

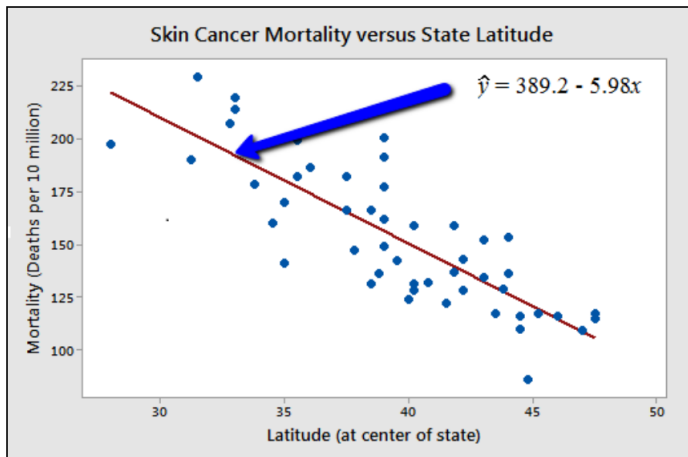
# Fundamental Methods of Data Science

Class 7

# Linear Classifiers



# Linear Regression



# Linear Regression in Python

```
import statsmodels.formula.api as smf
est = smf.ols(formula="TRB ~ AST + STL + BLK", data=nba_data).fit()
est.summary()
```

# Linear Regression in Python

```
import statsmodels.formula.api as smf
est = smf.ols(formula="TRB ~ AST + STL + BLK", data=nba_data).fit()
est.summary()
```

```
from sklearn import linear_model
X = wt_ht_data[['Height']]
Y = wt_ht_data['Weight']
lm = linear_model.LinearRegression()
lm.fit(X, Y)
print('Intercept is ' + str(lm.intercept_) + '\n')
print('Coefficient value of the height is ' + str(lm.coef_) + '\n')
print(pd.DataFrame(list(zip(X.columns, lm.coef_)),
                      columns = ['features', 'estimatedCoefficients'])))
```

# Linear Regression in Python

```
import statsmodels.formula.api as smf
est = smf.ols(formula="TRB ~ AST + STL + BLK", data=nba_data).fit()
est.summary()
```

```
from sklearn import linear_model
X = wt_ht_data[['Height']]
Y = wt_ht_data['Weight']
lm = linear_model.LinearRegression()
lm.fit(X, Y)
print('Intercept is ' + str(lm.intercept_) + '\n')
print('Coefficient value of the height is ' + str(lm.coef_) + '\n')
print(pd.DataFrame(list(zip(X.columns, lm.coef_)),
                      columns = ['features', 'estimatedCoefficients'])))
```

- After cleaning and normalizing the data

# Evaluating the Model

<b>Dep. Variable:</b>	TRB	<b>R-squared:</b>	0.634
<b>Model:</b>	OLS	<b>Adj. R-squared:</b>	0.632
<b>Method:</b>	Least Squares	<b>F-statistic:</b>	272.9
<b>Date:</b>	Fri, 06 Oct 2017	<b>Prob (F-statistic):</b>	1.10e-102
<b>Time:</b>	09:48:10	<b>Log-Likelihood:</b>	-853.73
<b>No. Observations:</b>	476	<b>AIC:</b>	1715.
<b>Df Residuals:</b>	472	<b>BIC:</b>	1732.
<b>Df Model:</b>	3		
<b>Covariance Type:</b>	nonrobust		

	coef	std err	t	P> t	[0.025	0.975]
<b>Intercept</b>	1.0288	0.128	8.020	0.000	0.777	1.281
<b>AST</b>	0.0884	0.054	1.633	0.103	-0.018	0.195
<b>STL</b>	1.3464	0.221	6.100	0.000	0.913	1.780
<b>BLK</b>	3.7348	0.154	24.179	0.000	3.431	4.038

