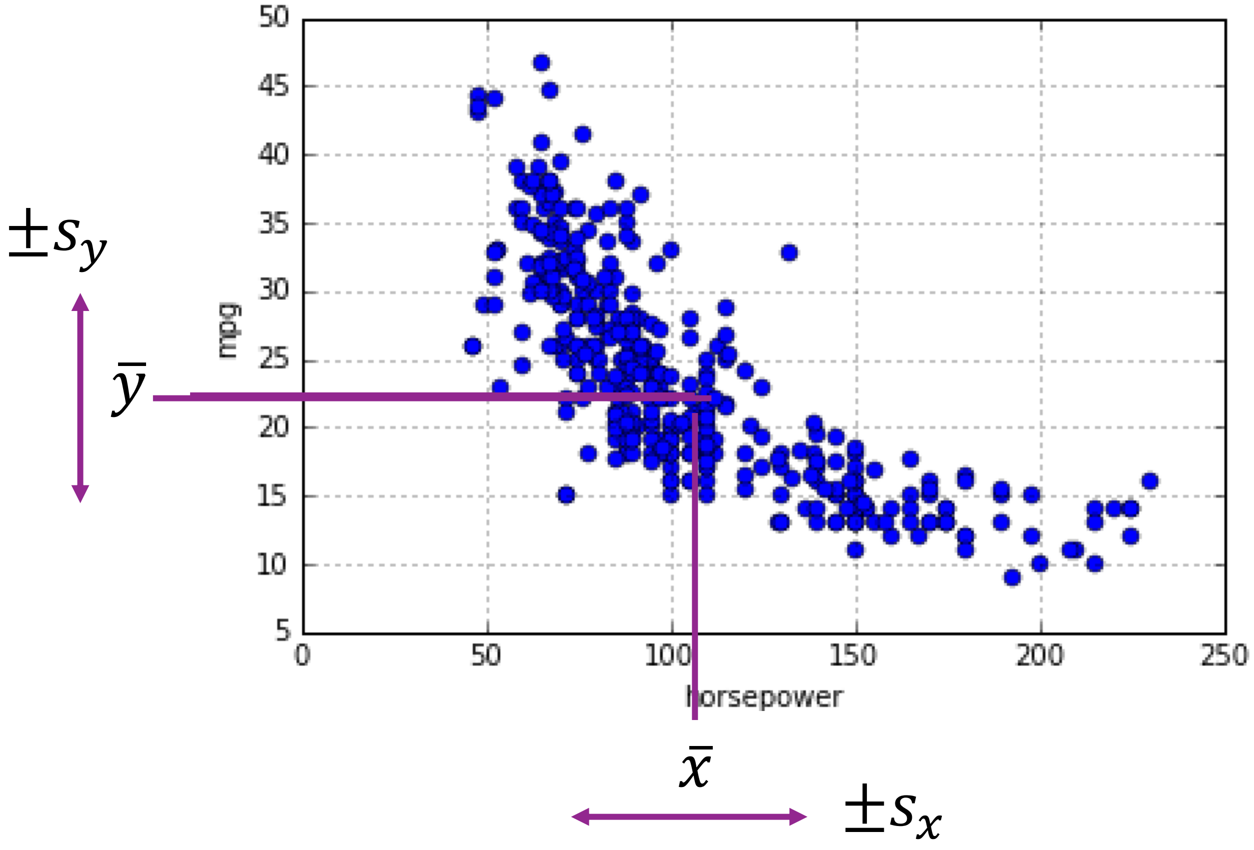
- ❑The sample std deviations: s_x, s_y



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

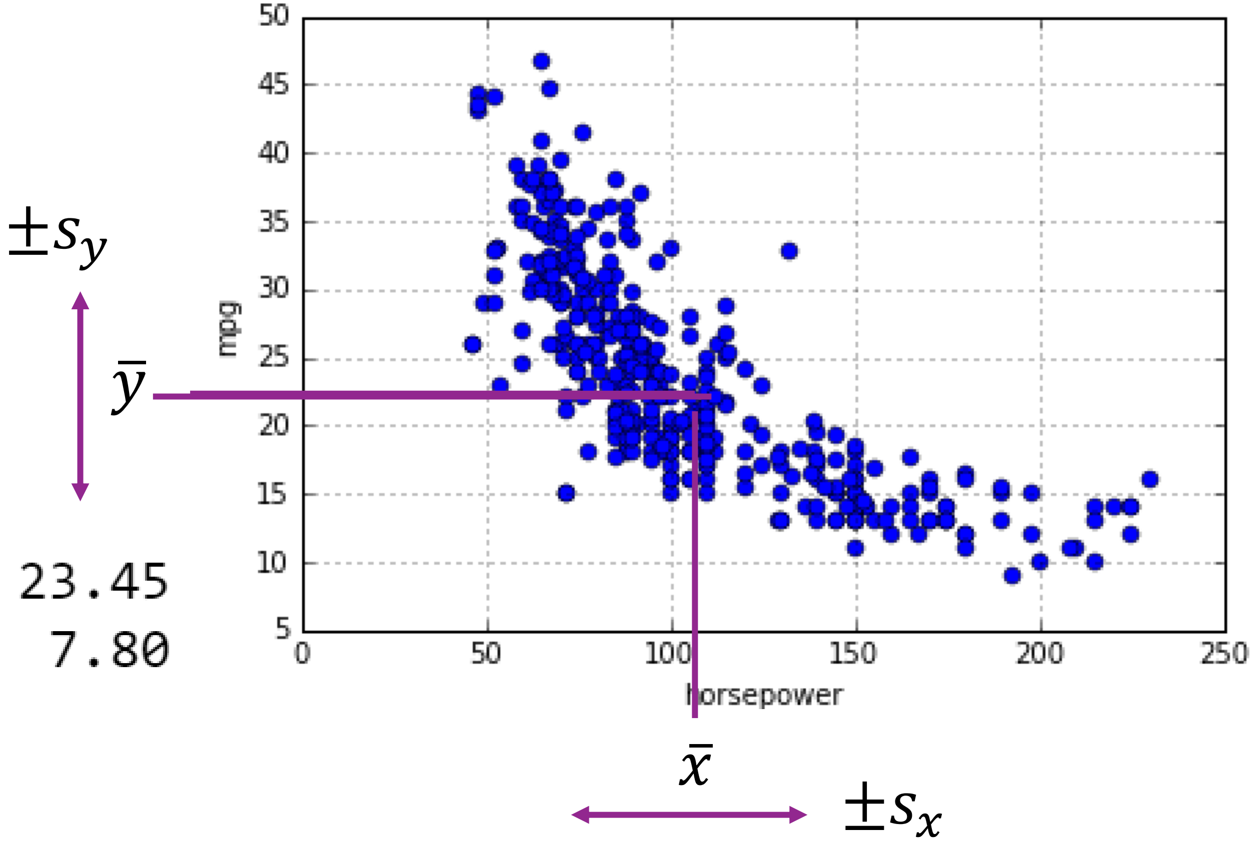


Computing Means and SD in Python

- 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-Schartz Law: $|s_{xy}| < s_x s_y$
- 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:
  - $\bar{x} = \langle x_i\rangle, \quad \bar{y} = \langle y_i\rangle$
