

Analysis of Engineering and Scientific Data

Semester 1 - 2019

Sabrina Streipert

s.streipert@uq.edu.au

Chapter 11: Simple Linear Regression

- Aim: Study or analysis of the relationship between two or more variables
 - e.g. Pressure of a gas in a container versus its temperature

We examine a dependent variable and one or more independent variables (= predictors).

 \implies Regression Analysis

• Key importance (conditional expectation):

$$\mathbb{E}[Y \mid x] = \mu_{Y|x}$$

Suppose for now, the variable Y depends linearly on only one predictor, i.e.:

$$\mathbb{E}[Y \mid x] = \mu_{Y|x} = \beta_0 + \beta_1 x$$

$$Y = \beta_0 + \beta_1 x + \epsilon,$$

where:

 \implies

- x is a (non-random) predictor, and
- ϵ is a R.V.(=noise) with $\mathbb{E}[\epsilon] = 0$, $\operatorname{Var}(\epsilon) = \sigma^2$.

Assumptions:

- Normality of residuals,
- Constant variance, and,
- Independence of observations

Method:

• Collect data:

$$(x_1, y_1), \ldots, (x_n, y_n).$$

• Assume linear relation:

$$y \approx \beta_0 + \beta_1 x \qquad \leftrightarrow \qquad y = \beta_0 + \beta_1 x + \epsilon$$

• Since we do not have all possible tuples, we can only estimate β_0 and β_1 by $\hat{\beta}_0$ and $\hat{\beta}_1$, respectively, i.e.,

$$y_i = \hat{\beta}_0 + \hat{\beta}_1 x_i + e_i, \quad i = 1, \dots, n.$$

• $e_i =$ residual.

Use $\hat{\beta}_0, \hat{\beta}_1$ for predictions.

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

Note that we can also compute predicted observations for our data $(x_i, y_i)_{\{1 \le i \le n\}}$.

Ideally, we would like to find $\hat{\beta}_0$ and $\hat{\beta}_1$, such that $y_i = \hat{y}_i$, that is, $e_i = 0$.



```
1 D <- read.delim("amazon-books.txt")
2 plot(D$NumPages, D$Thick)
3 abline(lm(D$Thick<sup>D</sup>$NumPages), col='red')
```

Total mean squared error



Total Mean Squared Error:

$$L = SS_E = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \quad \longrightarrow \quad \text{min}$$

The least squares estimators

• To find the best estimators $\hat{\beta}_0$ and $\hat{\beta}_1$, we would like to minimize

$$L = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2.$$

- Specifically, solve $\hat{\beta}_0, \hat{\beta}_1 = \operatorname{argmin}_{\beta_0,\beta_1} \sum_{i=1}^n (y_i \beta_0 \beta_1 x_i)^2$.
- The solution, called the *least squares estimators* must satisfy: Since we want to minimize L, we take the (partial) derivative and set them equal to zero.

(f)
$$0 = \frac{\partial}{\partial \beta_0} L = \frac{\partial}{\partial \beta_0} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i)^2 = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-1)$$

(2)
$$0 = \frac{\partial}{\partial \beta_1} L = \sum_{i=1}^n \frac{\partial}{\partial \beta_1} (y_i - \beta_0 - \beta_1 x_i)^2 = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

(1):
$$0 = \frac{1}{\sqrt{2}} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$\int_{\partial \beta_0} (1) = \sum_{i=1}^n \frac{\partial}{\partial \beta_0} (y_i - \beta_0 - \beta_1 x_i) = \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i) (-x_i)$$

$$J_{0}(2)^{n} = \sum y_{i}x_{i} - \sum \beta_{b}x_{i} - \sum \beta_{1}x_{i}^{2}$$

$$0 = \sum y_{i}x_{i} - \beta_{0}n\cdot\overline{x} - \beta_{1}\sum x_{i}^{2}$$

$$\beta_{1} = \frac{\sum y_{i}x_{i} - \beta_{0}n\overline{x}}{\sum x_{i}^{2}} = \frac{\sum y_{i}x_{i} - \overline{y}n\overline{x} + \beta_{1}\overline{x}n}{\sum x_{i}^{2}}$$

$$\beta_{1} - \beta_{1}\frac{\overline{x}^{2}n}{\Sigma x_{i}^{2}} = \frac{\sum y_{i}x_{i} - \overline{y}n\overline{x}}{\sum x_{i}^{2}}$$

$$\beta_{1} \left[\frac{\sum x_{i}^{2} - \overline{x}^{2}n}{\Sigma x_{i}^{2}}\right] = \frac{\sum y_{i}x_{i} - \overline{y}n\overline{x}}{\sum x_{i}^{2}}$$

$$\beta_{1} \left[\frac{\sum x_{i}^{2} - \overline{x}^{2}n}{\Sigma x_{i}^{2}}\right] = \frac{\sum y_{i}x_{i} - \overline{y}n\overline{x}}{\sum x_{i}^{2}}$$

$$\beta_{1} = \frac{\sum y_{i}x_{i} - n\overline{x}\overline{y}}{\sum x_{i}^{2}}$$