<b>Omnibus:</b>	110.206	<b>Durbin-Watson:</b>	1.716
<b>Prob(Omnibus):</b>	0.000	<b>Jarque-Bera (JB):</b>	314.747
<b>Skew:</b>	1.100	<b>Prob(JB):</b>	4.50e-69
<b>Kurtosis:</b>	6.321	<b>Cond. No.</b>	9.70

- Higher (Adj.) R-squared is normally better

# Evaluating the Model

<b>Dep. Variable:</b>	TRB	<b>R-squared:</b>	0.634
<b>Model:</b>	OLS	<b>Adj. R-squared:</b>	0.632
<b>Method:</b>	Least Squares	<b>F-statistic:</b>	272.9
<b>Date:</b>	Fri, 06 Oct 2017	<b>Prob (F-statistic):</b>	1.10e-102
<b>Time:</b>	09:48:10	<b>Log-Likelihood:</b>	-853.73
<b>No. Observations:</b>	476	<b>AIC:</b>	1715.
<b>Df Residuals:</b>	472	<b>BIC:</b>	1732.
<b>Df Model:</b>	3		
<b>Covariance Type:</b>	nonrobust		

	coef	std err	t	P> t	[0.025	0.975]
<b>Intercept</b>	1.0288	0.128	8.020	0.000	0.777	1.281
<b>AST</b>	0.0884	0.054	1.633	0.103	-0.018	0.195
<b>STL</b>	1.3464	0.221	6.100	0.000	0.913	1.780
<b>BLK</b>	3.7348	0.154	24.179	0.000	3.431	4.038

<b>Omnibus:</b>	110.206	<b>Durbin-Watson:</b>	1.716
<b>Prob(Omnibus):</b>	0.000	<b>Jarque-Bera (JB):</b>	314.747
<b>Skew:</b>	1.100	<b>Prob(JB):</b>	4.50e-69
<b>Kurtosis:</b>	6.321	<b>Cond. No.</b>	9.70

- ▶ Higher (Adj.) R-squared is normally better
- ▶ What does it mean?

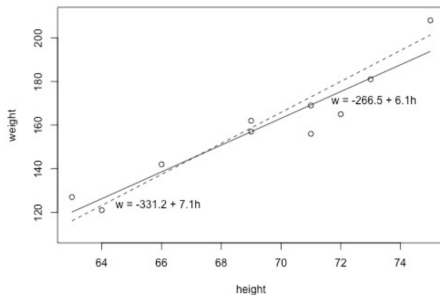


# Statistics

- ▶ Understanding the R-squared measure
- ▶ Understanding how to improve the model
  - ▶ Selecting correct features
- ▶ Following material is based on  
<https://onlinecourses.science.psu.edu/stat501/>
  - ▶ For better understanding, please follow further the online material

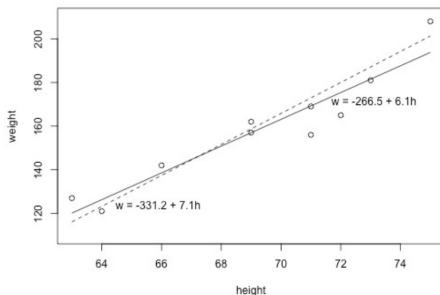
# Choosing the Best Line

- ▶ Looking for correlation between Height and Weight



# Choosing the Best Line

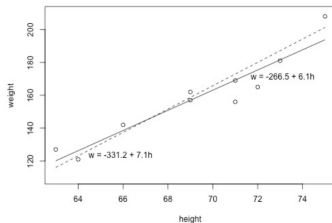
- ▶ Looking for correlation between Height and Weight



- ▶ Some notation
  - ▶  $y_i$  - observed response for instance  $i$
  - ▶  $x_i$  - predictor value for instance  $i$
  - ▶  $\hat{y}_i$  - predicted response for instance  $i$
  - ▶  $\hat{y}_i = b_0 + b_1x_i$  - linear formula

