BIE-PST – Probability and Statistics

Lecture 12: Linear regression

Winter semester 2023/2024

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12 Linear regression

12.1 Covariance and correlation

Suppose we want to examine the connection between two variables.

Sometimes we expect that there is a relation, sometimes we can assume there is not.

Examples 12.1.

- Heights of sons and heights of fathers.
- Bodily weight and height.
- Mean temperature and latitude from city to city.
- Income and the number of years spent studying.
- Number of storks and number of newborns in a city (see literature).

First we model this connection using *correlation*.
The *covariance* of two random variables X and Y is defined as

$$\operatorname{cov}(X,Y) = \mathrm{E}\left((X - \mathrm{E}\,X)(Y - \mathrm{E}\,Y)\right)$$

and can be computed as

$$\operatorname{cov}(X,Y) = \mathrm{E}\,(XY) - \mathrm{E}\,X\,\mathrm{E}\,Y.$$

The *correlation coefficient* is defined as

$$\rho_{X,Y} = \frac{\operatorname{cov}(X,Y)}{\sqrt{\operatorname{var} X}\sqrt{\operatorname{var} Y}}$$

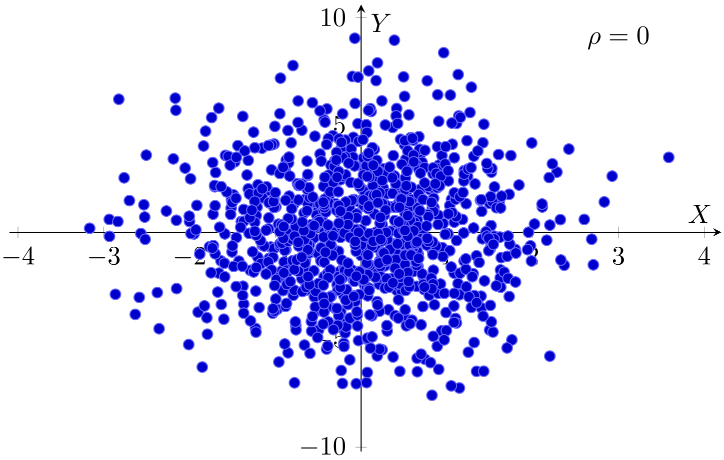
and gives a measure of the *linear dependence* between X and Y.

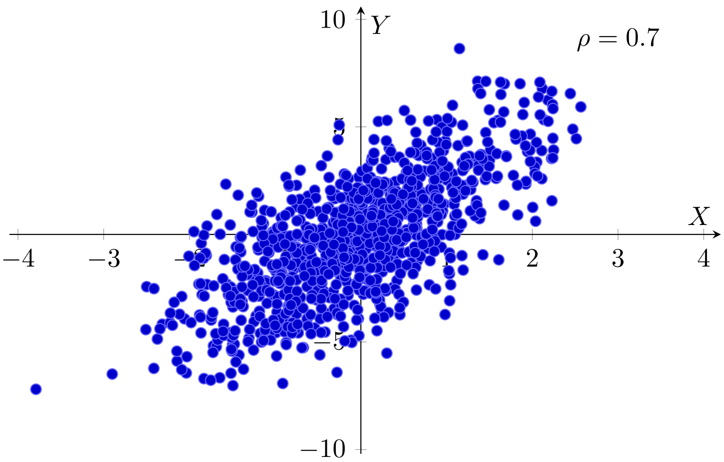
Theorem 12.2. *For the correlation coefficient $\rho_{X,Y}$ it holds that*

1. $\rho_{X,Y} \in [-1,1]$.
2. *If X and Y are independent, then $\rho_{X,Y} = 0$.*
3. *If $Y = a + bX$ for $b > 0$, then $\rho_{X,Y} = 1$.*
4. *If $Y = a + bX$ for $b < 0$, then $\rho_{X,Y} = -1$.*

Proof. See lecture 6. □

Correlation – sample of 1000 values





Based on a random sample of pairs $(X_1, Y_1), \ldots, (X_n, Y_n)$, the covariance can be estimated using the *sample covariance*:

$$s_{X,Y} = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X}_n)(Y_i - \bar{Y}_n).$$

The correlation coefficient can be estimated using the *sample correlation coefficient* as

$$r_{X,Y} = \frac{s_{X,Y}}{s_X s_Y},$$

where $s_X = \sqrt{s_X^2}$ and $s_Y = \sqrt{s_Y^2}$ are the sample standard deviations of X and Y, respectively.