The least squares solution

Using the sample means, **x** and **y**

$$\overline{x} = \frac{1}{n} \sum_{i=1}^{n} x_i, \quad \overline{y} = \frac{1}{n} \sum_{i=1}^{n} y_i,$$

the estimators are:

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n x_i y_i - \frac{(\sum_{i=1}^n x_i)(\sum_{i=1}^n y_i)}{n}}{\sum_{i=1}^n x_i^2 - \frac{(\sum_{i=1}^n x_i)^2}{n}}$$

Additional quantities of interest

$$\sum_{i=1}^{n} (x_i - \overline{x})^2 = \sum_{i=1}^{n} (x_i - \overline{x})^2 = \sum_{i=1}^{n} (x_i - \overline{x})^2 = \sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y}) = \sum_{i=1}^{n} (x_i - \overline{y})(y_i - \overline{y})(y_i - \overline{y}) = \sum_{i=1}^{n} (x_i - \overline{y})(y_i - \overline{y$$

That is,

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n x_i y_i - \frac{(\sum_{i=1}^n x_i)(\sum_{i=1}^n y_i)}{n}}{\sum_{i=1}^n x_i^2 - \frac{(\sum_{i=1}^n x_i)^2}{n}} = \frac{S_{XY}}{S_{XX}}.$$

In addition, we have:

$$SS_{T} = \sum_{i=1}^{n} (y_{i} - \overline{y})^{2} = \underbrace{\Sigma(y_{i}^{2} - 2y_{i}\overline{y} + \overline{y}^{2})}_{g_{i}} = \underbrace{\Sigma(y_{i}^{2} - n_{i}\overline{y}^{2})}_{g_{i}} = \underbrace{\Sigma(y_{i}^{2} - 2y_{i}\overline{y} + \overline{y}^{2})}_{g_{i}} = \underbrace{\Sigma(y_{i}^{2} - n_{i}\overline{y}^{2})}_{g_{i}} = \underbrace{\Sigma(y_{i}^{2$$

 $SS_T = SS_R + SS_E,$

The Analysis of Variance

• We did not consider the final unknown parameter in our regression model:

$$Y = \beta_0 + \beta_1 x + \epsilon,$$

namely, the $Var(\epsilon) = \sigma^2$.

- We use the residuals $e_i = \hat{y}_i y_i$, to obtain an estimate of σ^2 .
- Specifically,

$$SS_E = \sum_{i=1}^n \left(\hat{y}_i - y_i \right)^2,$$

and it can be shown that

$$\mathbb{E}[SS_E] = (n-2)\sigma^2,$$

so:

1

$$\hat{\sigma}^2 = \frac{SS_E}{n-2}.$$

How good is my regression model?

A widely used measure for a regression model is the following ratio of sum of squares, which is often used to judge the adequacy of a regression model:

$$R^{2} = \frac{SS_{R}}{SS_{T}} = 1 - \frac{SS_{E}}{SS_{T}}, \qquad R^{2} \in [0,1]$$

le $\lambda^{2} = 0.877$
"Modul accounts for $87.70/0$ of the variability
in data".

Properties of least square estimator

$$\mathbb{E}[\hat{\beta}_0] = \beta_0, \quad \operatorname{Var}\left(\hat{\beta}_0\right) = \sigma^2 \left[\frac{1}{n} + \frac{\overline{x}^2}{S_{XX}}\right],$$
$$\mathbb{E}[\hat{\beta}_1] = \beta_1, \quad \operatorname{Var}\left(\hat{\beta}_1\right) = \frac{\sigma^2}{S_{XX}},$$