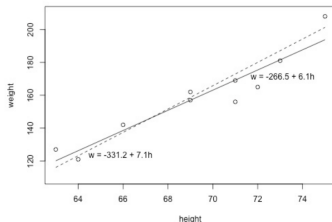
# Least Square Error

- For each instance, the residual error is  $e_i = y_i - \hat{y}_i$



# Least Square Error

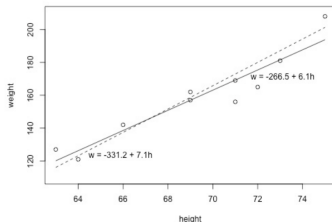
- ▶ For each instance, the residual error is  $e_i = y_i - \hat{y}_i$



- ▶ Least square error - find  $b_0$  and  $b_1$  which minimize
  - ▶  $\sum_{i=0}^n e_i^2$

# Least Square Error

- ▶ For each instance, the residual error is  $e_i = y_i - \hat{y}_i$



- ▶ Least square error - find  $b_0$  and  $b_1$  which minimize
  - ▶  $\sum_{i=0}^n e_i^2$
- ▶ Assuming we have:
  - ▶ dashed -  $\sum_{i=0}^n e_i^2 = 766$
  - ▶ solid -  $\sum_{i=0}^n e_i^2 = 597$
- ▶ Which line is better?

# Correlation

- ▶ Assume we've found the best line, can we now safely predict values?

# Correlation

- ▶ Assume we've found the best line, can we now safely predict values?
  - ▶ We don't know if our sample match the population (later)
  - ▶ We don't know if there is a correlation between the dependent and the independent variables at all

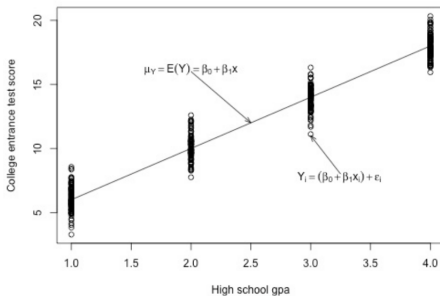


## Population Regression Line

- ▶ To know if our regression line is accurate, we can compare it against the “population” regression line

# Population Regression Line

- ▶ To know if our regression line is accurate, we can compare it against the “population” regression line



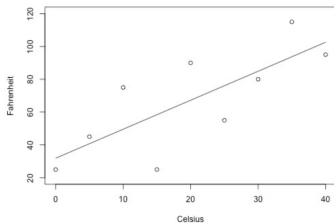
- ▶  $\mu_Y$  - the mean of the dependent variable for the whole population
- ▶ Each sample has an error  $\epsilon_i$
- ▶ We can see the errors  $\epsilon_i$  have equal variance ( $\sigma^2$ )

# Correlation in Population and Variance

- Assume we are comparing two thermometers

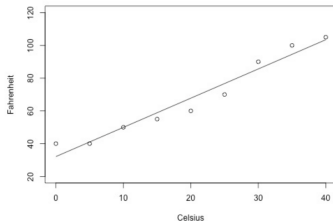
---

Thermometer A



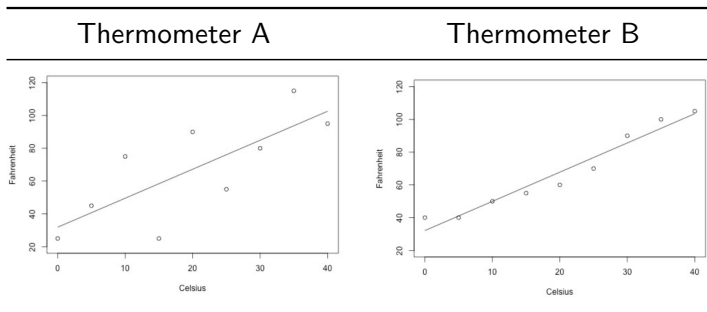
---

Thermometer B



# Correlation in Population and Variance

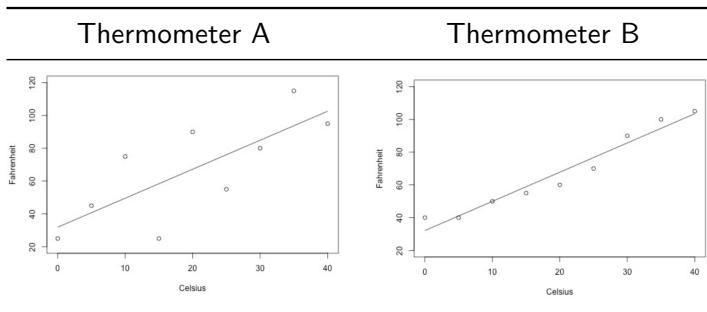
- Assume we are comparing two thermometers