  - $s_{xx} = \left\langle (x_i - \bar{x})^2\right\rangle, \; s_{yy} = \left\langle (y_i - \bar{y})^2\right\rangle$

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.

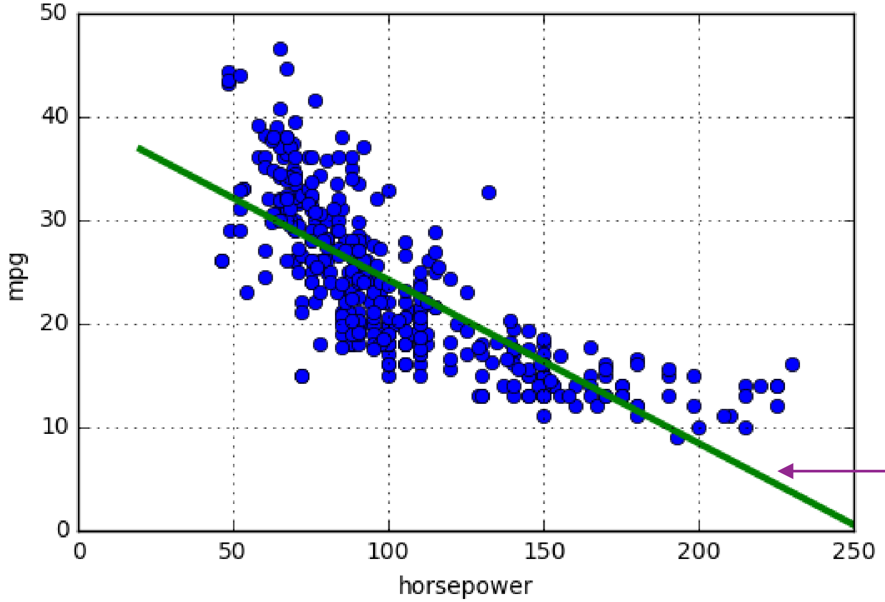
	Student	x_i	y_i	$(x_i - \bar{x})$	$(y_i - \bar{y})$	$(x_i - \bar{x})^2$	$(y_i - \bar{y})^2$	$(x_i - \bar{x})(y_i - \bar{y})$
	1	95	85	17	8	289	64	136
	2	85	95	7	18	49	324	126
	3	80	70	2	-7	4	49	-14
	4	70	65	-8	-12	64	144	96
	5	60	70	-18	-7	324	49	126
Sum		390	385			730	630	470
Mean		78	77					

