

Elementary Statistics Course

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1 Regresión y Correlación

1.1 Joint frequency distribution

Relations among variables

In the last chapter we saw how to describe the distribution of a single variable in a sample. However, in most cases, studies require to describe several variables that are often related. For instance, a nutritional study should consider all the variables that could be related to the weight, as height, age, gender, smoking, diet, physic exercise, etc.

To understand a phenomenon that involve several variables is not enough to study every variable by its own. We have to study all the variables together to describe how they interact and the type of relation among them.

Usually in a *dependency study* there is a **dependent variable** Y that it is supposed to be influenced by a set of variables X_1, \dots, X_n known as **independent variables**. The simpler case is a *simple dependency study* when there is only one independent variable, that is the case covered in this chapter.

Joint frequencies

To study the relation between two variables X and Y , we have to study the joint distribution of the **two-dimensional variable** (X, Y) , whose values are pairs (x_i, y_j) where the first element is a value of X and the second a value of Y .

Definition 1 (Joint sample frequencies). Given a sample of n values and a two-dimensional variable (X, Y) , for every value of the variable (x_i, y_j) is defined

- **Absolute frequency** n_{ij} : Is the number of times that the pair (x_i, y_j) appears in the sample.
- **Relative frequency** f_{ij} : Is the proportion of times that the pair (x_i, y_j) appears in the sample.

$$f_{ij} = \frac{n_{ij}}{n}$$

Watch out! For two-dimensional variables it make no sense cumulative frequencies.

Joint frequency distribution

The values of the two-dimensional variable with their frequencies is known as **joint frequency distribution**, and is represented in a joint frequency table.

$X \backslash Y$	y_1	\dots	y_j	\dots	y_q
x_1	n_{11}	\dots	n_{1j}	\dots	n_{1q}
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
x_i	n_{i1}	\dots	n_{ij}	\dots	n_{iq}
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots
x_p	n_{p1}	\dots	n_{pj}	\dots	n_{pq}

Joint frequency distribution

Example with grouped data

The height (in cm) and weight (in kg) of a sample of 30 students is:

(179,85), (173,65), (181,71), (170,65), (158,51), (174,66), (172,62), (166,60), (194,90), (185,75), (162,55),
 (187,78), (198,109), (177,61), (178,70), (165,58), (154,50), (183,93), (166,51), (171,65), (175,70), (182,60),
 (167,59), (169,62), (172,70), (186,71), (172,54), (176,68), (168,67), (187,80).

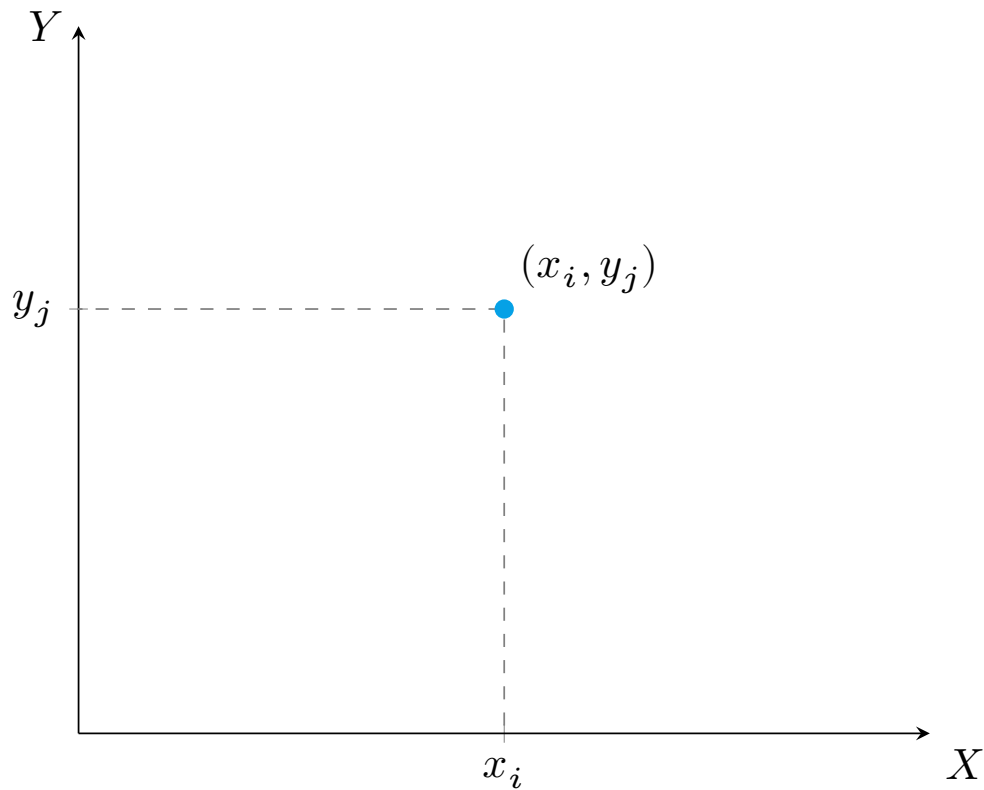
The joint frequency table is

X/Y	$[50, 60)$	$[60, 70)$	$[70, 80)$	$[80, 90)$	$[90, 100)$	$[100, 110)$
$(150, 160]$	2	0	0	0	0	0
$(160, 170]$	4	4	0	0	0	0
$(170, 180]$	1	6	3	1	0	0
$(180, 190]$	0	1	4	1	1	0
$(190, 200]$	0	0	0	0	1	1

Scatter plot

The joint frequency distribution can be represented graphically with a **scatter plot**, where data is displayed as a collections of points on a XY coordinate system.

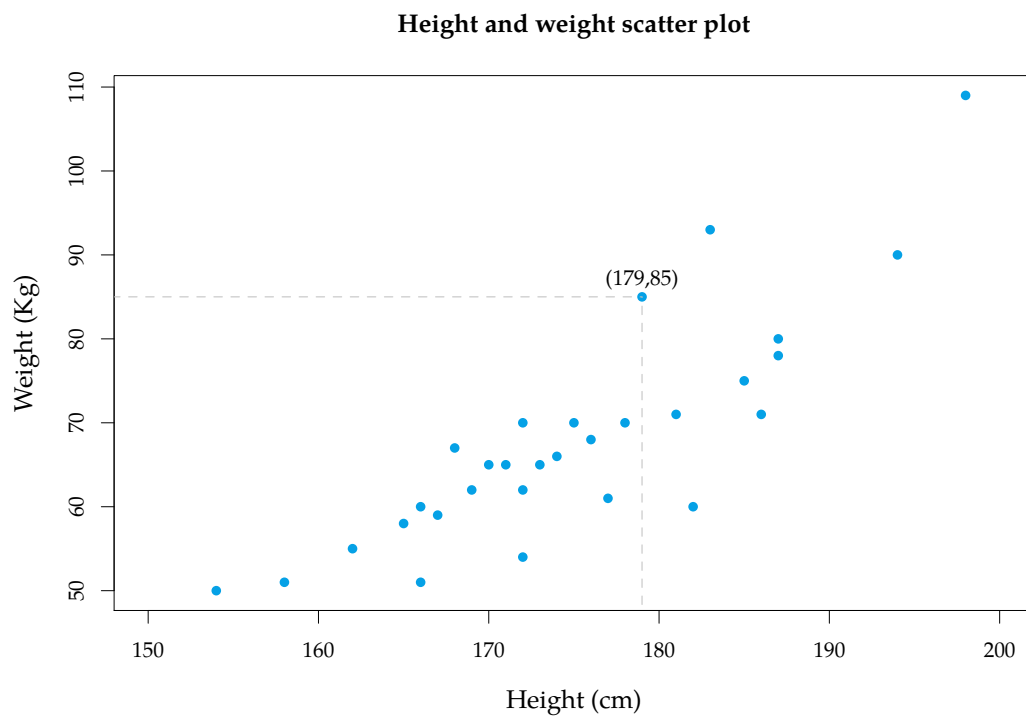
Usually the independent variable is represented in the X axis and the dependent variable in the Y axis. For every data pair (x_i, y_j) in the sample a dot is drawn on the plane with those coordinates.