- We know that  $\sigma^2 = 0$  in this case, which one is more precise?

# Correlation in Population and Variance

- Assume we are comparing two thermometers



- We know that  $\sigma^2 = 0$  in this case, which one is more precise?
- But if we didn't know  $\sigma^2 = 0$ ?

# Estimating the Variance

- ▶ In order to compute the variance, we need to take into account the whole population
  - ▶ Normally it is impossible, what can we do?

# Estimating the Variance

- ▶ In order to compute the variance, we need to take into account the whole population
  - ▶ Normally it is impossible, what can we do?
- ▶ We can estimate the variance
  - ▶  $s^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1}$ 
    - ▶  $n$  - number of samples
    - ▶  $y_i$  - response of sample  $i$
    - ▶  $\bar{y}$  - estimated mean

# Estimating the Variance

- ▶ In order to compute the variance, we need to take into account the whole population
  - ▶ Normally it is impossible, what can we do?
- ▶ We can estimate the variance
  - ▶  $s^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1}$ 
    - ▶  $n$  - number of samples
    - ▶  $y_i$  - response of sample  $i$
    - ▶  $\bar{y}$  - estimated mean
- ▶ Why  $n - 1$ ?



# Estimating the Variance

- ▶ In order to compute the variance, we need to take into account the whole population
  - ▶ Normally it is impossible, what can we do?
- ▶ We can estimate the variance
  - ▶  $s^2 = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-1}$ 
    - ▶  $n$  - number of samples
    - ▶  $y_i$  - response of sample  $i$
    - ▶  $\bar{y}$  - estimated mean
- ▶ Why  $n - 1$ ?
  - ▶ Since we only estimated the mean, we lose 1 “degree of freedom” and increase the variance

# Mean Square Error

- ▶ How can we estimate the mean -  $\bar{y}$ ?

# Mean Square Error

- ▶ How can we estimate the mean -  $\bar{y}$ ?
- ▶ We can estimate the mean for the set of responses for  $x_i$  using our model
  - ▶  $\hat{y}_i = b_0 + b_1 x_i$

# Mean Square Error

- ▶ How can we estimate the mean -  $\bar{y}$ ?
- ▶ We can estimate the mean for the set of responses for  $x_i$  using our model
  - ▶  $\hat{y}_i = b_0 + b_1 x_i$
- ▶ The estimated variance is
  - ▶  $MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-2}$

# Mean Square Error

- ▶ How can we estimate the mean -  $\bar{y}$ ?
- ▶ We can estimate the mean for the set of responses for  $x_i$  using our model
  - ▶  $\hat{y}_i = b_0 + b_1 x_i$
- ▶ The estimated variance is
  - ▶  $MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-2}$
- ▶ Why  $n - 2$ ?

# Mean Square Error

- ▶ How can we estimate the mean -  $\bar{y}$ ?
- ▶ We can estimate the mean for the set of responses for  $x_i$  using our model
  - ▶  $\hat{y}_i = b_0 + b_1 x_i$
- ▶ The estimated variance is
  - ▶  $MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-2}$
- ▶ Why  $n - 2$ ?
  - ▶ We are estimating two values now,  $b_0$  and  $b_1$

## Correlation Between Variables

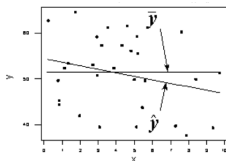
- ▶ How can we check if our model capture a possible correlation between the variables?
  - ▶ We check if it explains the variance in the sample

# Correlation Between Variables

- ▶ How can we check if our model capture a possible correlation between the variables?
  - ▶ We check if it explains the variance in the sample
- ▶ Below there are two examples containing a regression function, which one can be useful for prediction?

