*Curso de Formación de Personal Investigador Usuario de Animales para Experimentación* 

# SIMPLE LINEAR REGRESSION AND CORRELATION

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## **Learning objectives**

- Define the statistics related to the association between variables: correlation and regression.
- Explain how to explore the data: scatter plot (linear trend) and boxplots (evenness of the data) with R Commander.
- Define and calculate the correlation coefficient as a measure of association.
- Define linear regression as a statistic tool for prediction.
- Establish the model describing linear regression: intercept and slope, and the assumptions implied.
- Test the significance of the regression coefficients.
- Development of calculations by R Commander and interpretation of the outputs, including regression diagnostics.
- Define  $R^2$ , the coefficient of determination.
- Distinguish outliers from influential observations and define procedures to detect them.

## **Analysis of several variables**

#### Two main interests:

- Estimating the degree of association between two variables: CORRELATION analysis.
- 2. Predicting the values of one variable given that we know the realised value of another variable(s): REGRESSION analysis. This analysis can also be used to understand the relationship among variables.
  - a) A response variable and an independent variable: **simple (linear) regression**.
  - b) A response variable and two or more independent variables: multiple (linear) regression.
  - c) When the relationship among variables is not linear: **nonlinear regression**.
  - d) If the variable is a dichotomous or binary variable: **logistic regression**.

#### Data example

To analyse the relationship of two variables we will return to the catsWeight data base. In this case we will pick up the variables body weight in kilograms (BODYwt) as the independent or explanatory variable, and hearth weight expressed in grams (HEARTwt) as the dependent or response variable.

RC	atsWe	ight 🛛	- 0 X	
	Sex	BODYwt	HEARTHwt	
35	F	2.5	9.0	
36	F	2.5	10.9	
37	F	2.6	8.7	
38	F	2.6	10.1	
39	F	2.6	10.1	
40	F	2.7	8.5	
41	F	2.7	10.2	
42	F	2.7	10.8	
43	F	2.9	9.9	
44	F	2.9	10.1	
45	F	2.9	10.1	=
46	F	3.0	10.6	
47	F	3.0	13.0	
48	M	2.0	6.5	
49	M	2.0	6.5	
50	M	2.1	10.1	
51	M	2.2	7.2	
52	M	2.2	7.6	
53	M	2.2	7.9	
54	M	2.2	8.5	
55	M	2.2	9.1	
56	M	2.2	9.6	
57	M	2.2	9.6	
58	M	2.2	10.7	
59	M	2.3	9.6	
60	M	2.4	7.3	
61	M	2.4	7.9	
62	M	2.4	7.9	
63	M	2.4	9.1	
64	M	2.4	9.3	Ŧ

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## **Studying normality**

#### Data: catsWeight Graphs > Boxplot; Plot by: Sex Variable: BODYwt

#### Variable: HEARTHwt



Different distributions for males and females in both variables From now on, we will work only with the male's subset

#### Subsetting (for males, "M")

R Comm	ander			
File Edit	Data Statistics Graphs N	lodels Dis	tributions Tools He	lp
R Script R	New data set Load data set Merge data sets		:t) 🔞 View data set	Model: 2 <no< th=""></no<>
	Import data Data in packages	+		
	Active data set	•	View data	
	Manage variables in active	data set 🕨	Select active data se	et
		Refresh active data set		
			Help on active data	set (if available)
		Variables in active data set		
			Set case names	
			Subset active data s	et
			Sort active data set.	



