Regression analysis
Two variables

(Montgomery and Runger: ch 11
Brani Vidakovic: ch 14)

Reminder

Covariance Defined

Covariance is a number qunatifying average dependence between two random variables.

The covariance between the random variables X and Y, denoted as $\operatorname{cov}(X,Y)$ or σ_{XY} is

$$\sigma_{XY} = E\left[(X-\mu_X)(Y-\mu_Y)\right] = E(XY) - \mu_X\mu_Y \qquad (5\text{-}14)$$

The units of σ_{XY} are units of X times units of Y.

Unlike the range of variance, $-\infty < \sigma_{XY} < \infty$.

Correlation is "normalized covariance"

- Also called:
  Pearson correlation coefficient

  $\rho_{XY} = \sigma_{XY} / \sigma_X \sigma_Y$
  is the covariance normalized to be $-1 \leq \rho_{XY} \leq 1$

Karl Pearson (1852– 1936)
English mathematician and biostatistician

Covariance and Scatter Patterns

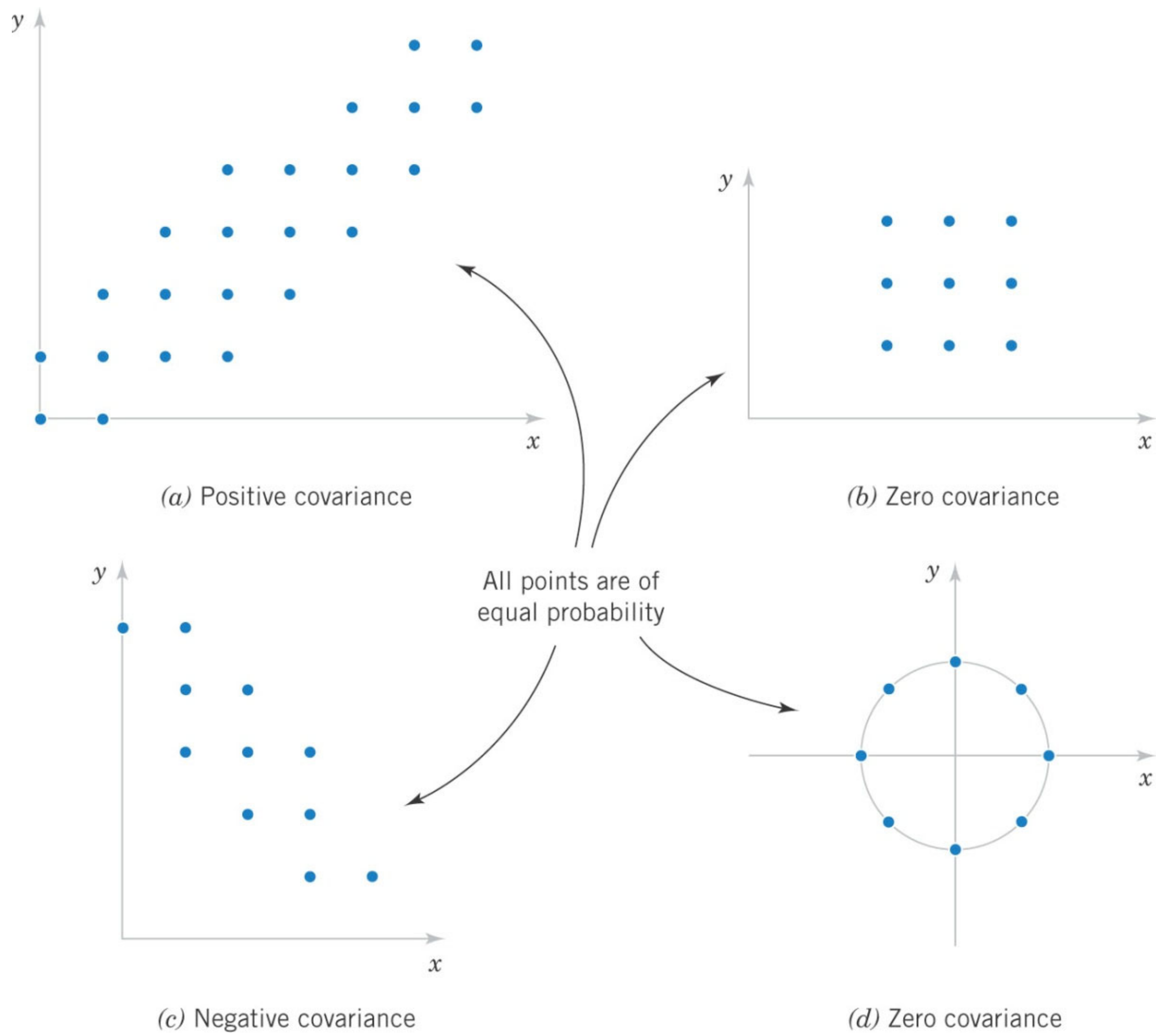


Figure 5-13 Joint probability distributions and the sign of cov(X, Y). Note that covariance is a measure of linear relationship. Variables with non-zero covariance are correlated.

