Simple Linear Regression

June 8, 2023

Problem

What is relationship between

- the tar content in the outlet stream in a chemical process is and the inlet temperature
- gas mileage and engine volume
- house price and square footage of living space

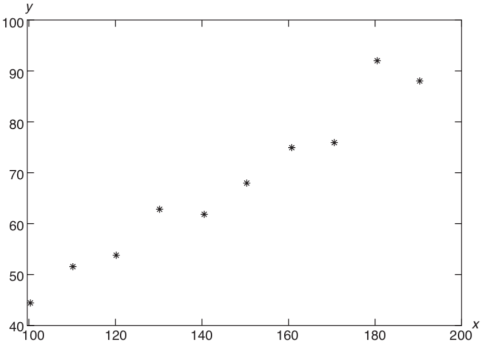
- inlet temperature, engine volume, square feet of living space ... are **independent variable (or regressor)**, x
- Tar content, gas mileage, house price ... are **dependent variable (or response)**, Y

How to find out relationship between regressor and response

Data observation

i	x_i	y_i	i	x_i	y_i
1	100	45	6	150	68
2	110	52	7	160	75
3	120	54	8	170	76
4	130	63	9	180	92
5	140	62	10	190	88

y: the percent yield of a laboratory experiment
x: the temperature at which the experiment



It seems that y is a linear function of x with some noise

Linear relationship

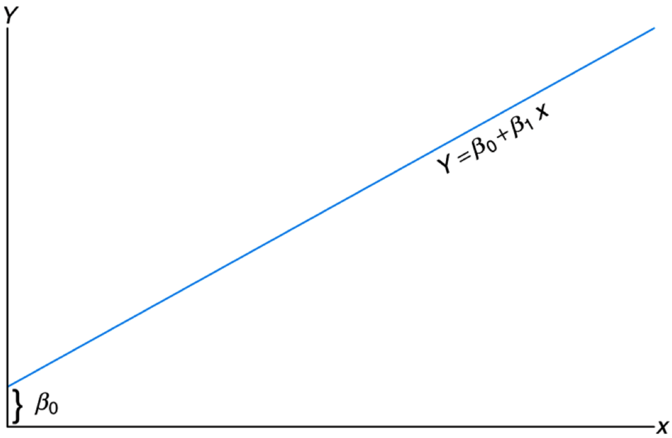


Figure: intercept β_0, slope β_1

However

- run several experiment with the same inlet temperature, tar content wil not be the same
- several automobiles with the same engine will not all have the same gas mileage.
- Houses with the same square footage are sold with different prices

- Response Y is not a determisnistic function of regressor x

$$Y \neq f(x)$$

- But

$$Y = f(x) + \text{ noise}$$

Regression Analysis

- Find the best ”fit” relationship between Y and x
- Qualify the strength of relationship
- Explain impact of x on Y
- Predict Y given some specific value of x

(Simple) Linear regression model

Dependent Variable

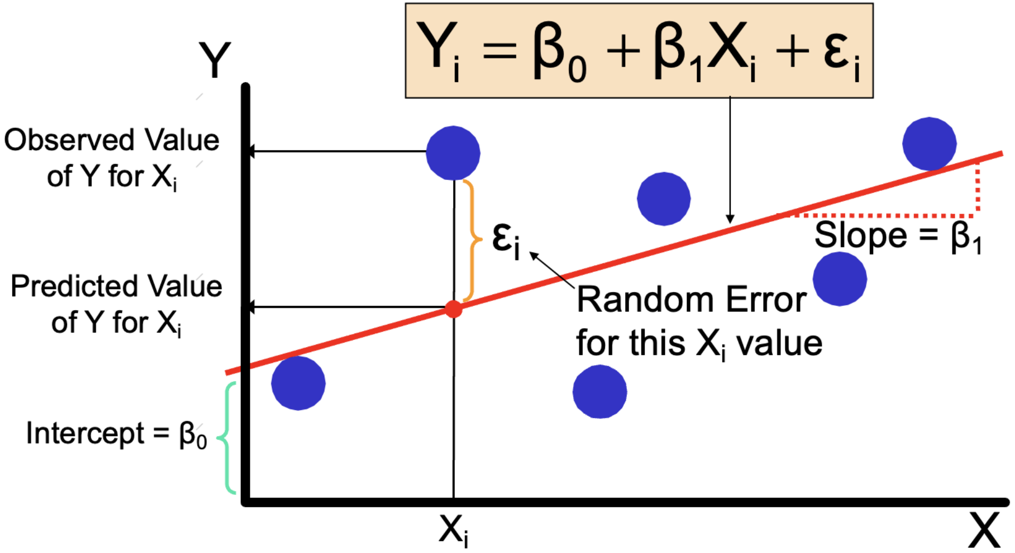
Population Y intercept

Population Slope Coefficient

Independent Variable

Random Error term

$$\boxed{Y_i = \underbrace{\beta_0 + \beta_1 X_i}_{\text{Linear component}} + \underbrace{\varepsilon_i}_{\text{Random Error component}}}$$