R Subset Data Set
Include all variables OR Variables (select one or more)
BODYwt HEARTHwt Sex
Subset expression Sex=="M"
Name for new data set catsWeightM
🔁 Help 🖌 OK 🗱 Cancel



Rc	atsWeig	htM 🔄		
	Sex E	ODYwt H	EARTHwt	
48	М	2.0	6.5	*
49	М	2.0	6.5	
50	М	2.1	10.1	
51	М	2.2	7.2	
52	М	2.2	7.6	
53	М	2.2	7.9	E
54	М	2.2	8.5	
55	М	2.2	9.1	
56	М	2.2	9.6	
57	М	2.2	9.6	μ
58	М	2.2	10.7	
59	М	2.3	9.6	
60	М	2.4	7.3	
61	М	2.4	7.9	
62	М	2.4	7.9	
63	М	2.4	9.1	
64	М	2.4	9.3	
65	М	2.5	7.9	
66	М	2.5	8.6	
67	М	2.5	8.8	
68	М	2.5	8.8	
69	М	2.5	9.3	
70	М	2.5	11.0	
71	М	2.5	12.7	
72	М	2.5	12.7	
73	М	2.6	7.7	
74	М	2.6	8.3	
75	М	2.6	9.4	
76	М	2.6	9.4	
77	М	2.6	10.5	-

## Plot of data from males

A plot for a pair of variables gives us a first impression about their relationship.

Data: catsWeightM

Graphs > Scatterplot

x-variable: BODYwt; y-variable: HEARTHwt; Options: Least-squares line



A linear relationship is observed

#### **Correlation** (Pearson)

The correlation is a measure of the degree of association between two variables. It is calculated as

$$r = \frac{\operatorname{cov}(x, y)}{\sqrt{s_x^2 s_y^2}} = \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_i (x_i - \overline{x})^2 \sum_i (y_i - \overline{y})^2}}$$

0.7930296

r

#### Statistics > Summaries > Correlation test Variables: BODYwt and HEARTHwt

Pearson's product-moment correlation
data: BODYwt and HEARTHwt
t = 12.688, df = 95, p-value < 2.2e-16
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
 0.7051085 0.8569367
sample estimates:
 cor</pre>

 $H_0$ : ( $\rho$  = 0), is rejected

*r* is an estimator of  $\rho$ , the population parameter.

The denominator is the geometric mean of the sample variances estimates. This makes r to range from -1 to 1. As close is an estimate to -1 or 1, the correlation is larger.

#### **Correlation** – sample size -

The **sample size** required to have a particular correlation statistically different from 0 depends upon the same correlation coefficient:

 $z' = 0.5 \ln \left| \frac{1-r}{1+r} \right|$  Fisher's classic z-transformation to normalize the distribution of Pearson correlation coefficient.

$$n = \left[\frac{z_{1-\alpha/2} + z_{1-\beta}}{|z'_{r_0} - z'_{r_1}|}\right] + 3$$

 $r_0 = 0$  and  $r_1$  is the magnitude of the coefficient we want to estimate.

	Sample size for a power of		
ρ	80%	90%	
0.1	781	1044	
0.2	194	258	
0.3	85	113	
0.4	47	62	
0.5	29	38	
0.6	20	25	
0.7	14	17	
0.8	10	12	
0.9	7	8	

#### **Correlation** – sample size with R -

```
> library(pwr)
> pwr.r.test(r = 0.5, sig.level = 0.05, power = 0.80)
```

approximate correlation power calculation (arctangh transformation)

n = 28.24841
r = 0.5
sig.level = 0.05
power = 0.8
alternative = two.sided

#### Simple linear regression - the model -



To estimate  $\beta_0$  and  $\beta_1$  we resort to the Least Squares methodology, i.e., minimize the sum of the squares of the deviations (red arrows) between actual (blue diamond) an predicted values (on the slope).



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

 $\beta_1$  is the increase of the dependent variable when the independent variable increases 1 unit

### **Assumptions in regression analysis**

- 1. The variables *x* and *y* are linearly related (definition of the model).
- 2. Both variables are measured for each of *n* observations.
- 3. Variable *x* is measured without error (fixed).
- 4. Variable *y* is a set of random observations measured with error.
- 5. The errors are independent and normally distributed with homogeneous variance:

$$\boldsymbol{\varepsilon} \sim N(\boldsymbol{0}, \mathbf{I}\sigma_e^2)$$

Some of the above conditions can be seen in the figure. For each value (fixed) of *x*, there is a normal distribution of *y* (random), with mean on the regression line.