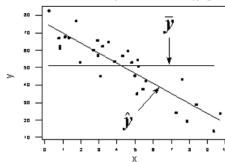
---

Example A



---

Example B



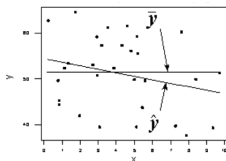


# Correlation Between Variables

- ▶ How can we check if our model capture a possible correlation between the variables?
  - ▶ We check if it explains the variance in the sample
- ▶ Below there are two examples containing a regression function, which one can be useful for prediction?

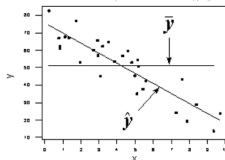
---

Example A



---

Example B



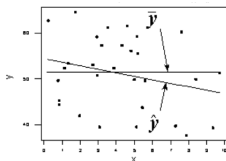
- 
- ▶ How can we determine that it is useful?

# Correlation Between Variables

- ▶ How can we check if our model capture a possible correlation between the variables?
  - ▶ We check if it explains the variance in the sample
- ▶ Below there are two examples containing a regression function, which one can be useful for prediction?

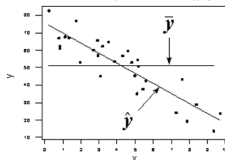
---

Example A



---

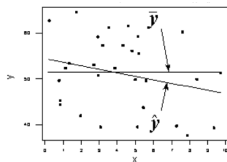
Example B



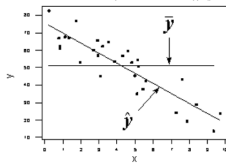
- 
- ▶ How can we determine that it is useful?
    - ▶ We compare it against another model

# The Null Model

Example A



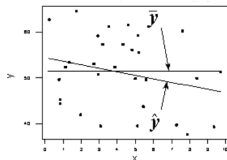
Example B



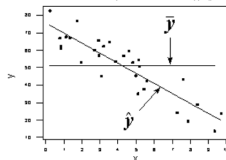
- ▶ In the above examples, we compare both functions against a constant model
  - ▶ Such a model is called the null model and it always predict  $\hat{y}_i = \bar{y}$

# R-squared

Example A



Example B



- ▶ We can now compute for each example and model the following three values

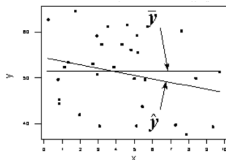
- ▶  $SSR = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{n-2}$

- ▶  $MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-2}$

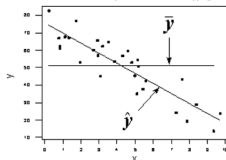
- ▶  $Tot = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-2}$

# R-squared

Example A



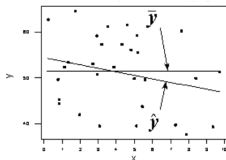
Example B



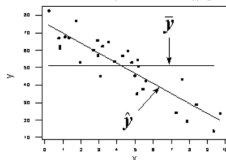
- ▶ We can now compute for each example and model the following three values
  - ▶  $SSR = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{n-2}$
  - ▶  $MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-2}$
  - ▶  $Tot = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-2}$
- ▶  $SSR_A = 12, MSE_A = 170, Tot_A = 182$

# R-squared

Example A



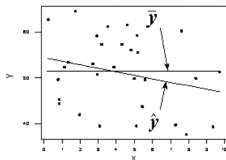
Example B



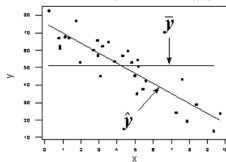
- ▶ We can now compute for each example and model the following three values
  - ▶  $SSR = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{n-2}$
  - ▶  $MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n-2}$
  - ▶  $Tot = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{n-2}$
- ▶  $SSR_A = 12, MSE_A = 170, Tot_A = 182$
- ▶  $SSR_B = 670, MSE_B = 170, Tot_B = 840$