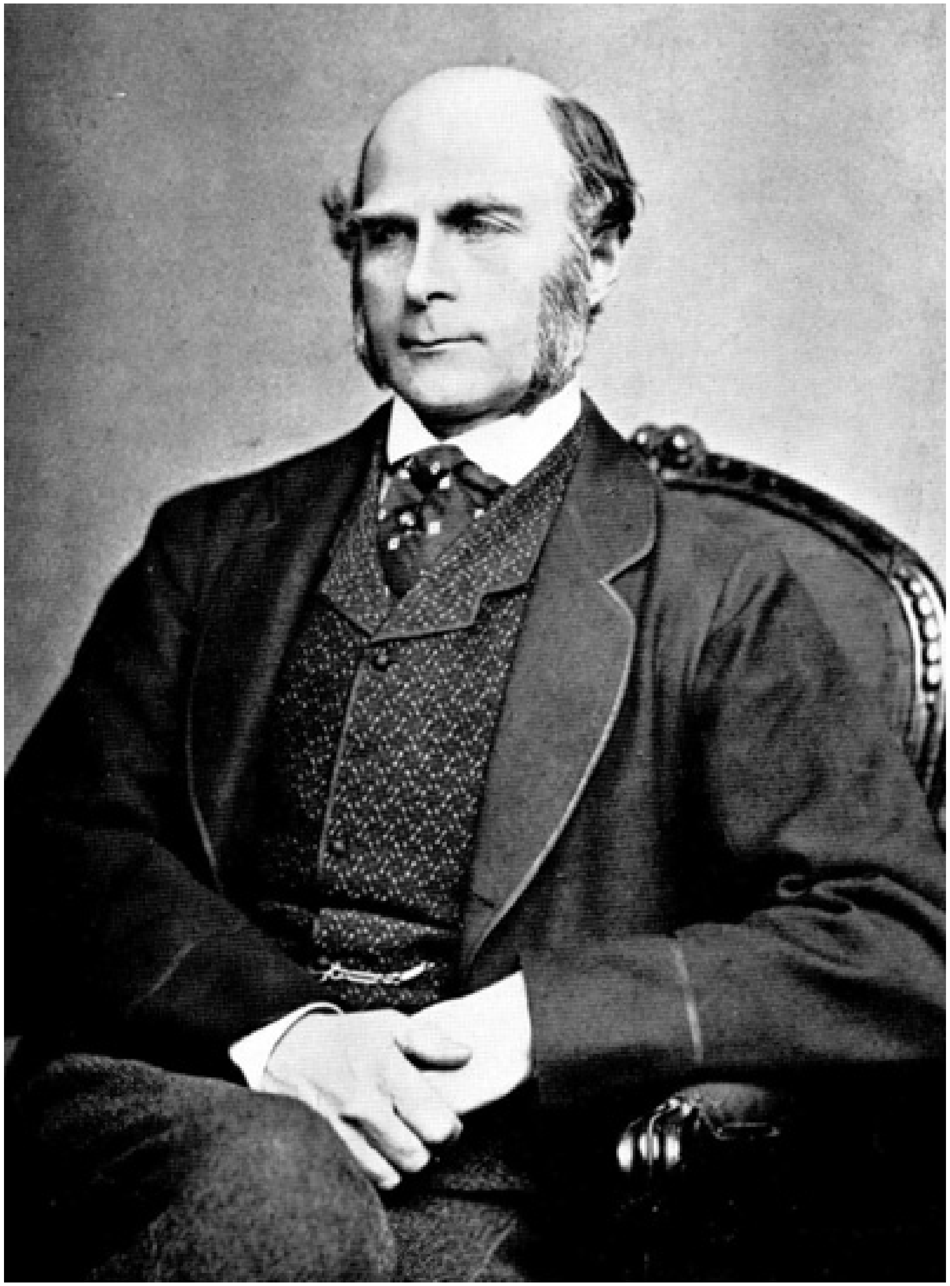
Regression analysis

- Many problems in engineering and science involve sample in which two or more variables were measured. They may not be independent from each other and one (or several) of them can be used to predict another