The result is a set of points that usually is known as a *point cloud*.

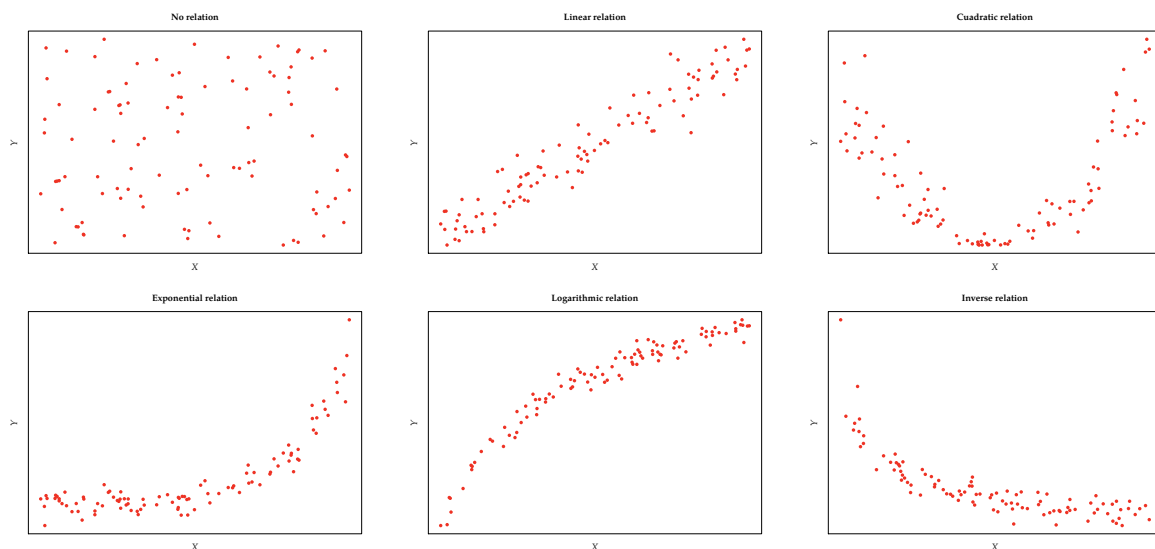
Scatter plot

Example of heights and weights



Scatter plot interpretation

The shape of the point cloud in a scatter plot gives information about the type of relation between the variables.



Marginal frequency distributions

The frequency distributions of each variable of the two-dimensional variable are known as **marginal frequency distributions**.

We can get the marginal frequency distributions from the joint frequency table summing frequencies by rows and columns.

$X \backslash Y$	y_1	\cdots	y_j	\cdots	y_q	n_x
x_1	n_{11}	\cdots	n_{1j}	\cdots	n_{1q}	n_{x_1}
\vdots	\vdots	\vdots	$\downarrow +$	\vdots	\vdots	\vdots
x_i	n_{i1}	$\rightarrow +$	n_{ij}	$\rightarrow +$	n_{iq}	n_{x_i}
\vdots	\vdots	\vdots	$\downarrow +$	\vdots	\vdots	\vdots
x_p	n_{p1}	\cdots	n_{pj}	\cdots	n_{pq}	n_{x_p}
n_y	n_{y_1}	\cdots	n_{y_j}	\cdots	n_{y_q}	n

Marginal frequency distributions

Example of heights and weights

The marginal frequency distributions for the previous sample of heights and weights are

X/Y	[50, 60]	[60, 70]	[70, 80]	[80, 90]	[90, 100]	[100, 110]	n_x
(150, 160]	2	0	0	0	0	0	2
(160, 170]	4	4	0	0	0	0	8
(170, 180]	1	6	3	1	0	0	11
(180, 190]	0	1	4	1	1	0	7
(190, 200]	0	0	0	0	1	1	2
n_y	7	11	7	2	2	1	30

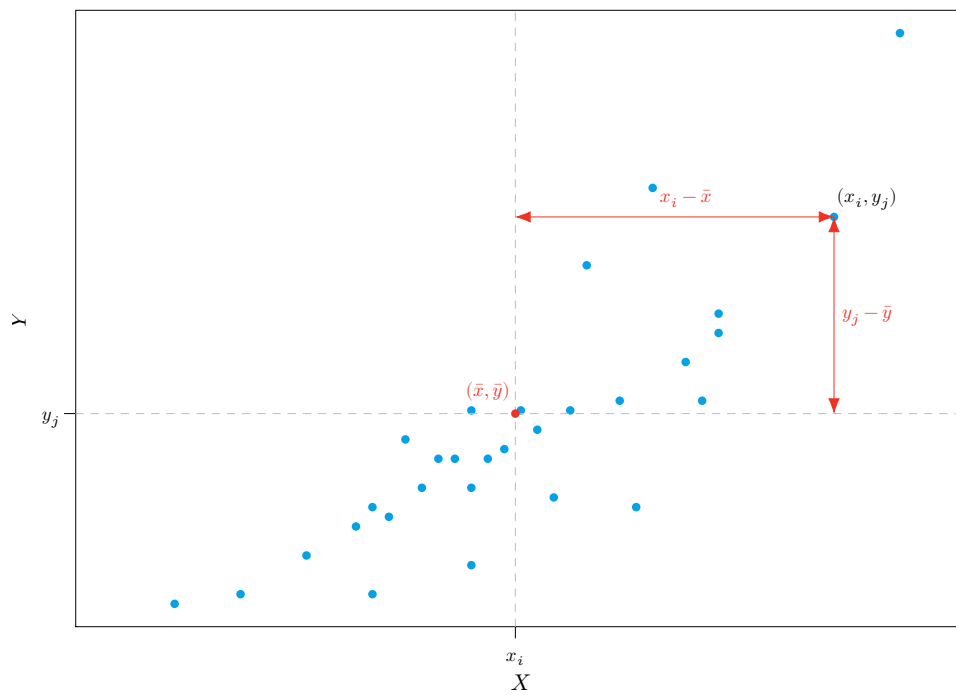
and the corresponding statistics are

$$\begin{aligned} \bar{x} &= 174.67 \text{ cm} & s_x^2 &= 102.06 \text{ cm}^2 & s_x &= 10.1 \text{ cm} \\ \bar{y} &= 69.67 \text{ Kg} & s_y^2 &= 164.42 \text{ Kg}^2 & s_y &= 12.82 \text{ Kg} \end{aligned}$$