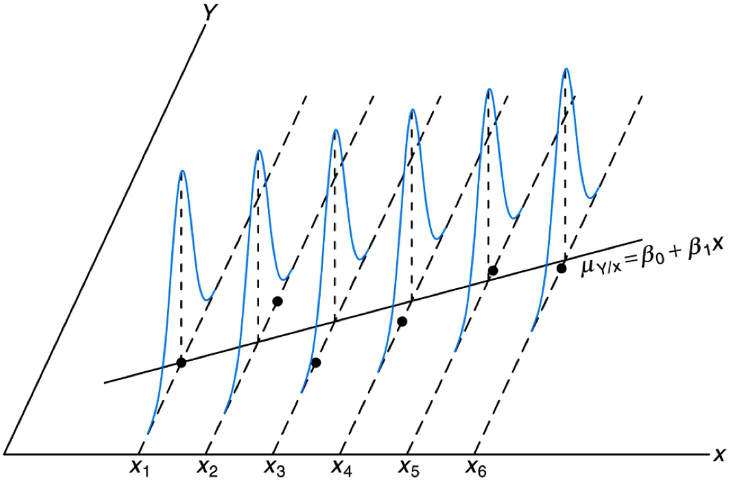


$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$
Y
Observed Value of Y for X_i
ε_i
Predicted Value of Y for X_i
Slope = β_1
Random Error for this X_i value
Intercept = β_0
X_i
X

Model assumption

- Error $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ are i.i.d
- Given x, response Y is normally distributed $\mathcal{N}(\beta_0 + \beta_1 x, \sigma^2)$
- True regression line $\mu_{Y|x} = \beta_0 + \beta_1 x$

The true regression line **go through the means of the response** but actually unknown



Fitted regression line

Estimated (or predicted) y value for observation i

Estimate of the regression intercept

Estimate of the regression slope

Value of x for observation i

$$\hat{y}_i = b_0 + b_1 x_i$$

One can use a fitted regression line to estimate predict or forecast y value given observaton x

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Least square and fitted model

Residual - error in fit

- Given
  - Data set $\{(x_i, y_i), i = 1, \ldots, n\}$
  - Fitted regression line

$$\hat{y}_i = b_0 + b_1 x_i$$

- Residual

$$e_i = y_i - \hat{y}_i$$

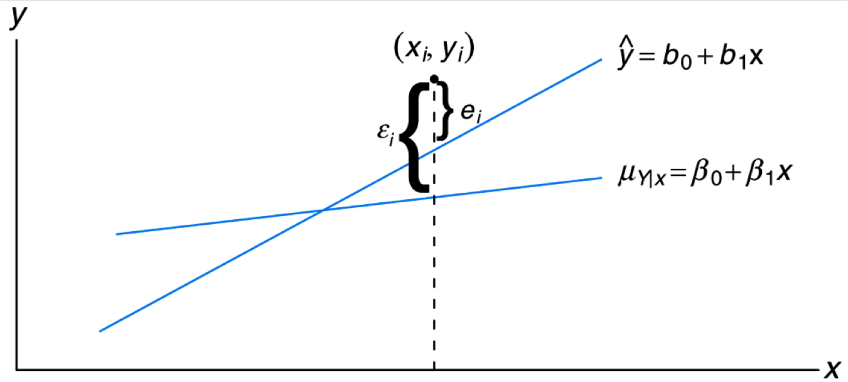
Important relationship

$$
\begin{aligned}
y_i &= b_0 + b_1 x_i + e_i \\
&= \hat{y}_i + e_i
\end{aligned}
$$

In word

actual value = fitted value + residual

Residual vs Error



Residual e_i is observed but error term ϵ_i is unobservable

Remark

- β_0, β_1 are unknown
- true regression line $\mu_{Y|x} = \beta_0 + \beta_1 x$ is then unknown
- **Need to estimate** β_0, β_1 from observed data

Least square method

- Sum of square of residual

$$SSE = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - b_0 - b_1 x_i)^2$$

- Minimize SSE to get estimates b_0, b_1 for β_0 and β_1
- Solve the optimization problem

$$\frac{\partial SSE}{\partial b_0} = 0; \quad \frac{\partial SSE}{\partial b_1} = 0$$

Least square estimators

- $$b_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$
  or equivalent
  $$b_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$
- $b_0 = \bar{Y} - b_1\bar{x}$
  where $\bar{y} = \sum_{i=1}^{n} y_i/n$, $\bar{x} = \sum_{i=1}^{n} x_i/n$