- Everyday example: in most samples height and weight of people are related to each other

- Biological example: in a cell sorting experiment the copy number of a protein may be measured alongside its volume

- Regression analysis uses a sample to build a model to predict protein copy number given a cell volume

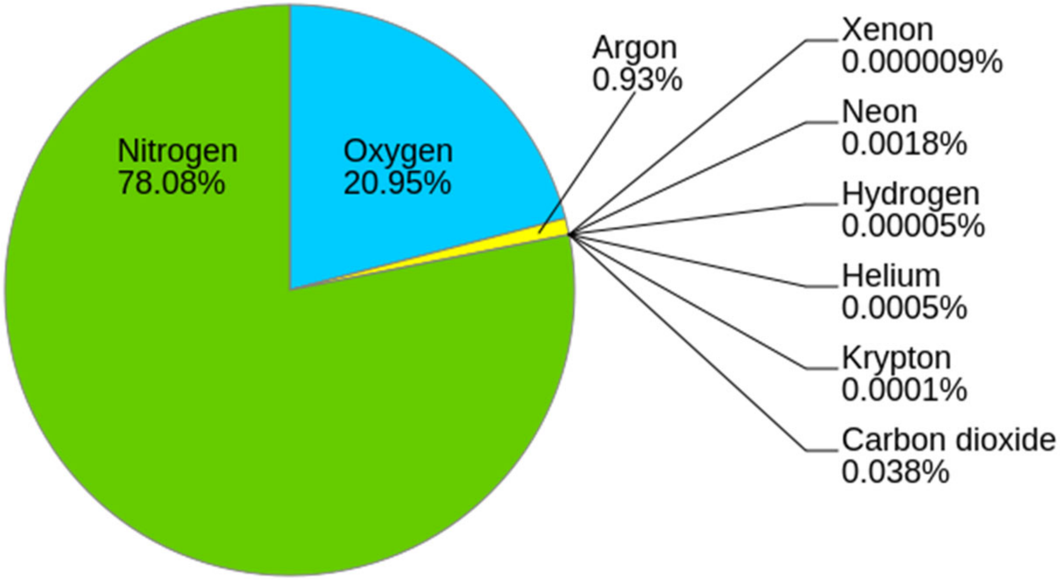


Sir Francis Galton,
(1822 -1911) was an English statistician, anthropologist, proto-geneticist, psychometrician, eugenicist, ("Nature vs Nurture", inheritance of intelligence), tropical explorer, geographer, inventor (Galton Whistle to test hearing), meteorologist (weather map, anticyclone).

Invented both correlation and regression analysis when studied heights of fathers and sons

Found that fathers with height above average tend to have sons with height also above average but closer to the average.
Hence "regression" to the mean

Two variable samples



- Oxygen can be distilled from the air
- Hydrocarbons need to be filtered out or the whole thing would go kaboom!!!
- When more hydrocarbons were removed, the remaining oxygen stays cleaner
- Except we don't know how dirty was the air to begin with

Table 11-1 Oxygen and Hydrocarbon Levels

Observation Number	Hydrocarbon Level x (%)	Purity y (%)
1	0.99	90.01
2	1.02	89.05
3	1.15	91.43
4	1.29	93.74
5	1.46	96.73
6	1.36	94.45
7	0.87	87.59
8	1.23	91.77
9	1.55	99.42
10	1.40	93.65
11	1.19	93.54
12	1.15	92.52
13	0.98	90.56
14	1.01	89.54
15	1.11	89.85
16	1.20	90.39
17	1.26	93.25
18	1.32	93.41
19	1.43	94.98
20	0.95	87.33