1.2 Covariance

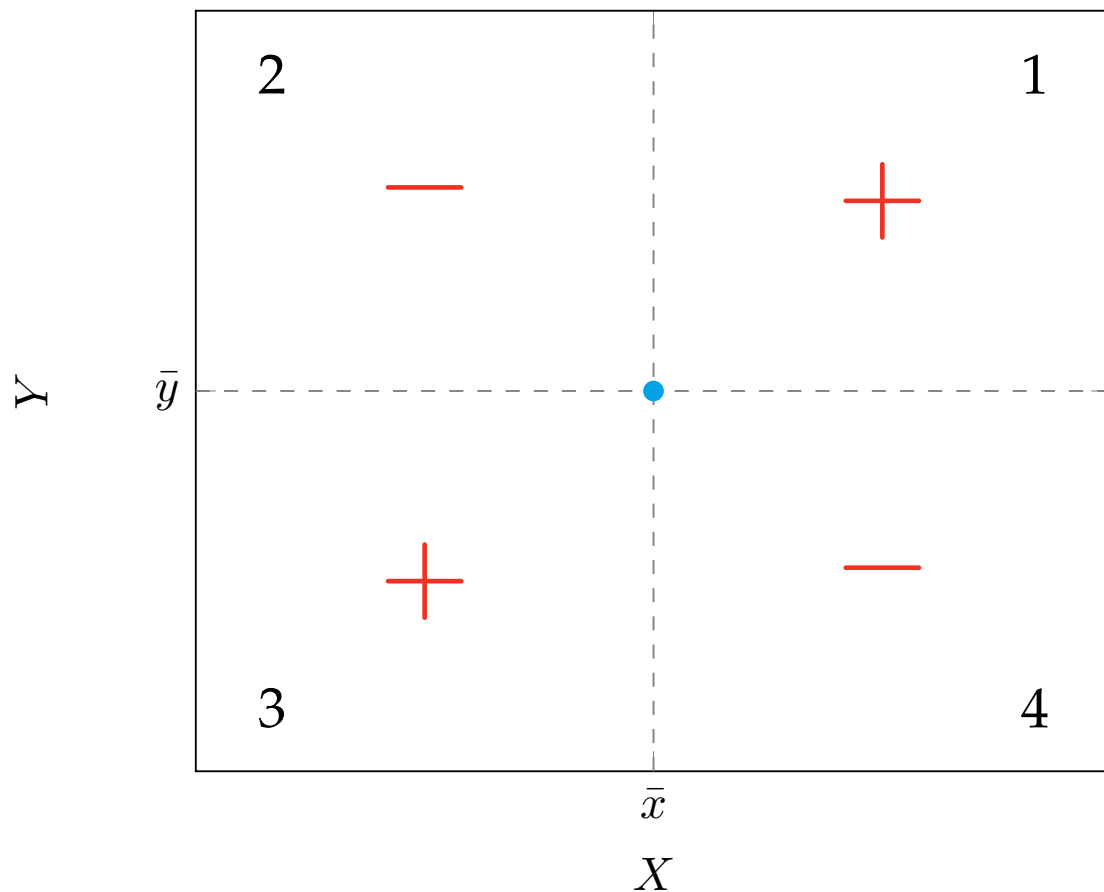
Deviations from the means

To study the relation between two variables, we have to analyze the joint variation of them.



Sign of deviations from the mean

Dividing the point cloud of the scatter plot in 4 quadrants centered in the mean point (\bar{x}, \bar{y}) , the sign of deviations from the mean is:

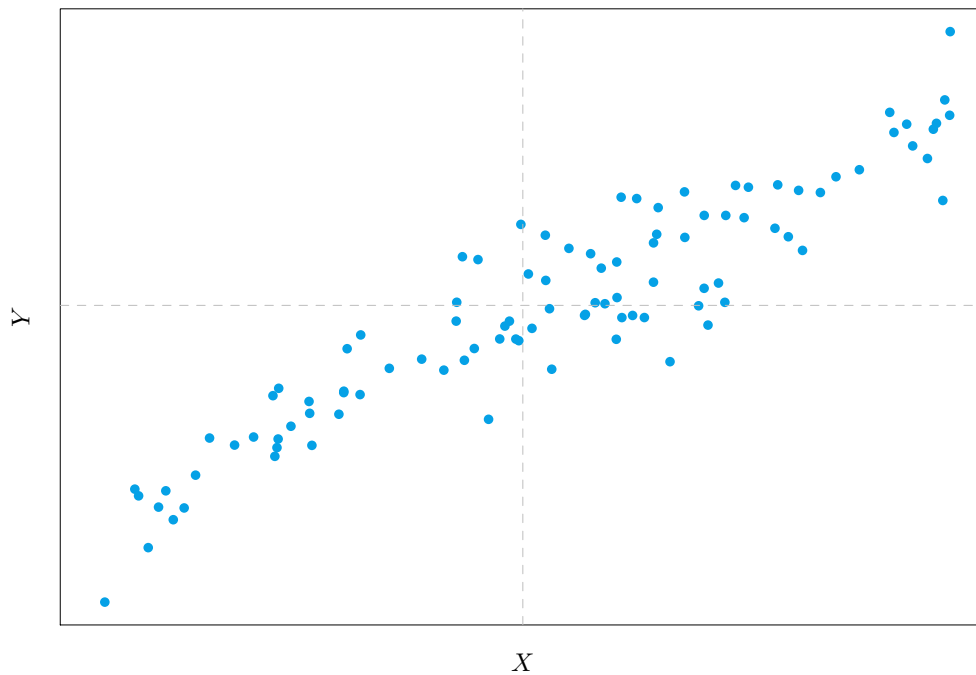


Quadrant	$(x_i - \bar{x})$	$(y_j - \bar{y})$	$(x_i - \bar{x})(y_j - \bar{y})$
1	+	+	+
2	-	+	-
3	-	-	+
4	+	-	-

Sign of the product of deviations from the mean

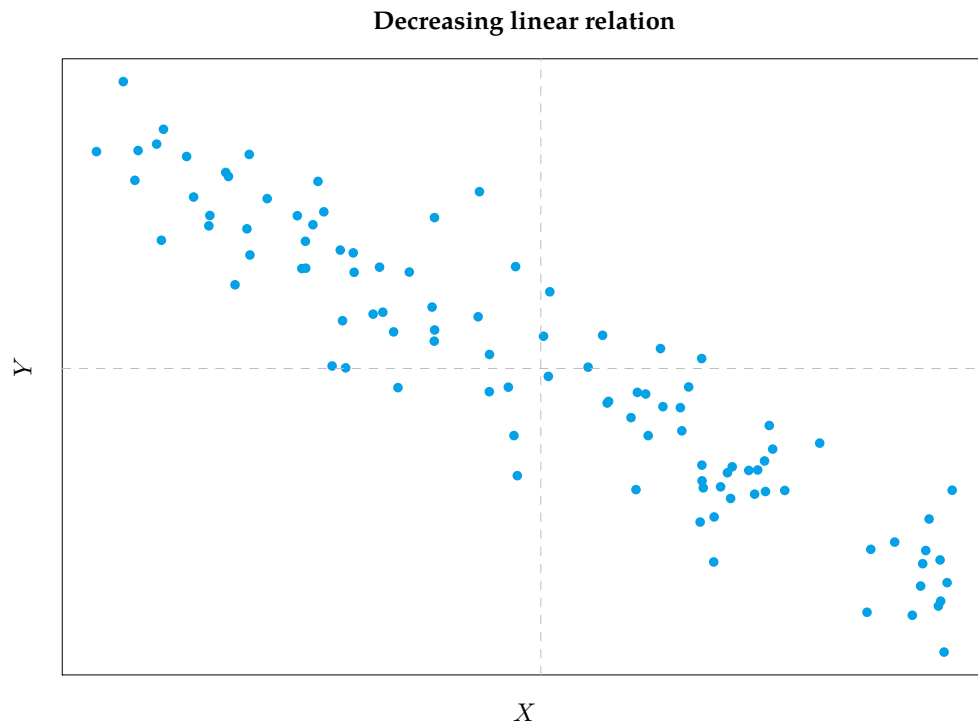
If there is an *increasing linear* relationship between the variables, most of the points will fall in quadrants 1 and 3, and the sum of the products of deviations from the mean will be positive.

Increasing linear relation



$$\sum (x_i - \bar{x})(y_j - \bar{y}) = +$$

If there is an *decreasing linear* relationship between the variables, most of the points will fall in quadrants 2 and 4, and the sum of the products of deviations from the mean will be negative.



$$\sum (x_i - \bar{x})(y_j - \bar{y}) = -$$

Covariance

Using the products of deviations from the mean we get the statistic

Definition 2 (Sample covariance). The *sample covariance* of a two-dimensional variable (X, Y) is the average of the products of deviations from the respective means.

$$s_{xy} = \frac{\sum (x_i - \bar{x})(y_j - \bar{y})n_{ij}}{n}$$

It can also be calculated using the formula

$$s_{xy} = \frac{\sum x_i y_j n_{ij}}{n} - \bar{x}\bar{y}.$$

The covariance measures the linear relation between two variables:

- If $s_{xy} > 0$ there exists an increasing linear relation.
- If $s_{xy} < 0$ there exists a decreasing linear relation.
- If $s_{xy} = 0$ there is no linear relation.