# R-squared

Example A



Example B



- ▶  $SSR_A = 12$ ,  $MSE_A = 170$ ,  $Tot_A = 182$
- ▶  $SSR_B = 670$ ,  $MSE_B = 170$ ,  $Tot_B = 840$
- ▶ We can now define *R – squared*

$$\text{▶ } R - \text{squared} = \frac{SSR}{Tot} = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

# R-squared and Pearson Correlation Coefficient

- ▶ Remember that Pearson correlation coefficient is denoted by  $R$
- ▶ What is the relationship between  $R$  and  $R - squared$ ?



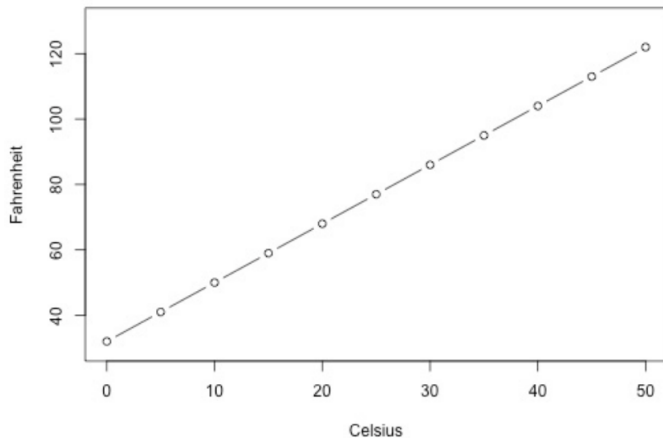
# R-squared and Pearson Correlation Coefficient

- ▶ Remember that Pearson correlation coefficient is denoted by  $R$
- ▶ What is the relationship between  $R$  and  $R - \text{squared}$ ?
- ▶ Couldn't we just square  $R$  then?

# R-squared and Pearson Correlation Coefficient

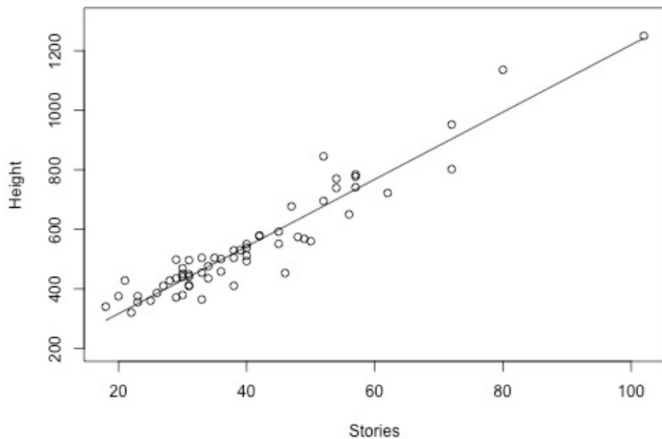
- ▶ Remember that Pearson correlation coefficient is denoted by  $R$
- ▶ What is the relationship between  $R$  and  $R - squared$ ?
- ▶ Couldn't we just square  $R$  then?
  - ▶ Only for simple regression functions

## Examples



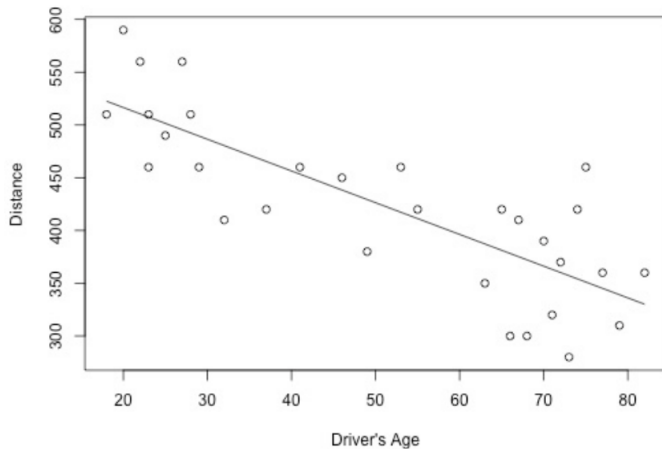
- Can you estimate R-squared? R?