$$Y = \beta_0 + \beta_1 X + \epsilon$$

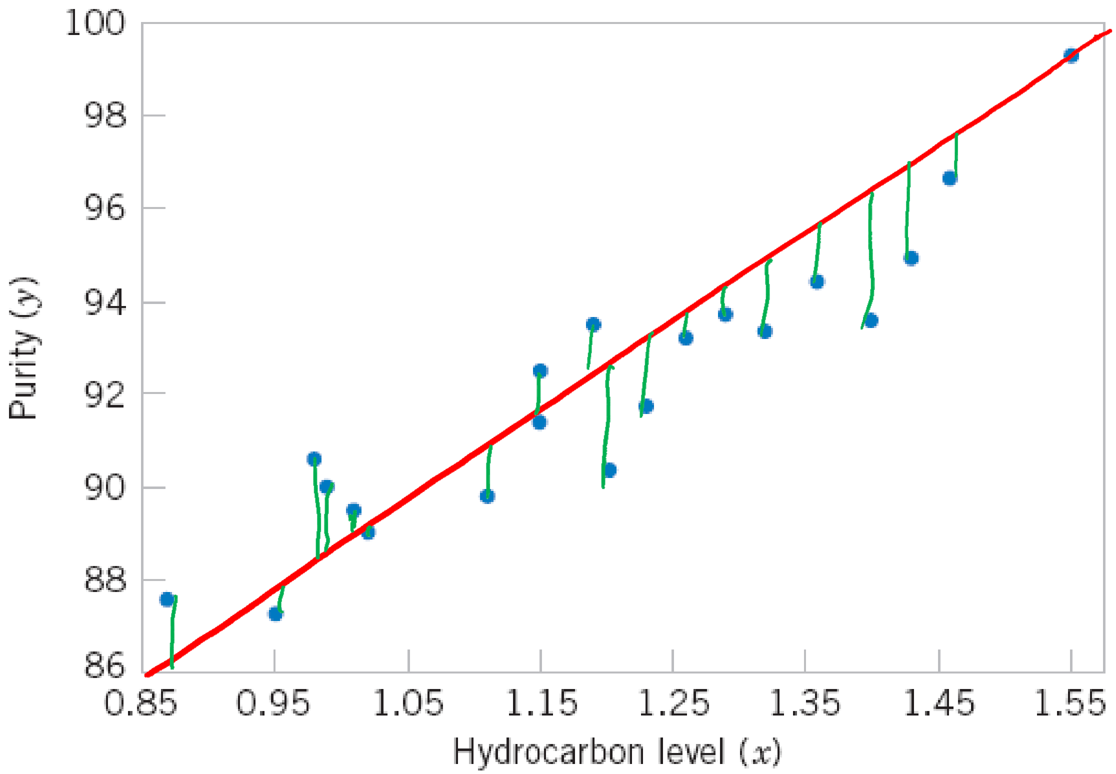


Figure 11-1 Scatter diagram of oxygen purity versus hydrocarbon level from Table 11-1.

$$Y = 75 + 15 \cdot X + \epsilon$$

Linear regression

The **simple linear regression model** is given by

$$Y = \beta_0 + \beta_1 X + \mathrm{E} = \hat{Y} + \mathrm{E}$$

E is the **random error**

slope β_1 and intercept β_0 of the line are called **regression coefficients**

Note: Y , $\hat{Y}$, X and E are random variables

Let's assume that E(E| x)=0 →
E(Y| x) =$\beta_0 + \beta_1 x$ + E(E| x) =$\beta_0 + \beta_1 x$

$Y = \beta_0 + \beta_1 X + \epsilon \; ; \quad E(\epsilon \mid x) = 0 \quad \forall x$

How does one find β_0 & β_1?

$$Cov(Y, X) = Cov((\beta_0 + \beta_1 X + \epsilon), X) =$$

$$= \cancel{Cov(\beta_0, X)} + \beta_1 Cov(X, X) + \cancel{Cov(\epsilon, X)}$$

$Cov(\beta_0, X) = 0$ since β_0 is constant

$$Cov(X, X) = E(X^2) - E(X)^2 = Var(X)$$

$$Cov(\epsilon, X) = E(\epsilon \cdot X) - E\cancel{(\epsilon)} \cdot E(X) =$$

$$= E(\epsilon \cdot X) = \sum_{\text{all } x} x \cdot E\cancel{(\epsilon \mid x)} = 0$$

Thus $\boxed{\beta_1 = \frac{Cov(X, Y)}{Var(X)}}$, $\boxed{\beta_0 = E(Y) - \beta_1 E(X)}$

Method of least squares

- The **method of least squares** is used to estimate the parameters, β_0 and β_1 by minimizing the sum of the squares of the vertical deviations in Figure 11-3.

Figure 11-3 Deviations of the data from the estimated regression model.