Example

Estimate regression line for raw material data

Relative humidity	46	53	29	61	36	39	47	49	52	38	55	32	57	54	44
Moisture content	12	15	7	17	10	11	11	12	14	9	16	8	18	14	12

Solution

- Independent variable x: relative humidity
- Dependent variable y: moisture content
- $n = 15$

$$\sum x_i = 692 \qquad \sum y_i = 186$$

$$\sum x_i^2 = 33212 \qquad \sum x_i y_i = 8997$$

$$\bar{x} = 46.133 \qquad \bar{y} = 12.4$$

$$b_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$= \frac{15 \times 8997 - 692 \times 186}{15 \times 33212 - 692^2} = 0.323$$

and

$$b_0 = \bar{y} - b_1\bar{x} = 12.4 - 0.232 \times 46.133 = -2.51$$

Fitted line equation

$$\hat{y} = 0.323x - 2.51$$

- b_0: the estimated average value of Y when $x = 0$
- b_1 measures the estimated change in the average value of Y as a result of a one-unit change in x
    - $b_1 = 0.323$: the average value of moisture content increases by 0.323, on average, for each additional one relative humidity

Exercise

Compressive strength x and intrinsic permeability y are related according to a simple linear regression model. Summary quantities of a sample data are $n = 14$, $\sum y_i = 572$, $\sum y_i^2 = 23,530$, $\sum x_i = 43$, $\sum x_i^2 = 157.42$ and $\sum x_i y_i = 1697.80$.

1. Calculate the least squares estimates b_0 and b_1
2. Use the fitted line to predict permeability when the compressive strength $x = 4.3$
3. Suppose that the observed value of permeability at $x = 3.7$ is $y = 46.1$. Calculate the value of the corresponding residual.

Exercise

The following data are chloride concentration x (in milligrams per roadway area in the watershed y (in percentage)

x	4.4	6.6	9.7	10.6	10.8	10.9
y	0.19	0.15	0.57	0.70	0.67	0.63

Fit the linear regression model with least square method.

Linear regression with Excel

Input data → Choose Data → Data Analysis →choose Regression and click Ok → select range for x and Y and click Ok

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	-2.5104577	1.31542339	-1.9084788	0.07865561	-5.3522571	0.33134181	-5.3522571	0.33134181
X Variable 1	0.32320356	0.02795527	11.5614542	3.2619E-08	0.26280988	0.38359725	0.26280988	0.38359725

Figure: Estimate parameter result in report

Practice

Estimate the regression line for pollution data

Solids Reduction, x (%)	Oxygen Demand Reduction, y (%)	Solids Reduction, x (%)	Oxygen Demand Reduction, y (%)
3	5	36	34
7	11	37	36
11	21	38	38
15	16	39	37
18	16	39	36
27	28	39	45
29	27	40	39
30	25	41	41
30	35	42	40
31	30	42	44
31	40	43	37
32	32	44	44
33	34	45	46
33	32	46	46

A Measure of Quality of Fit: Coefficient of Determination

Coefficient of Determination

the proportion of variability explained by the fitted model

$$R^2 = 1 - \frac{SSE}{SSR}$$

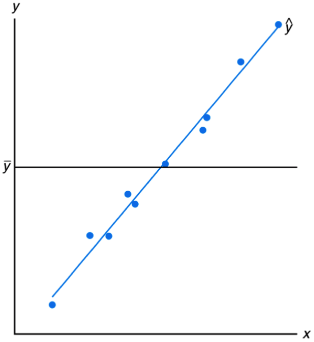
- $SSE = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$: error sum of squares
- $SSR = \sum_{i=1}^{n}(y_i - \bar{y})^2$: total corrected sum of squares

Meaning

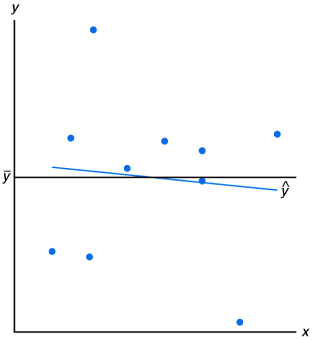
R^2 expresses the proportion of the total variation in the values of the variable Y that can be accounted for or explained by a linear relationship with the values of the random variable X