Therefore, the estimated standard error of the slope and the estimated standard error of the intercept are:

$$se\left(\hat{\beta}_{0}\right) = \sqrt{\sigma^{2}\left[\frac{1}{n} + \frac{\overline{x}^{2}}{S_{XX}}\right]},$$

$$se\left(\hat{\beta}_{1}\right) = \sqrt{\frac{\sigma^{2}}{S_{XX}}}.$$

EXAMPLE

A study considers the microstructure of the ultrafine powder of partially stabi-

lized zirconia as a function of temperature. The data is as follows:

x (Temperature)	1100	1200	1300	1100	1500	1200	1300
y (Porosity)	30.8	19.2	6.0	13.5	11.4	7.7	3.6

n= 7

Given \overline{X} find $\overline{2}_{x_i}^s = \overline{X} \cdot n$

$$\begin{split} \hat{\beta}_{0} = \overline{y} - \hat{\beta} \overline{x} \\ \hat{\beta}_{1} &= \frac{Z x_{1} y_{1} - Z x_{1} \cdot Z y_{1}}{Z x_{1}^{2} - (Z x_{1})^{2}} \\ \widehat{\beta}_{1} &= \frac{110590 - n \overline{x} \cdot x_{1} \overline{y}}{\overline{x}} \\ = \frac{110590 - 7 \cdot 1242.9 \cdot 13.1714}{10930000 - 7 \cdot (1242.9)^{2}} = -0.0344 \\ \hat{\beta}_{0} = \overline{y} - \hat{\beta}_{1} \overline{x} = \beta_{1} 1714 - (-0.0344) \cdot \beta_{2} 42.9 = \\ &= 55.9272 \\ \hat{\gamma}_{1} = \hat{\beta}_{0} + \hat{\beta}_{1} x_{1} \end{split}$$

Estimate the porosity for a temperature of 1400 degrees Celcius.

 $\hat{\gamma} = 55.9272 - 0.0344.1400 =$ = 7.7672 Find SS_E (= error sum of squares).

$$S_{\Sigma} = S_{\Sigma} - \hat{\beta}_{1} S_{XY} = 385.52.30$$
where $S_{\Sigma} = \overline{\Sigma}y_{1}^{2} - n\overline{y}^{2} = 1737.7 - 7 \cdot (13.1714)^{2}$
 $S_{XY} = \overline{\Sigma}X_{1}Y_{1} - N\overline{y}\overline{y} = 110590 - 7 \cdot (1242.9) \cdot (131714)$
 $\hat{\beta}_{1} = -0.0344$
Find the least square optimates for y with respect to the predictor $x_{1}^{*} = x_{1} + B$
 $\hat{X}^{*} = X_{1} + \overline{X}$
 $\hat{\alpha}_{1} = \overline{T}_{11} d \hat{\beta}_{0}, \hat{\beta}_{1} = S_{1} \cdot \overline{y} = \hat{\beta}_{0} + \hat{\beta}_{1} X_{1}^{*}$
 $\hat{\gamma} = \hat{\beta}_{0} + \hat{\beta}_{1} (X_{1} + \overline{X}) = \hat{\beta}_{0} + \hat{\beta}_{1} X_{1}^{*} + \hat{\beta}_{1} \overline{X}$
 $\hat{\gamma} = (\hat{\beta}_{0} + \hat{\beta}_{1}, \overline{X}) + \hat{\beta}_{1} X_{1}$
 $\hat{\beta}_{0} = -\hat{\beta}_{0} - \hat{\beta}_{1} \overline{X} = 55$
 $\frac{1}{7}(712 + 0.0344 + 12429)$
 $\hat{\Omega}_{1} = \hat{\beta}_{0} + \hat{\beta}_{1} \overline{X} = \hat{\beta}_{0} \Rightarrow \hat{\beta}_{0} = \hat{\beta}_{0} - \hat{\beta}_{1} \overline{X} = 55$
 $\frac{1}{7}(712 + 0.0344 + 12429)$
 $\hat{\Omega}_{1} = \hat{\beta}_{1} + \hat{\beta}_{1} \overline{X} = \hat{\beta}_{0} \Rightarrow \hat{\beta}_{0} = \hat{\beta}_{0} - \hat{\beta}_{1} \overline{X} = 55$
 $\frac{1}{7}(712 + 0.0344 + 12429)$
 $\hat{\Omega}_{1} = \hat{\beta}_{1} + \hat{\beta}_{1} \overline{X} = \hat{\beta}_{1} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} - \hat{\beta}_{1} \overline{X} = 55$
 $\frac{1}{7}(712 + 0.0344 + 12429)$
 $\hat{\Omega}_{2} = \hat{\beta}_{1} + \hat{\beta}_{1} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{0} - \hat{\beta}_{1} \overline{X} = 55$
 $\hat{\Omega}_{1} = \hat{\beta}_{1} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{1} - \hat{\beta}_{1} \overline{X} = 55$
 $\hat{\Omega}_{2} = \hat{\beta}_{1} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} - \hat{\beta}_{1} \overline{X} = 55$
 $\hat{\Omega}_{1} = \hat{\beta}_{1} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} - \hat{\beta}_{1} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} - \hat{\beta}_{1} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} \Rightarrow \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_{2} \overline{X} = \hat{\beta}_{2} + \hat{\beta}_{2} + \hat{\beta}_{2} + \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_{2} + \hat{\beta}_{2} = \hat{\beta}_{2} + \hat{\beta}_$