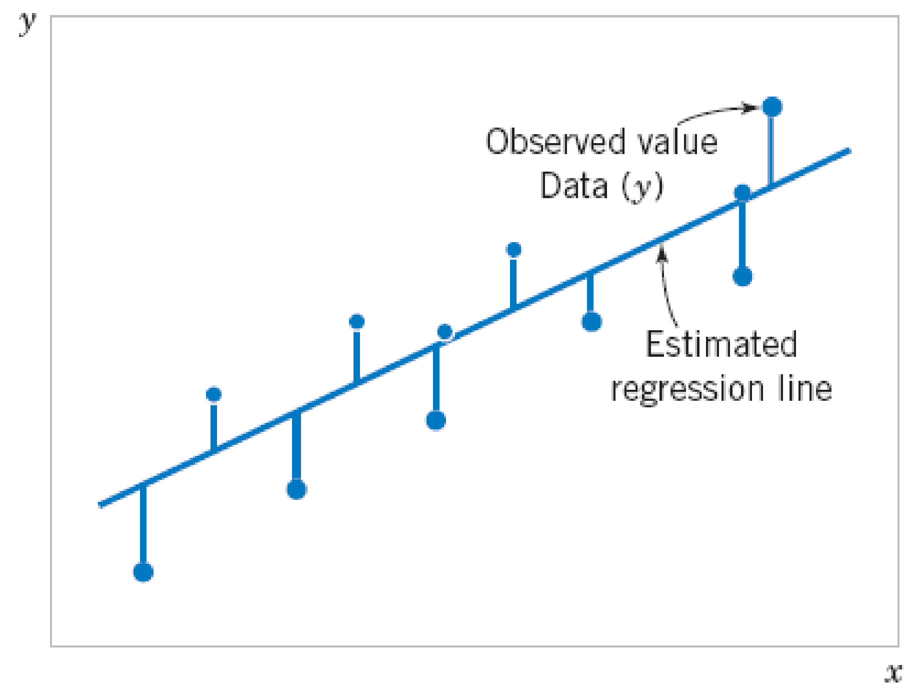


Figure 11-3 Deviations of the data from the estimated regression model.

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \qquad i = 1, 2, \ldots, n \tag{11-3}$$

and the sum of the squares of the deviations of the observations from the true regression line is

$$L = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 \tag{11-4}$$

The least squares estimators of β_0 and β_1, say, $\hat{\beta}_0$ and $\hat{\beta}_1$, must satisfy

$$\left.\frac{\partial L}{\partial \beta_0}\right|_{\hat{\beta}_0, \hat{\beta}_1} = -2 \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) = 0$$

$$\left.\frac{\partial L}{\partial \beta_1}\right|_{\hat{\beta}_0, \hat{\beta}_1} = -2 \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) x_i = 0 \tag{11-5}$$

$$\hat{\beta}_0 \sum x_i = -\hat{\beta}_1 \frac{(\sum x_i)^2}{n}$$

$$n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$\hat{\beta}_0 \sum_{i=1}^{n} x_i + \hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i \tag{11-6}$$

$$+ \frac{\sum y_i \sum x_i}{n}$$

Traditional notation

Definition

The **least squares estimates** of the intercept and slope in the simple linear regression model are

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \tag{11-7}$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} y_i x_i - \frac{\left(\sum_{i=1}^{n} y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n}}{\sum_{i=1}^{n} x_i^2 - \frac{\left(\sum_{i=1}^{n} x_i\right)^2}{n}} = \frac{S_{xy}}{S_{xx}} \tag{11-8}$$

where $\bar{y} = (1/n)\sum_{i=1}^{n} y_i$ and $\bar{x} = (1/n)\sum_{i=1}^{n} x_i$.

11-2: Simple Linear Regression

Definition

The **least squares estimates** of the intercept and slope in the simple linear regression model are

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \tag{11-7}$$

$$\hat{\beta}_1 = \frac{\dfrac{\sum_{i=1}^{n} y_i x_i}{n} - \dfrac{\left(\sum_{i=1}^{n} y_i\right)\left(\sum_{i=1}^{n} x_i\right)}{n^2}}{\dfrac{\sum_{i=1}^{n} x_i^2}{n} - \dfrac{\left(\sum_{i=1}^{n} x_i\right)^2}{n^2}} = \frac{Cov(X, Y)}{Var(X)} \tag{11-8}$$

where $\bar{y} = (1/n)\sum_{i=1}^{n} y_i$ and $\bar{x} = (1/n)\sum_{i=1}^{n} x_i$.

11-4: Hypothesis Tests in Simple Linear Regression

11-4.2 Analysis of Variance Approach to Test Significance of Regression

The analysis of variance identity is

$$\sum_{i=1}^{n}(y_i - \bar{y})^2 = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2 + \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \qquad (11\text{-}24)$$

Symbolically,

$$SS_T = SS_R + SS_E \qquad (11\text{-}25)$$

11-7: Adequacy of the Regression Model

11-7.2 Coefficient of Determination (R^2)

VERY COMMONLY USED

- The quantity

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

is called the **coefficient of determination** and is often used to judge the adequacy of a regression model.

- $0 \le R^2 \le 1$;
- We often refer (loosely) to R^2 as the amount of variability in the data explained or accounted for by the regression model.