Covariance calculation

Example of heights and weights

Using the joint frequency table of the sample of heights and weights

X/Y	[50, 60)	[60, 70)	[70, 80)	[80, 90)	[90, 100)	[100, 110)	n_x
(150, 160]	2	0	0	0	0	0	2
(160, 170]	4	4	0	0	0	0	8
(170, 180]	1	6	3	1	0	0	11
(180, 190]	0	1	4	1	1	0	7
(190, 200]	0	0	0	0	1	1	2
n_y	7	11	7	2	2	1	30

$$\bar{x} = 174.67 \text{ cm} \quad \bar{y} = 69.67 \text{ Kg}$$

the covariance is

$$\begin{aligned} s_{xy} &= \frac{\sum x_i y_j n_{ij}}{n} - \bar{x}\bar{y} = \frac{155 \cdot 55 \cdot 2 + 165 \cdot 55 \cdot 4 + \dots + 195 \cdot 105 \cdot 1}{30} - 174.67 \cdot 69.67 = \\ &= \frac{368200}{30} - 12169.26 = 104.07 \text{ cm} \cdot \text{Kg}, \end{aligned}$$

This means that there is a increasing linear relation between the weight and the height.

1.3 Regression

Regression

In most cases the goal of a dependency study is not only to detect a relation between two variables, but also to express that relation with a mathematical function,

$$y = f(x)$$

in order to predict the dependent variable for every value of the independent one.

The part of Statistics in charge of constructing such a function is **regression**, and the function is known as **regression function** or **regression model**.

Simple regression models

Depending on the type of function there are a lot of types of regression models. The most common are shown in the table below.

Model	Equation
Linear	$y = a + bx$
Quadratic	$y = a + bx + cx^2$
Cubic	$y = a + bx + cx^2 + dx^3$
Potential	$y = a \cdot x^b$
Exponential	$y = e^{a+bx}$
Logarithmic	$y = a + b \log x$
Inverse	$y = a + \frac{b}{x}$
Sigmoidal	$y = e^{a+\frac{b}{x}}$

The model choice depends on the shape of the points cloud in the scatterplot.

Residuals or predictive errors

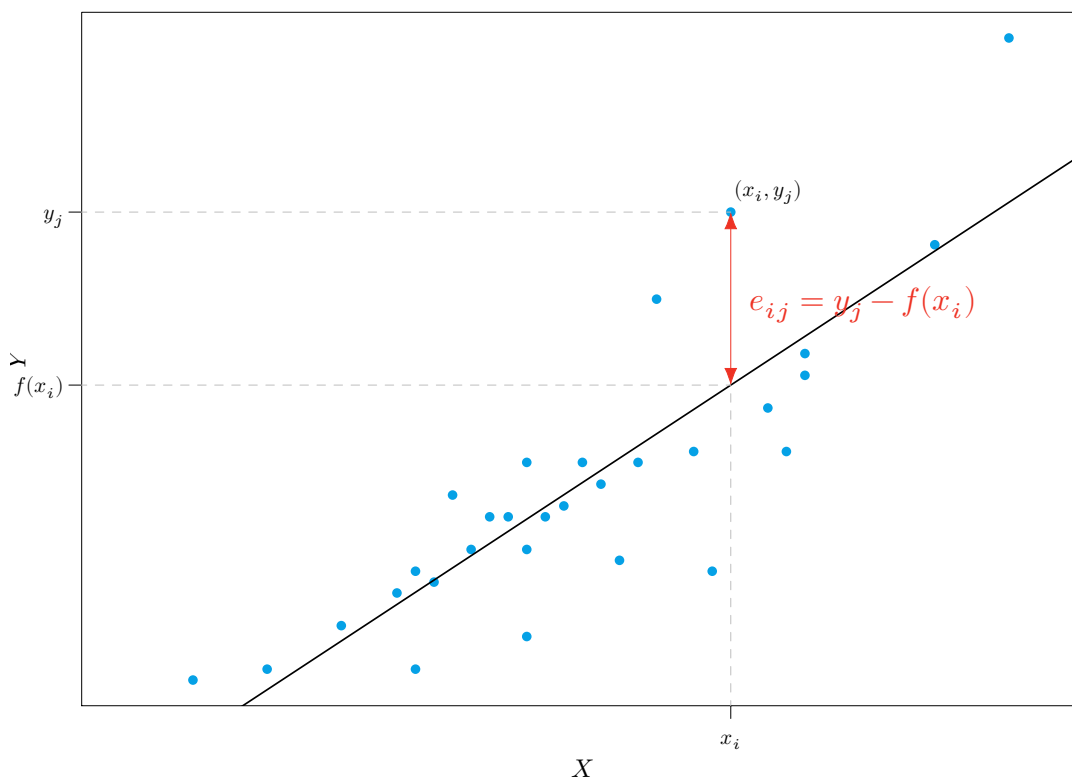
Once chosen the type of regression model, we have to determine which function of that family explains better the relation between the dependent and the independent variables, that is, the function that predicts better the dependent variable.

That function is the function that minimize the distances from the observed values for Y in the sample to the predicted values of the regression function. These distances are known as *residuals* or *predictive errors*.

Definition 3 (Residuals or predictive errors). Given a regression model $y = f(x)$ for a two-dimensional variable (X, Y) , the *residual* or *predictive error* for every pair (x_i, y_j) of the sample is the difference between the observed value of the dependent variable y_j and the predicted value of the regression function for x_i ,

$$e_{ij} = y_j - f(x_i).$$

Residuals or predictive errors on Y



Least squares fitting

A way to get the regression function is the *least squares method*, that determine the function that minimize the squared residuals.

$$\sum e_{ij}^2.$$

For a linear model $f(x) = a + bx$, the sum depends on two parameters, the intercept a , and the slope b of the straight line,

$$\theta(a, b) = \sum e_{ij}^2 = \sum (y_j - f(x_i))^2 = \sum (y_j - a - bx_i)^2.$$

This reduces the problem to determine the values of a and b that minimize this sum.

1.4 Regression line

Least squares fitting of a linear model

To solve the minimization problem, we have to set to zero the partial derivatives with respect to a and b .

$$\begin{aligned}\frac{\partial \theta(a, b)}{\partial a} &= \frac{\partial \sum (y_j - a - bx_i)^2}{\partial a} = 0 \\ \frac{\partial \theta(a, b)}{\partial b} &= \frac{\partial \sum (y_j - a - bx_i)^2}{\partial b} = 0\end{aligned}$$

And solving the equation system, we get

$$a = \bar{y} - \frac{s_{xy}}{s_x^2} \bar{x} \quad b = \frac{s_{xy}}{s_x^2}$$

This values minimize the residuals on Y and give us the optimal linear model.

Regression line

Definition 4 (Regression line). Given a sample of a two-dimensional variable (X, Y) , the *regression line* of Y on X is

$$y = \bar{y} + \frac{s_{xy}}{s_x^2} (x - \bar{x}).$$

The regression line of Y on X is the straight line that minimize the predictive errors on Y , therefore is the linear regression model that gives better predictions of Y .