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




```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
```

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

Regression line:

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

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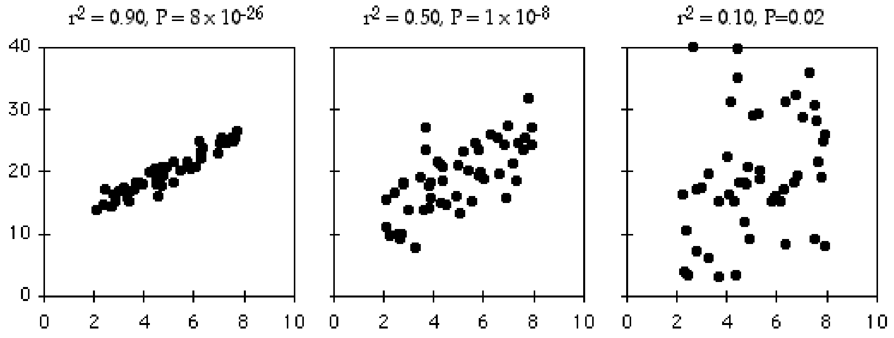
Minimum RSS

- Minimum RSS (Proof on board)

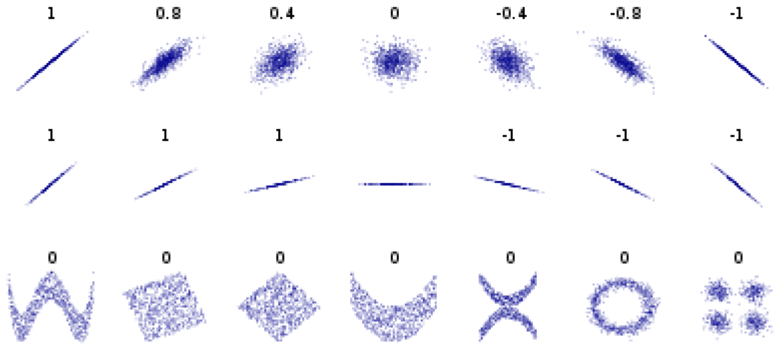
$$\min_{\beta_0,\beta_1} \mathrm{RSS}(\beta_0,\beta_1) = N\left(1 - r_{xy}^2\right)s_y^2$$



- Coefficient of Determination: $R^2 = r_{xy}^2$
  - Explains portion of variance in y explained by x
  - s_y^2=variance in target y
  - $\left(1 - R^2\right)s_y^2$=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})

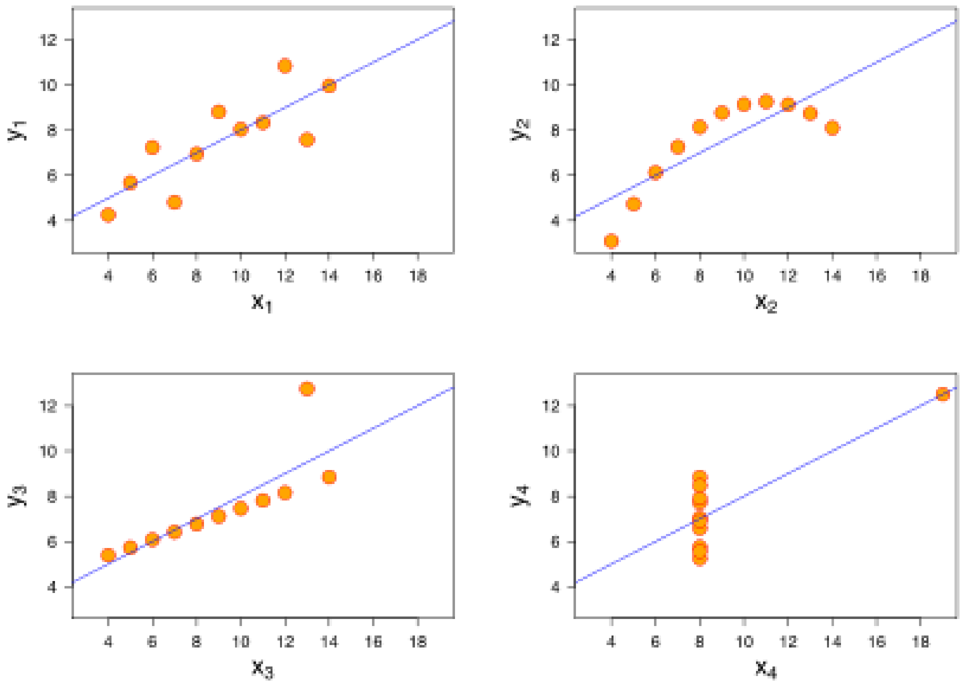


Linear models with varying levels of r_{xy}

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