Adjusted R-Squared

- Adjusted R-Squared uses unbiased estimates of σ_ε^2 and σ_Y^2:

$$= 1 - \frac{\sigma_\varepsilon^2}{s_Y^2} = 1 - \frac{\frac{SS_E}{n-2}}{\frac{SS_T}{n-1}}$$

- For small samples it is different from the regular R-Squared: $R^2 = 1 - \frac{SS_E}{SS_T}$

11-7: Adequacy of the Regression Model

11-7.2 Coefficient of Determination (R^2)

- For the oxygen purity regression model,

$$
\begin{aligned}
R^2 &= SS_R/SS_T \\
&= 152.13/173.38 \\
&= 0.877
\end{aligned}
$$

- Thus, the model accounts for 87.7% of the variability in the data.

11-2: Simple Linear Regression

Estimating σ_ε^2

An **unbiased estimator** of σ_ε^2 is

$$\hat{\sigma}_\varepsilon^2 = \frac{SS_E}{n-2} \qquad (11\text{-}13)$$

where SS_E can be easily computed using

$$SS_E = SS_T - \hat{\beta}_1 S_{xy} \qquad (11\text{-}14)$$

11-3: Properties of the Least Squares Estimators

- Slope Properties

$$E(\hat{\beta}_1) = \beta_1 \qquad V(\hat{\beta}_1) = \frac{\hat{\sigma}_\varepsilon^2}{S_{xx}} = \frac{\hat{\sigma}_\epsilon^2}{n\,\sigma_x^2}$$

Large $n \rightarrow$ small variance of β_1

- Intercept Properties

$$E(\hat{\beta}_0) = \beta_0 \quad \text{and} \quad V(\hat{\beta}_0) = \hat{\sigma}_\varepsilon^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}} \right] =$$

$$= \hat{\sigma}_\varepsilon^2 \left[1 + \frac{\mu_x^2}{\sigma_x^2} \right] \times \frac{1}{n}$$

11-4: Hypothesis Tests in Simple Linear Regression

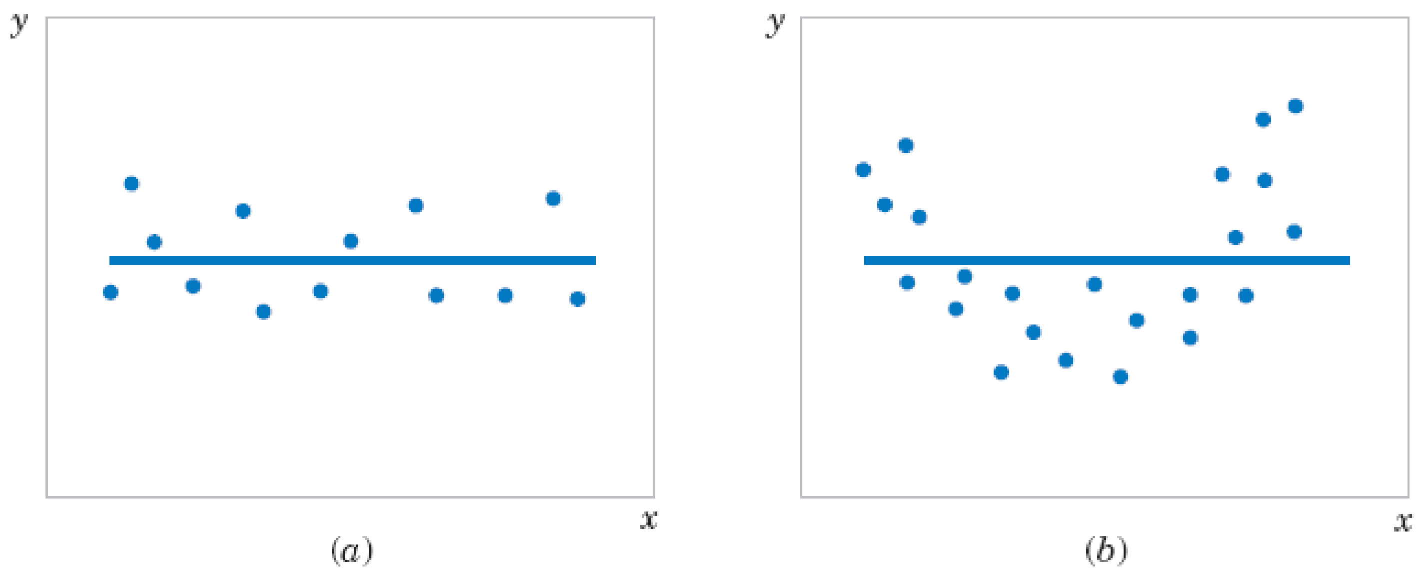


Figure 11-5 The hypothesis H_0: $\beta_1 = 0$ is not rejected.