Regression line calculation

Example of heights and weights

Using the previous sample of heights (X) and weights (Y) with the following statistics

$$\begin{aligned}\bar{x} &= 174.67 \text{ cm} & s_x^2 &= 102.06 \text{ cm}^2 & s_x &= 10.1 \text{ cm} \\ \bar{y} &= 69.67 \text{ Kg} & s_y^2 &= 164.42 \text{ Kg}^2 & s_y &= 12.82 \text{ Kg} \\ & & s_{xy} &= 104.07 \text{ cm} \cdot \text{Kg}\end{aligned}$$

the regression line of weight on height is

$$y = \bar{y} + \frac{s_{xy}}{s_x^2} (x - \bar{x}) = 69.67 + \frac{104.07}{102.06} (x - 174.67) = -108.49 + 1.02x$$

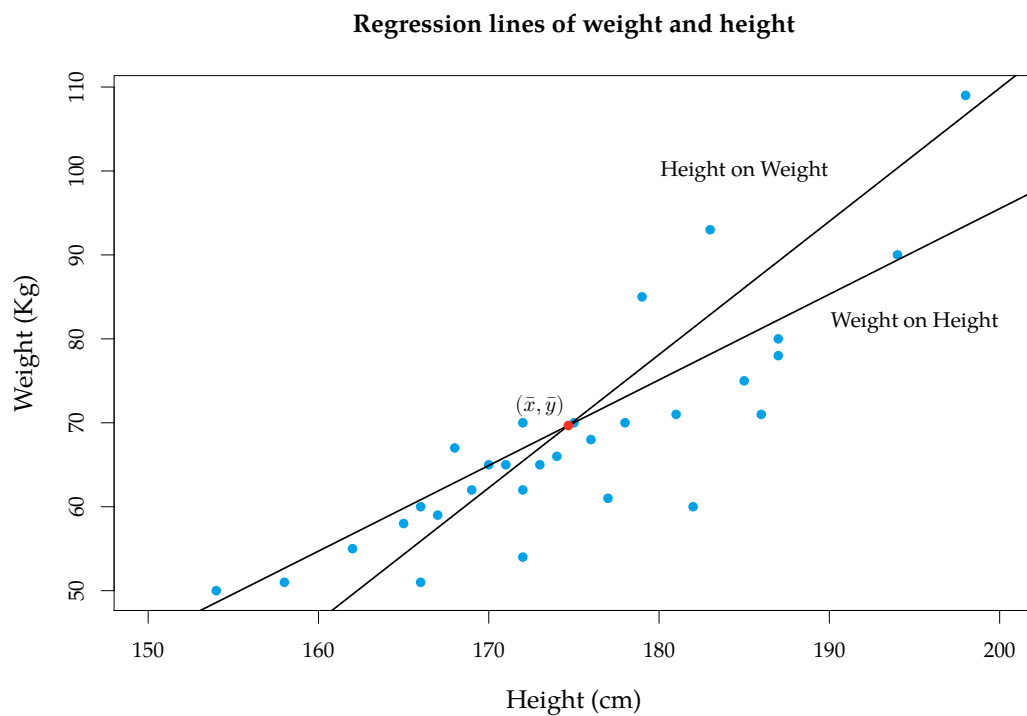
And the regression line of height on weight is

$$x = \bar{x} + \frac{s_{xy}}{s_y^2} (y - \bar{y}) = 174.67 + \frac{104.07}{164.42} (y - 69.67) = 130.78 + 0.63y$$

Observe that the regression lines are different!

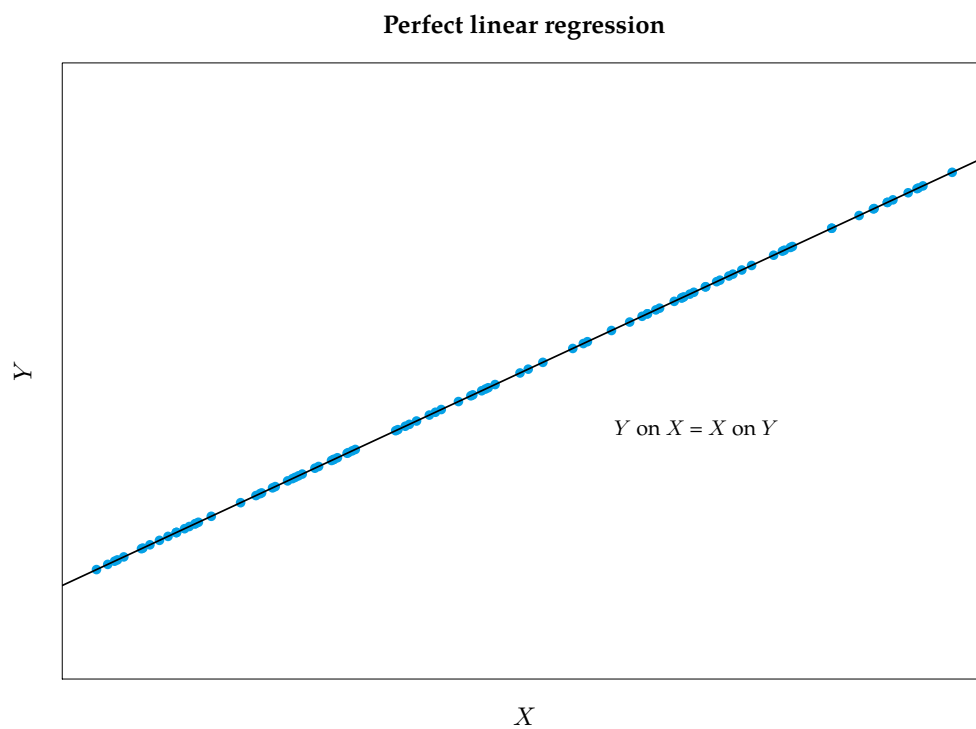
Regression lines

Example of heights and weights



Relative position of the regression lines

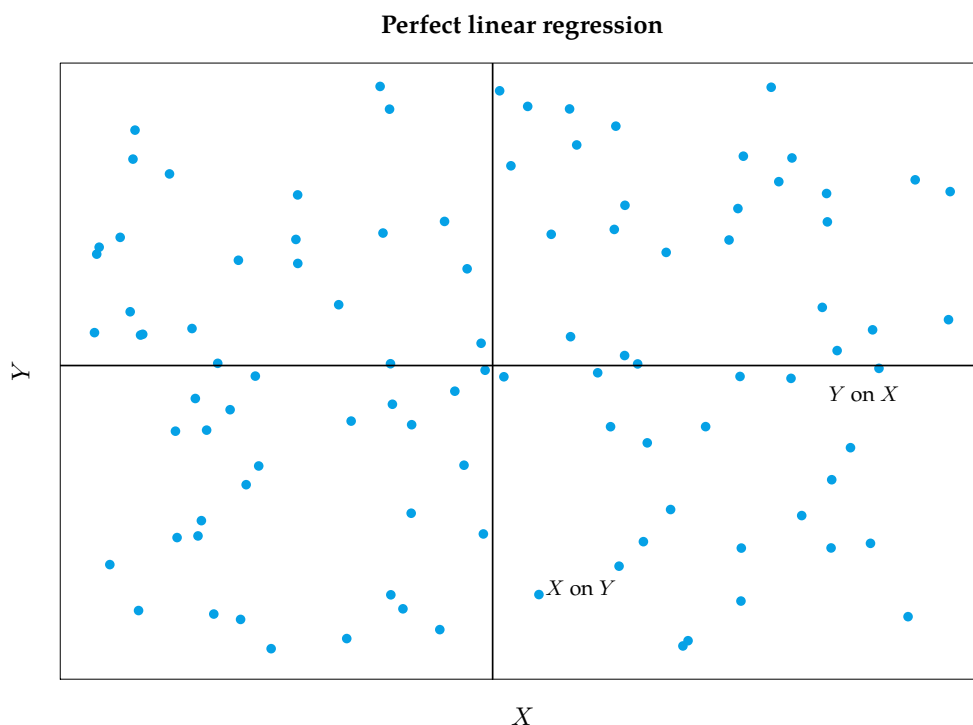
Usually, the regression line of Y on X and the regression line of X on Y are not the same, but they always intersect in the mean point (\bar{x}, \bar{y}) . If there is a perfect linear relation between the variables, then both regression lines are the same, as that line makes both X -residuals and Y -residuals zero.



If there is no linear relation between the variables, then both regression lines are constant and equals to the respective means,

$$y = \bar{y}, \quad x = \bar{x},$$

So, they intersect perpendicularly.