Good fit vs Poor fit

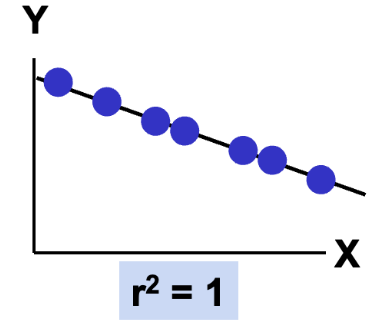
$$0 \leq R^2 \leq 1$$

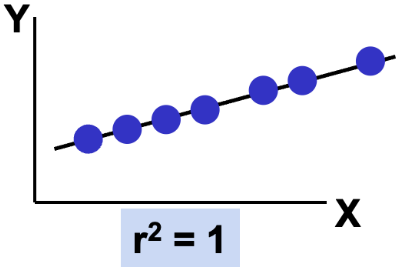


(a) $R^2 \approx 1.0$



(b) $R^2 \approx 0$

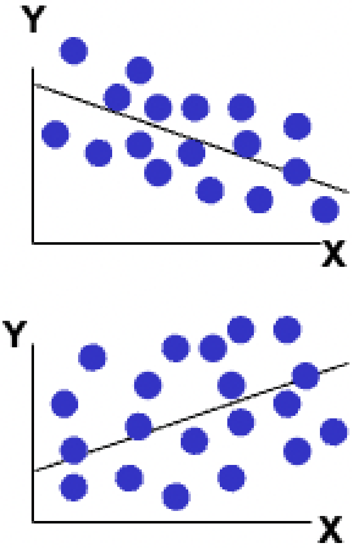




$r^2 = 1$

Perfect linear relationship between X and Y:

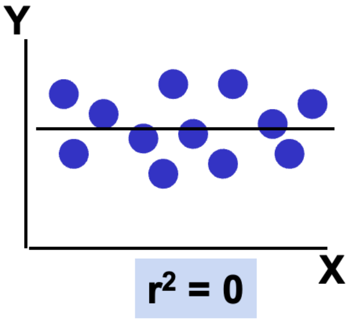
100% of the variation in Y is explained by variation in X



$0 < r^2 < 1$

Weaker linear relationships between X and Y:

Some but not all of the variation in Y is explained by variation in X



$r^2 = 0$

No linear relationship between X and Y:

The value of Y does not depend on X. (None of the variation in Y is explained by variation in X)

Compute R - square

Relative humidity	46	53	29	61	36	39	47	49	52	38	55	32	57	54	44
Moisture content	12	15	7	17	10	11	11	12	14	9	16	8	18	14	12

- Fitted regression line

$$\hat{y} = -2.51 + 0.323x$$

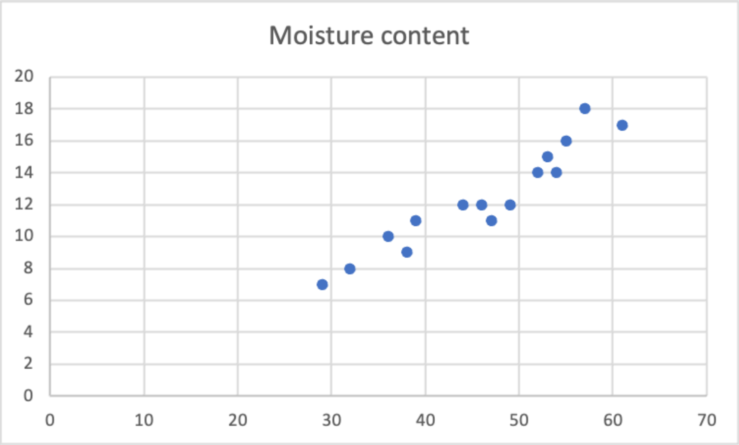
- $\bar{y} = 12.4$

x	$\hat{y}$	y	$y - \hat{y}$	$y - \bar{y}$
46	-2.51 + (0.323)(46) =12.348	12	12 - 12.348 = - 0.348	12 - 12.4 -0.4
53	14.609	15	0.391	2.6
...				

- $SSE = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = 13.08$
- $SSR = \sum_{i=1}^{n}(y_i - \bar{y})^2 = 147.6$
- $$R^2 = 1 - \frac{SSE}{SSR} = 1 - \frac{13.08}{147.8} = 0.911$$

Comment

- The coefficient of determination suggests that the model fit to the data explains 91.1% of the variability observed in the response.
- $R^2 \approx 1$ indicates that linear model is a good fit model
- It is reasonable to use this model to estimate or predict moisture content given a value of relative humidity


Moisture content
20
18
16
14
12
10
8
6
4
2
0
0
10
20
30
40
50
60
70

Excel Report

SUMMARY OUTPUT	
Regression Statistics	
Multiple R	0.95465385
R Square	0.91136397
Adjusted R S	0.90454582
Standard Err	1.00317487
Observations	15

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	134.517322	134.517322	133.667224	3.26188E-08
Residual	13	13.0826776	1.00635981		
Total	14	147.6			

	Coefficients	*Standard Erroi*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-2.5104577	1.31542339	-1.9084788	0.07865561	-5.352257109	0.33134181	-5.3522571	0.33134181
Relative hun	0.32320356	0.02795527	11.5614542	3.2619E-08	0.262809875	0.38359725	0.26280988	0.38359725