Hypothesis tests in linear regression

• Suppose we would like to test:

$$H_0: \beta_1 = \beta_{1,0}, \quad H_1: \beta_1 \neq \beta_{1,0}.$$
 Q-sided test recall

• The Test Statistic for the Slope is



- Under H_0 , the test statistic T follows a t distribution with n-2 degree of freedom.
- Reject H_0 if $|t| > t_{\frac{\alpha}{2}, n-2}$



• Suppose we would like to test:

$$H_0: \beta_0 = \beta_{0,0}, \quad H_1: \beta_0 \neq \beta_{1,0}.$$

• The Test Statistic for the intercept is

$$T = \frac{\hat{\beta}_0 - \beta_{0,0}}{\sqrt{\hat{\sigma}^2 \left[\frac{1}{n} + \frac{\overline{x}^2}{S_{XX}}\right]}} = \underbrace{\begin{array}{c} & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

- Under H_0 , the test statistic T follows a t distribution with n-2 degree of freedom.
- Reject H_0 if $|t| > t_{\frac{\alpha}{2}, n-2}$

An important special case of the hypotheses is:

$$H_0: \beta_1 = 0, \quad H_1: \beta_1 \neq 0.$$

If we fail to reject H_0 : $\beta_1 = 0$, this indicates that there is no linear

relationship between x and y.

Example:

Suppose we have 20 samples regarding oxygen purity (y) with respect to hydrocarbon levels (x) such that

$$\sum_{i=1}^{20} x_i = 23.92, \qquad \sum_{i=1}^{20} y_i = 1,843.21, \qquad \bar{x} = 1.1960, \qquad \bar{y} = 92.1605$$

$$\sum_{i=1}^{20} y_i^2 = 170,044.5321, \qquad \sum_{i=1}^{20} x_i^2 = 29.2892, \qquad \sum_{i=1}^{20} x_i y_i = 2,214.6566$$
Test: $H_0: \quad \beta_1 = 0$ $H_1: \quad \beta_1 \neq 0$ $n=2.0$
for $\alpha = 0.01.$

$$N=2.0$$
for $\alpha = 0.01.$

$$N=2.0$$

$$S_{XX} = \Sigma X_1^2 - N \cdot \overline{X}^2 = 29.2892 - 20 \cdot (1.1960)^2$$



The F distribution

- An alternative is to use the F statistic as is common in ANOVA (Analysis of Variance) (not covered fully in the course).
- Under H_0 , the test statistic

$$F = \frac{SS_R/1}{SS_E/(n-2)} = \frac{MS_R}{MS_E},$$

follows an F - distribution with 1 degree of freedom in the numerator and n-2 degrees of freedom in the denominator.

• Here,

 $MS_R = SS_R/1, \quad MS_E = SS_E/(n-2).$

Not coured

Ar	nalysis of	Variance Table	for Testin	ıg Signi	ificance of
gr	ession				
	Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
	Regression	$SS_R = \hat{\beta}_1 S_{xy}$	1	MS_R MS	MS_R/MS_E

Additional remarks

- There are also confidence intervals for $\hat{\beta}_0$ and $\hat{\beta}_1$ as well as prediction intervals for observations. We do not cover these formulas.
- To check the regression model assumptions, we plot the residuals e_i and check for:
 - Normality,

 - Independence

Transformations

Non-linear models can sometimes be "intrinsically" linear. -> can apply "nice" transformation to data and get linear relation

Examples:

• $Y = \beta_0 x^{\beta_1} \epsilon$, where $\epsilon \sim N(0, \sigma^2)$.