Regression coefficient

The most important parameter of a regression line is the slope.

Definition 5 (Regression coefficient b_{yx}). Given a sample of a two-dimensional variable (X, Y) , the *regression coefficient* of the regression line of Y on X is its slope,

$$b_{yx} = \frac{s_{xy}}{s_x^2}$$

The regression coefficient has always the same sign than the covariance.

It measures how the dependent variable changes in relation to the independent one according to the regression line. In particular, it gives the number of units that the dependent variable increases or decreases for every unit that increases the independent variable.

Regression coefficient

Example of heights and weights

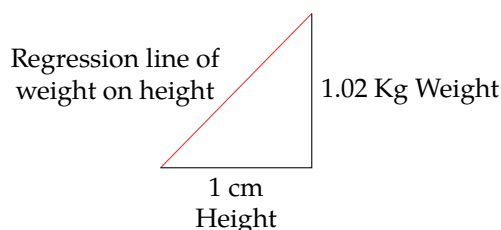
In the sample of heights and weights, the regression line of weight on height was

$$y = -108.49 + 1.02x.$$

Thus, the regression coefficient of weight on height was

$$b_{yx} = 1.02 \text{Kg/cm}.$$

That means that, according to the regression line of weight on height, the weight will increase 1.02 Kg for every cm that increases the height.



Regression predictions

Example of heights and weights

Usually the regression models are used to predict the dependent variable for some values of the independent variable.

Watch out! To get the best predictions of a variable you have to use the regression line where that variable plays the dependent variable role.

Thus, in the sample of heights and weights, to predict the weight of a person with a height of 180 cm, we have to use the regression line of weight on height,

$$y = -108.49 + 1.02 \cdot 180 = 75.11 \text{ Kg.}$$

But to predict the height of a person with a weight of 79 Kg, we have to use the regression line of height on weight,

$$x = 130.78 + 0.63 \cdot 79 = 180.55 \text{ cm.}$$

However, how reliable are these predictions?

1.5 Correlation

Correlation

Once we have a regression model, in order to see if it is a good predictive model we have to assess the goodness of fit of the model and the strength of the relation set by it. The part of Statistics in charge of this is **correlation**.

The correlation study the residuals of a regression model: the smaller the residuals, the greater the goodness of fit, and the stronger the relation set by the model.

Residual variance

To measure the goodness of fit of a regression model is common to use the *residual variance*.

Definition 6 (Sample residual variance s_{ry}^2). Given a regression model $y = f(x)$ de of a two-dimensional variable (X, Y) , its *sample residual variance* is the average of the squared residuals,

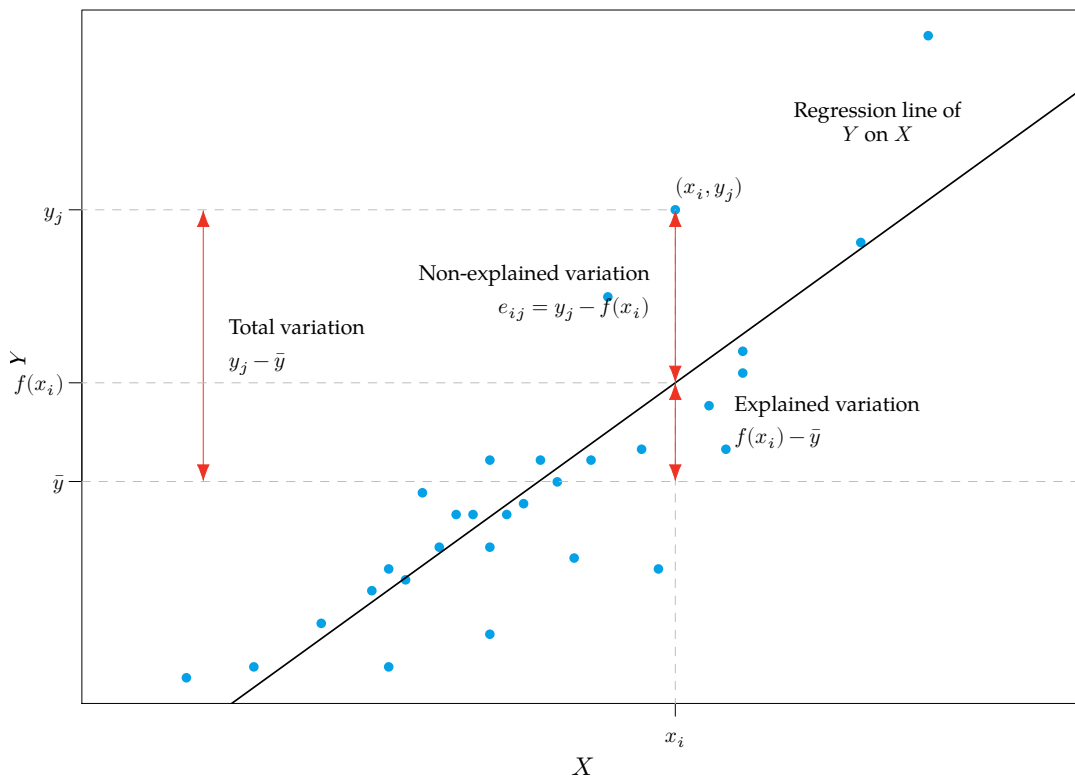
$$s_{ry}^2 = \frac{\sum e_{ij}^2 n_{ij}}{n} = \frac{\sum (y_j - f(x_i))^2 n_{ij}}{n}.$$

The greater the residuals, the greater the residual variance and the smaller the goodness of fit.

When the linear relation is perfect, the residuals are zero and the residual variance is zero. Conversely, when there are no relation, the residuals coincide with deviations from the mean, and the residual variance is the same than the variance of the dependent variable.

$$0 \leq s_{ry}^2 \leq s_y^2$$

Explained and non-explained variation



1.6 Correlation coefficients

Coefficient of determination

From the residual variance is possible to define another correlation statistic easier to interpret.

Definition 7 (Sample coefficient of determination r^2). Given a regression model $y = f(x)$ of a two-dimensional variable (X, Y) , its *coefficient of determination* is

$$r^2 = 1 - \frac{s_{ry}^2}{s_y^2}$$

As the residual variance ranges from 0 to s_y^2 ,

$$0 \leq r^2 \leq 1$$

The greater r^2 is, the greater the goodness of fit of the regression model, and more reliable will be its predictions. In particular,

- If $r^2 = 0$ then there is no relation as set by the regression model.
- If $r^2 = 1$ then the relation set by the model is perfect.

Linear coefficient of determination

When the regression model is linear, the residual variance is

$$\begin{aligned}
 s_{ry}^2 &= \sum e_{ij}^2 f_{ij} = \sum (y_j - f(x_i))^2 f_{ij} = \sum \left(y_j - \bar{y} - \frac{s_{xy}}{s_x^2} (x_i - \bar{x}) \right)^2 f_{ij} = \\
 &= \sum \left((y_j - \bar{y})^2 + \frac{s_{xy}^2}{s_x^4} (x_i - \bar{x})^2 - 2 \frac{s_{xy}}{s_x^2} (x_i - \bar{x})(y_j - \bar{y}) \right) f_{ij} = \\
 &= \sum (y_j - \bar{y})^2 f_{ij} + \frac{s_{xy}^2}{s_x^4} \sum (x_i - \bar{x})^2 f_{ij} - 2 \frac{s_{xy}}{s_x^2} \sum (x_i - \bar{x})(y_j - \bar{y}) f_{ij} = \\
 &= s_y^2 + \frac{s_{xy}^2}{s_x^4} s_x^2 - 2 \frac{s_{xy}}{s_x^2} s_{xy} = s_y^2 - \frac{s_{xy}^2}{s_x^2}.
 \end{aligned}$$

and the coefficient of determination is

$$r^2 = 1 - \frac{s_{ry}^2}{s_y^2} = 1 - \frac{s_y^2 - \frac{s_{xy}^2}{s_x^2}}{s_y^2} = 1 - 1 + \frac{s_{xy}^2}{s_x^2 s_y^2} = \frac{s_{xy}^2}{s_x^2 s_y^2}.$$

Linear coefficient of determination calculation

Example of heights and weights

In the sample of heights and weights, we had

$$\begin{aligned}
 \bar{x} &= 174.67 \text{ cm} & s_x^2 &= 102.06 \text{ cm}^2 \\
 \bar{y} &= 69.67 \text{ Kg} & s_y^2 &= 164.42 \text{ Kg}^2 \\
 s_{xy} &= 104.07 \text{ cm} \cdot \text{Kg}
 \end{aligned}$$

Thus, the linear coefficient of determination is

$$r^2 = \frac{s_{xy}^2}{s_x^2 s_y^2} = \frac{(104.07 \text{ cm Kg})^2}{102.06 \text{ cm}^2 \cdot 164.42 \text{ Kg}^2} = 0.65.$$

This means that the linear model of weight on height explains the 65% of the variation of weight, and the linear model of height on weight also explains 65% of the variation of height.