# Examples



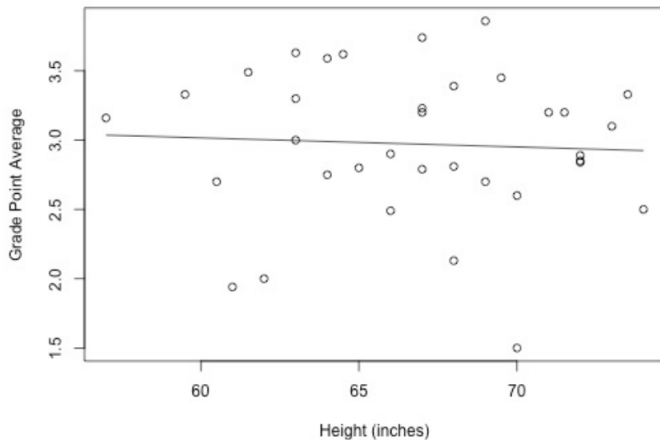
- Can you estimate R-squared? R?

# Examples



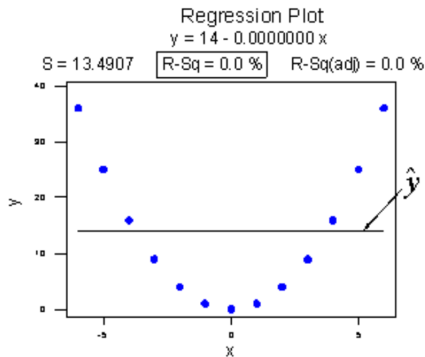
- Can you estimate R-squared? R?

## Examples



- Can you estimate R-squared? R?

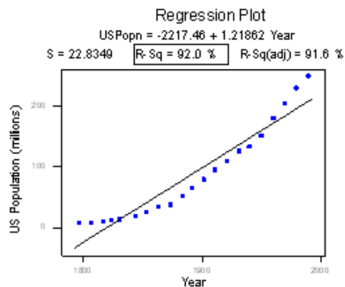
# R-squared Warnings



Pearson correlation of x and y = 0.000

- R-squared relates to linear relationship

# R-squared Warnings

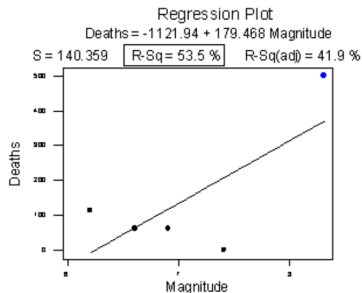


Pearson correlation of Year and USPopn = 0.959

- There might be a better function



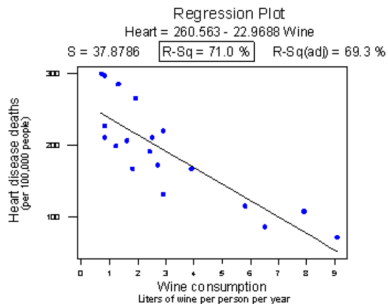
# R-squared Warnings



Pearson correlation of Deaths and Magnitude = 0.732

- Sensitive to outliers

# R-squared Warnings



Pearson correlation of Wine and Heart = -0.843

- Correlation does not imply causation

# Hypothesis Test for the Population Correlation Coefficient

- ▶ All our computations so far were based on sample data
- ▶ How can we generalize our observations to the whole population?