Figure 11-5 The null hypothesis H_0: $\beta_1 = 0$ is accepted.

11-4: Hypothesis Tests in Simple Linear Regression

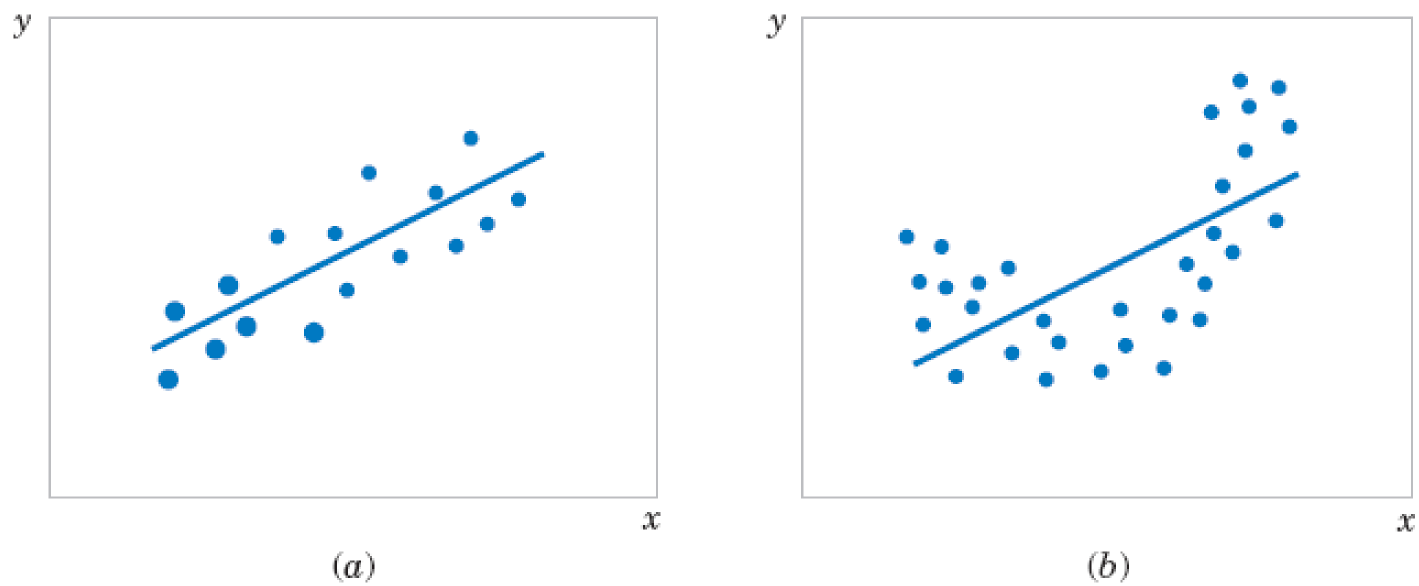


Figure 11-6 The hypothesis H_0: $\beta_1 = 0$ is rejected.

Figure 11-6 The **null hypothesis H_0: β_1 = 0 is rejected**.

11-4: Hypothesis Tests in Simple Linear Regression

11-4.1 Use of *Z*-tests for large n

An important special case of the hypotheses of Equation 11-18 is

$$H_0\colon \beta_1 = 0$$
$$H_1\colon \beta_1 \neq 0$$

These hypotheses relate to the **significance of regression**. *Failure* to reject H_0 is equivalent to concluding that there is no linear relationship between *X* and *Y*.

11-4: Hypothesis Tests in Simple Linear Regression

$$H_0: \beta_1 = 0$$
$$H_1: \beta_1 \neq 0$$

Choose α
(e.g. $\alpha = 5\%$
for 95%
confidence
in rejecting
H_0)

$$Z = \frac{\hat{\beta}_1}{\frac{\hat{\sigma}_\epsilon}{\hat{\sigma}_x} \cdot \frac{1}{\sqrt{n}}}$$

for $\alpha = 5\%$

Reject H_0 if $|Z| > Z_{\alpha/2} = 1.96$

11-4: Hypothesis Tests in Simple Linear Regression

11-4.1 Use of *t*-tests for smaller n.