### Simple linear regression - Results (1) -

Statistics > Fit models > Linear regression Response variable: HEARTHwt; Explanatory variables: BODYwt



For each increment of 1 kg of body weight, hearth weight increases 4.3127 g

$$\hat{y}_i = -1.1841 + 4.3127 x_i$$

 $H_0: \beta_0 = \beta_1 = 0$ , is rejected

$$t(\hat{\beta}_{1}) = \frac{\hat{\beta}_{1}}{s.e.(\hat{\beta}_{1})}$$
$$= \frac{4.3127}{0.3399} = 12.688$$

#### Simple linear regression - Results (1 cont.) -

Residual standard error: 1.557 on 95 degrees of freedom Multiple R-squared: 0.6289, Adjusted R-squared: 0.625 F-statistic: 161 on 1 and 95 DF, p-value: < 2.2e-16

*R-Squared* is the square of the correlation coefficient. It represents the fraction of the total variation in blood pressure that is explained by the linear relationship with age. In this case 62.89% of the variation of blood pressure is explained by age.

Adj R-Sq includes a correction to overcome the increment in R-Squared with the number of regressors (k).

$$R^{2} = SS_{AGE} / SS_{TOTAL}$$
$$R^{2}_{adj} = 1 - (1 - R^{2}) \frac{N - 1}{N - k - 1}$$

### **Diagnostics - Some plots of residuals**



Model should involve curvature



Heterogeneous variance



### Simple linear regression – Results (2) -

#### Models > Graphs > Basic diagnostic plots

#### Im(HEARTHwt ~ BODYwt)



Residuals are distributed approximately at random around 0: homogeneity of variance met No important deviations in Q-Q plot: response variable normal

## Some graphics about influential observations



High leverage, influential

Low leverage, influential



High leverage, not influential



Low leverage, not influential



X

## Some statistics useful for regression analysis

#### **Standardized residual**

Weak outlier,  $|rs_i| > 2$  (95% confidence) Strong outlier,  $|rs_i| > 3$  (95% confidence)

$$rs_i = \frac{r_i}{\sqrt{MSE(1-h_i)}} \sim t_{N-k-1}$$

#### Leverage $(h_i)$

Standardized value of how much an observation deviates from the centre of the space of *x* values. Observations with high leverage can indicate an outlier in the *x* and are potentially influent. Computed as the diagonal elements of  $\mathbf{X}(\mathbf{X}^{*}\mathbf{X})^{-1}\mathbf{X}^{*}$ .

$$DFFITS_{i} = \frac{\hat{y}_{i} - \hat{y}_{i,-i}}{s_{-i}\sqrt{h_{i}}} = R - student_{i} \left[\frac{h_{i}}{1 - h_{i}}\right]^{\frac{1}{2}} \qquad DFBETAS_{j,i} = \frac{\hat{\beta}_{j} - \hat{\beta}_{j,-i}}{s_{-i}\sqrt{c_{jj}}}$$

where  $c_{jj}$  are the diagonal elements of  $(\mathbf{X}^{*}\mathbf{X})^{-1}$ . Analyse only *DFBETAS* corresponding to high values of *DFFITS*.

#### Cook's D

Essentially a DFFITS statistic scaled and squared to make extreme values stand out more clearly.

## Simple linear regression – Results (3) -

#### Models > Graphs > Basic diagnostic plots



The  $\sqrt{\text{standardized residual of}}$ obs. 140 is greater than  $\sqrt{2}$ (=1.41): weak outlier; the one of obs. 144 is greater than  $\sqrt{3}$ (=1.73): strong outlier

None of the points is outside the high Cook's distance contour(s), the dashed red lines: none of the observations is influential

See also: http://www.sthda.com/english/articles/39-regression-model-diagnostics/161-linear-regression-assumptionsand-diagnostics-in-r-essentials