# Hypothesis Test for the Population Correlation Coefficient

- ▶ All our computations so far were based on sample data
- ▶ How can we generalize our observations to the whole population?
- ▶ We test our hypothesis that our data behaves in a certain way

# Criminal Trial Analogy

- ▶ Null hypothesis ( $H_0$ ) - Defendant is not guilty
- ▶ Alternative hypothesis ( $H_1$ ) - Defendant is guilty

# Criminal Trial Analogy

- ▶ Null hypothesis ( $H_0$ ) - Defendant is not guilty
- ▶ Alternative hypothesis ( $H_1$ ) - Defendant is guilty
- ▶ Jury uses evidence (sample data) to make a decision
  - ▶ If there is sufficient evidence to refute the assumption of innocence, they deem the defendant as guilty (they reject the null hypothesis)
  - ▶ If there is insufficient evidence, they do not reject the null evidence and the defendant is deemed innocent

# Test Statistic and P-values

- ▶ How do we make decision?
  - ▶ We obtain the evidence (sample data) as a value denoting the behavior of the data
    - ▶ This value is called the **test statistic**
  - ▶ We check the probability of the test statistic to be this value given the null hypothesis
    - ▶ This is the **P-value**
  - ▶ If it is very low, we reject the null hypothesis and accept the alternative one

# Hypothesis Test for the Population Correlation Coefficient

- ▶ When testing for population correlation
  - ▶ Test statistic:  $t^* = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}}$
  - ▶ Null hypothesis: there is no correlation
  - ▶ Alternative hypothesis: there is some correlation
  - ▶ Compute the probability (P-value) that we have  $t^*$  given the null hypothesis
  - ▶ If the P-value is sufficiently small, reject the null hypothesis



# Hypothesis Test for the Population Correlation Coefficient

- Our dependent variable is total rebounds

	coef	std err	t	P> t	[0.025	0.975]
<b>Intercept</b>	1.0288	0.128	8.020	0.000	0.777	1.281
<b>AST</b>	0.0884	0.054	1.633	0.103	-0.018	0.195
<b>STL</b>	1.3464	0.221	6.100	0.000	0.913	1.780
<b>BLK</b>	3.7348	0.154	24.179	0.000	3.431	4.038

# Adjusted R-squared in Multiple Linear Regression

- ▶ For every additional feature added to the model, the R-squared increases
  - ▶ Our model can never explain less variance
- ▶ In addition, having more features increases the chance of over-fitting

# Adjusted R-squared in Multiple Linear Regression

- ▶ For every additional feature added to the model, the R-squared increases
  - ▶ Our model can never explain less variance
- ▶ In addition, having more features increases the chance of over-fitting
- ▶ Adjusted R-squared takes the number of used features into account
  - ▶  $R_{adj}^2 = 1 - (\frac{n-1}{n-p})(1 - R^2)$

# Having “Wrong” Predictors

- ▶ By including features which do not improve our model we incur several issues
  - ▶ We reduce the degree of freedom, which increases the estimated variance and lowers the power of our tests
  - ▶ Visualization and understanding are harder
  - ▶ Longer computation time

## Example - IQ and Physical Characteristics

- ▶ Are a person's brain size and body size predictive of his or her intelligence?
- ▶ MLR Model:  $IQ = b_0 + b_1 * Br + b_2 * Hht + b_3 * Wht$

## Example - IQ and Physical Characteristics

- ▶ Are a person's brain size and body size predictive of his or her intelligence?
- ▶ MLR Model:  $IQ = b_0 + b_1 * Br + b_2 * Hht + b_3 * Wht$

Model Summary

S	R-sq	R-sq(adj)
19.7944	29.49%	23.27%

## Example - IQ and Physical Characteristics

- ▶ Are a person's brain size and body size predictive of his or her intelligence?
- ▶ MLR Model:  $IQ = b_0 + b_1 * Br + b_2 * Hht + b_3 * Wht$

### Model Summary

S	R-sq	R-sq(adj)
19.7944	29.49%	23.27%

Term	Coef	SE Coef	T-Value	P-Value
Constant	111.4	63.0	1.77	0.086
Brain	2.060	0.563	3.66	0.001
Height	-2.73	1.23	-2.22	0.033
Weight	0.001	0.197	0.00	0.998