The number of degrees of freedom in **n-2**

One can always fit a straight line through two points so one needs n>=3

11-4: Hypothesis Tests in Simple Linear Regression

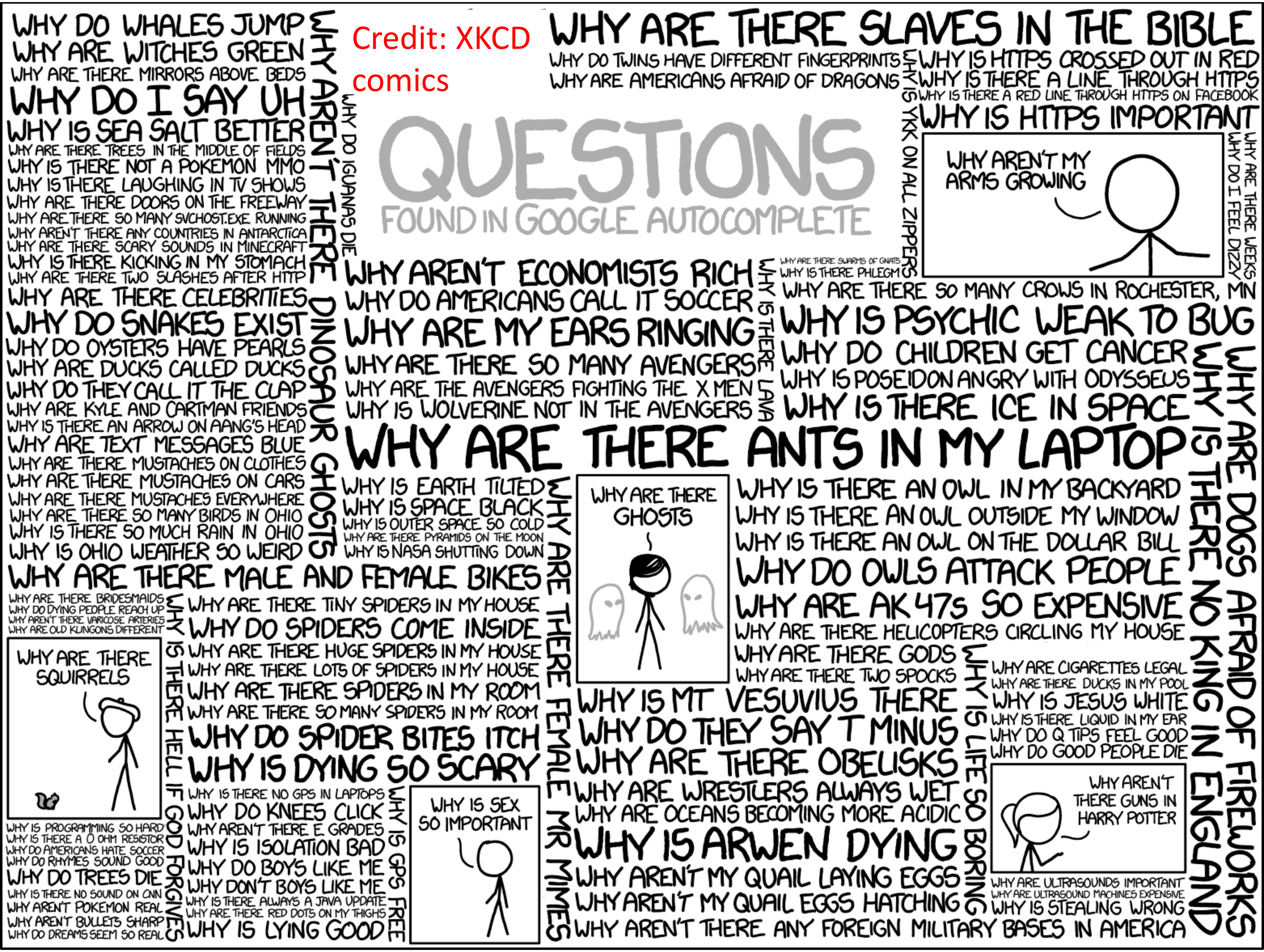
$$H_0: \beta_1 = 0$$
$$H_1: \beta_1 \neq 0$$

Choose α (e.g. $\alpha = 5\%$ for 95% confidence in rejecting H_0)

$$T = \frac{\hat{\beta}_1}{\frac{\hat{\sigma}_\epsilon}{\hat{\sigma}_x} \cdot \frac{1}{\sqrt{n}}}$$

$t_{\alpha/2, n-2}$ is such $1 - \frac{\alpha}{2} = \mathrm{tcdf}(t_{\alpha/2, n-2}, n-2)$

Reject H_0 if $|T| > t_{\alpha/2, n-2}$



Credit: XKCD comics