Normality,
Constant variance, and,
Independence

Why is this "intrinsically" linear?

$$\log (Y) = \log (\beta_0 X^{\beta_1} \mathcal{E}) = \log (\beta_0) + \log (X^{\beta_1}) + \log (c) \mathcal{E} \sim \mathcal{N}(0, 0^2)$$

$$\log (Y) = \log (\beta_0) + \beta_1 \cdot \log (x) + \log (c) \mathcal{E} \sim \mathcal{N}(0, 0^2)$$

$$Z_1 = \mathcal{L}_0 + \mathcal{L}_1 \quad \mathcal{N}_1 + \mathcal{E}$$

• $Y = \beta_0 + \beta_1 x + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$.

Why is this "intrinsically" linear?

$$\begin{array}{l}
 Y = \frac{x}{x\beta_0 + \beta_1 + x\epsilon} & \frac{1}{y_1} = \frac{x\beta_0 + \beta_1 + x\epsilon}{x} = \beta_0 + \beta_1 \frac{1}{x} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{x\beta_0 + \beta_1 + x\epsilon}{x} = \beta_0 + \beta_1 \frac{1}{x} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} = \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon & \frac{1}{y_1} + \epsilon \\
 \frac{x}{y_1} + \epsilon$$

Boyle's Law

```
1 D <- read.delim("boyle.txt")
2 plot(D$Height, D$Pressure, pch=16)</pre>
```



plot(log(D\$Height), log(D\$Pressure), pch=16)



1

Logistic Regression

- Take the response variable, Y_i as a Bernoulli random variable.
- In this case notice that $\mathbb{E}[Y] = P(Y = 1)$.
- The logit response function has the form $\mathbb{E}[Y] = \underbrace{e^{\beta_0 + \beta_1 x}}_{1 + e^{\beta_0 + \beta_1 x}}.$
- Fitting a logistic regression model to data yields estimates of β_0 and β_1 .
- The following formula is called the odds:

$$\frac{\mathbb{E}[Y]}{1 - \mathbb{E}[Y]} = e^{\beta_0 + \beta_1 x}.$$

Example:

Source: $https://dasl.datadescription.com/datafiles/?_sf_s=stream&_sfm_cases=4+59943$

1 D <- read.delim("streams.txt")
2 D1 <- D %>% mutate(lime = ifelse(Substrate=='Limestone',1,0)
3 plot(D1\$pH, D1\$lime, pch=16)



Multiple Regression

What if there are more variables that explain the value of the output?

 \longrightarrow Use multiple regression models

Example - revisited:

pairs(~pH+Hard+Alkali, data=D)



Following material not rovered in class.

Try to fit the following linear model:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

with $\epsilon \sim N(0, \sigma^2)$ and $y = \text{Hard}, x_1 = \text{pH}, x_2 = \text{Alkali}.$

As before, we set up

$$L = \sum_{i} (y_i - \hat{y}_i)^2 = \sum_{i} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1,i} - \hat{\beta}_2 x_{2,i})^2$$

and try to minimize it.

As before, we find the critical value by setting the partial derivatives equal to zero, that is

$$0 = \frac{\partial}{\partial \beta_0} L = \sum_i 2(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1,i} - \hat{\beta}_2 x_{2,i})(-1)$$

$$0 = \frac{\partial}{\partial \beta_1} L = \sum_i 2(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1,i} - \hat{\beta}_2 x_{2,i})(-x_{1,i})$$

$$0 = \frac{\partial}{\partial \beta_2} L = \sum_i 2(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{1,i} - \hat{\beta}_2 x_{2,i})(-x_{2,i})$$

which simplifies to

$$\begin{aligned} 0 &= n\bar{y} - \hat{\beta}_0 - \hat{\beta}_1 \bar{x_1} - \hat{\beta}_2 \bar{x_2} \\ 0 &= \sum_i y_i x_{1,i} - \hat{\beta}_0 n \bar{x_1} - \hat{\beta}_1 \sum_i x_{1,i}^2 - \hat{\beta}_2 \sum_i x_{2,i} x_{1,i} \\ 0 &= \sum_i y_i x_{2,i} - \hat{\beta}_0 n \bar{x}_2 - \hat{\beta}_1 \sum_i x_{1,i} x_{2,i} - \hat{\beta}_2 \sum_i x_{2,i}^2 \end{aligned}$$

Solving these three equations for the three unknowns $\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2$ yields the estimators.

Back to example:



In general, one could express the problem in Matrix notation:

So we have $\vec{y} = X\vec{\beta} + \vec{\epsilon}$

Aim: Find $\vec{\beta}$ so that $L = \sum_i \epsilon_i^2 = \vec{\epsilon}^T \vec{\epsilon}$ is minimal

We have $X^T X \vec{\beta} = X^T \vec{y}$