Correlation coefficient

Definition 8 (Sample correlation coefficient). Given a sample of a two-dimensional variable (X, Y) , the *sample correlation coefficient* is the square root of the linear coefficient of determination, with the sign of the covariance,

$$r = \sqrt{r^2} = \frac{s_{xy}}{s_x s_y}.$$

As r^2 ranges from 0 to 1, r ranges from -1 to 1,

$$-1 \leq r \leq 1$$

The correlation coefficient measures the strength of the linear association but also its direction (increasing or decreasing):

- If $r = 0$ then there is no linear relation.
- Si $r = 1$ then there is a perfect increasing linear relation.
- Si $r = -1$ then there is a perfect decreasing linear relation.

Correlation coefficient

Example of heights and weights

In the sample of heights and weights, we had

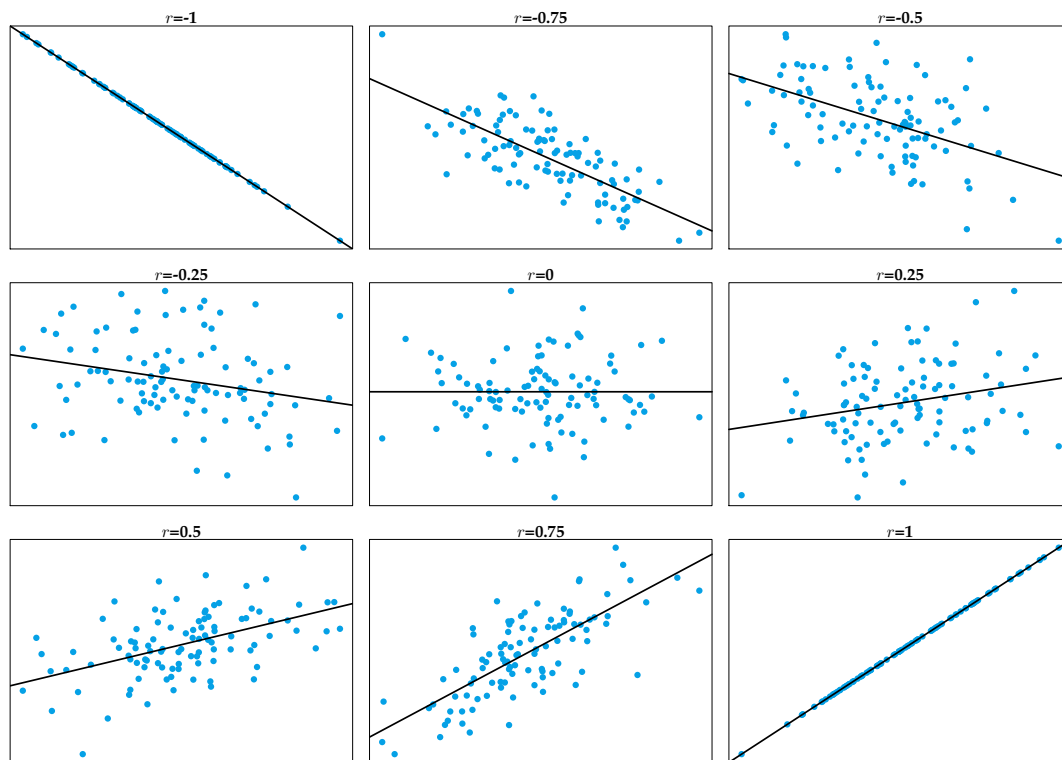
$$\begin{aligned}\bar{x} &= 174.67 \text{ cm} & s_x^2 &= 102.06 \text{ cm}^2 \\ \bar{y} &= 69.67 \text{ Kg} & s_y^2 &= 164.42 \text{ Kg}^2 \\ s_{xy} &= 104.07 \text{ cm} \cdot \text{Kg}\end{aligned}$$

Thus, the correlation coefficient is

$$r = \frac{s_{xy}}{s_x s_y} = \frac{104.07 \text{ cm Kg}}{10.1 \text{ cm} \cdot 12.82 \text{ Kg}} = +0.8.$$

This means that there is a rather strong linear increasing relation between height and weight.

Different correlations



Reliability of regression predictions

The coefficient of determination explains the goodness of fit of a regression model, but there are other factors that influence the reliability of regression predictions:

- The coefficient of determination: The greater r^2 , the greater the goodness of fit and the more reliable the predictions.
- The variability of the population distribution: The greater the variation, the more difficult to predict and the less reliable the predictions.
- The sample size: The greater the sample size, the more information we have and the more reliable the predictions.

In addition, we have to take into account that a regression model is only valid for the range of values observed by the sample. That means that, as we don't have any information outside that range, we must not do predictions for values far from that range.

1.7 Non-linear regression

Non-linear regression

The fit of a non-linear regression can be also done by least square fitting method.

However, in some cases the fitting of a non-linear model can be reduced to the fitting of a linear model applying a simple transformation to the variables of the model.

Transformations of non-linear regression models

- **Logarithmic model:** A logarithmic model $y = a + b \log x$ can be transformed in a linear model with the change $t = \log x$:

$$y = a + b \log x = a + bt.$$

- **Exponential model:** An exponential model $y = e^{a+bx}$ can be transformed in a linear model with the change $z = \log y$:

$$z = \log y = \log(e^{a+bx}) = a + bx.$$

- **Potential model:** A potential model $y = ax^b$ can be transformed in a linear model with the changes $t = \log x$ and $z = \log y$:

$$z = \log y = \log(ax^b) = \log a + b \log x = a' + bt.$$

- **Inverse model:** An inverse model $y = a + b/x$ can be transformed in a linear model with the change $t = 1/x$:

$$y = a + b(1/x) = a + bt.$$

- **Sigmoidal model:** A sigmoidal model $y = e^{a+b/x}$ can be transformed in a linear model with the changes $t = 1/x$ and $z = \log y$:

$$z = \log y = \log(e^{a+b/x}) = a + b(1/x) = a + bt.$$

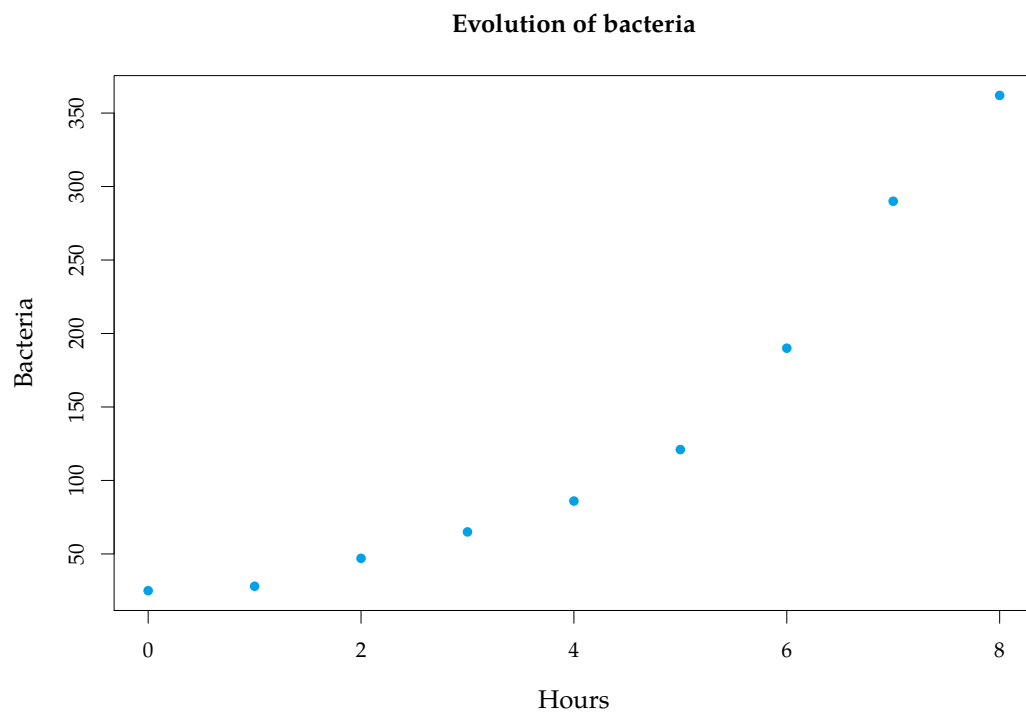
Exponential relation

Example of evolution of a bacterial culture

The number of bacteria in a culture evolves with time according to the table below.

Hours	Bacteria
0	25
1	28
2	47
3	65
4	86
5	121
6	190
7	290
8	362

The scatter plot of the sample is showed below.



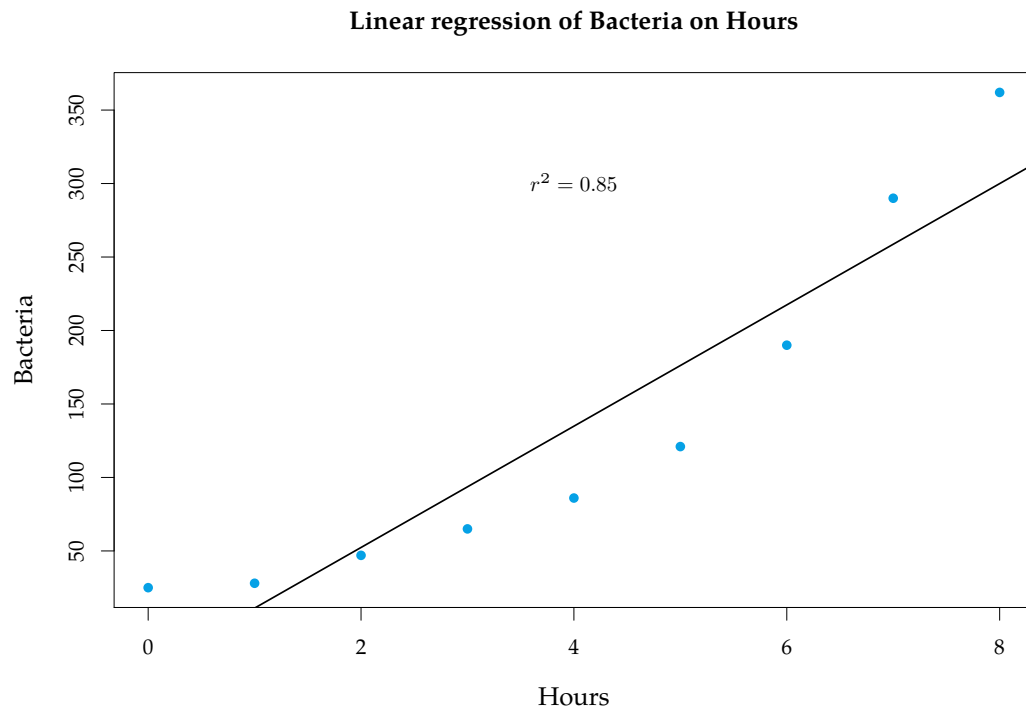
Exponential relation

Example of evolution of a bacterial culture

Fitting a linear model we get

Hours	Bacteria
0	25
1	28
2	47
3	65
4	86
5	121
6	190
7	290
8	362

Bacteria = $-30.18 + 41,27 \text{ Hours}$, with $r^2 = 0.85$.



Is a good model?

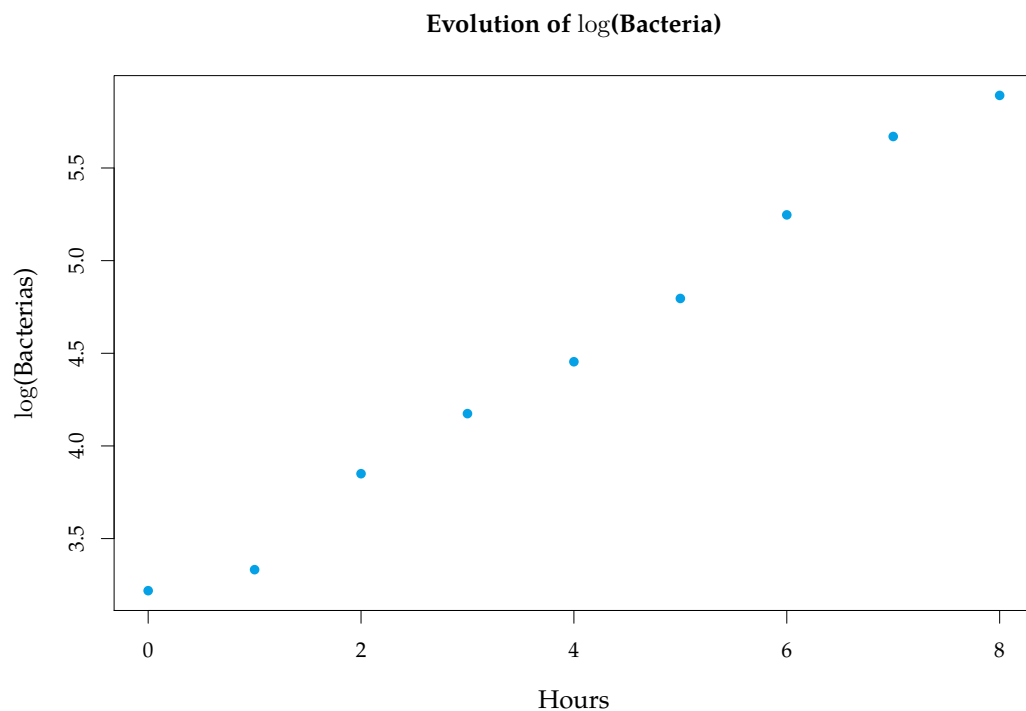
Fitting an exponential regression model

Example of evolution of a bacterial culture

Although the linear model is not bad, according to the shape of the point cloud of the scatter plot, an exponential model looks more suitable.

To construct an exponential model $y = e^{a+bx}$ we can apply the transformation $z = \log y$, that is, applying a logarithmic transformation to the dependent variable.

Hours	Bacteria	$\log(\text{Bacteria})$
0	25	3.22
1	28	3.33
2	47	3.85
3	65	4.17
4	86	4.45
5	121	4.80
6	190	5.25
7	290	5.67
8	362	5.89



Fitting an exponential regression model

Example of evolution of a bacterial culture

Now it only remains to compute the regression line of the logarithm of bacteria on hours,

$$\log(\text{Bacteria}) = 3.107 + 0.352 \text{ Horas},$$

and, undoing the change of variable,

$$\text{Bacteria} = e^{3.107+0.352 \text{ Horas}},$$

with $r^2 = 0.99$.

Thus, the exponential model fits much better than the linear model.