The sample covariance can be rewritten as

$$\begin{aligned} s_{X,Y} &= \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)(Y_i - \bar{Y}_n) \\ &= \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i Y_i - n\bar{X}_n\bar{Y}_n\right) \\ &= \frac{n}{n-1}\left(\frac{1}{n}\sum_{i=1}^{n} X_i Y_i - \bar{X}_n\bar{Y}_n\right). \end{aligned}$$

From the law of large numbers it follows that it is a consistent estimator of the covariance.

Because the sample variances are consistent estimators of the real variances, the sample correlation is therefore a consistent estimator of the correlation coefficient itself.

Example 12.3 (– comparing heights of fathers and sons)**.** Suppose we want to estimate the correlation between the heights of fathers and their sons. We have observed five pairs of fathers and their sons, now adults. Their heights were measured as follows:

height of father [cm]	X_i	172	176	180	184	186
height of son [cm]	Y_i	178	183	180	188	190

We have computed the following characteristics from the data:

$$\sum_{i=1}^{n} X_i = 898, \qquad \sum_{i=1}^{n} Y_i = 919,$$

$$\sum_{i=1}^{n} X_i^2 = 161412, \qquad \sum_{i=1}^{n} Y_i^2 = 169017,$$

$$\sum_{i=1}^{n} X_i Y_i = 165156.$$

From the observed characteristics we compute the sample means, variances and the covariance:

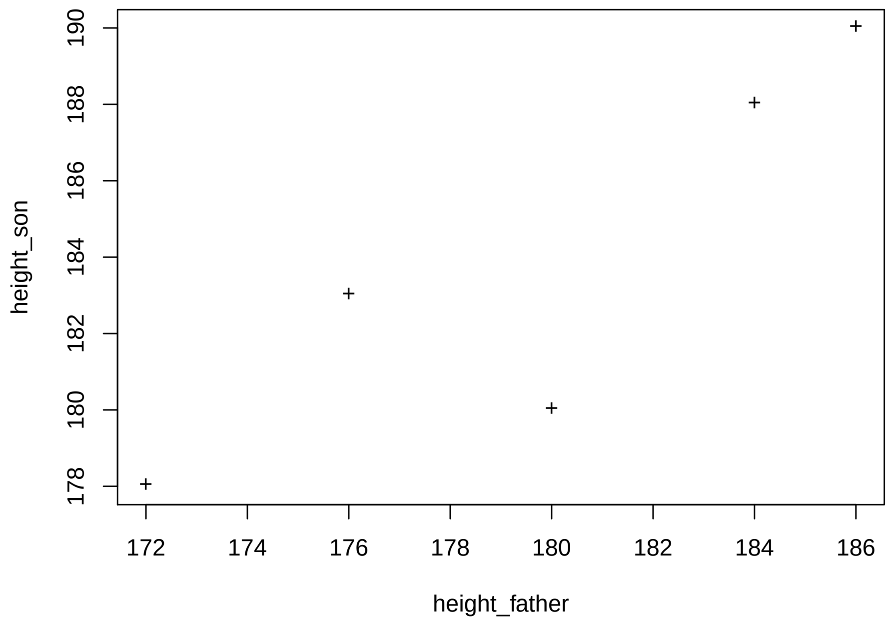
$$\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i = \frac{898}{5} = 179.6, \qquad \bar{Y}_n = \frac{1}{n}\sum_{i=1}^{n} Y_i = \frac{919}{5} = 183.8,$$

$$\begin{aligned} s_X^2 &= \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i^2 - n\bar{X}_n^2\right) = \frac{1}{4}\left(161412 - 5\cdot 179.6^2\right) = 32.8, \\ s_Y^2 &= \frac{1}{n-1}\left(\sum_{i=1}^{n} Y_i^2 - n\bar{Y}_n^2\right) = \frac{1}{4}\left(169017 - 5\cdot 183.8^2\right) = 26.2, \\ s_{X,Y} &= \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i Y_i - n\bar{X}_n\bar{Y}_n\right) = \frac{1}{4}\left(165156 - 5\cdot 179.6\cdot 183.8\right) = 25.9. \end{aligned}$$

The sample correlation coefficient is obtained as

$$r_{X,Y} = \frac{s_{X,Y}}{\sqrt{s_X^2 s_Y^2}} = \frac{25.9}{\sqrt{32.8\cdot 26.2}} \doteq 0.883.$$

We can conclude that there is a positive correlation between the height of sons and their fathers. The sample correlation coefficient can be computed in `R` using `cor(height_father,height_son)`.



We want to be able to determine whether the correlation between the variables is *statistically significant.*

Theorem 12.4. *When observing* independent normally distributed pairs*, then when* $\rho_{X,Y} = 0$*, the statistic*

$$T = \frac{r_{X,Y}}{\sqrt{1 - r_{X,Y}^2}}\sqrt{n-2}$$

has the Student's t-distribution with $n-2$ *degrees of freedom.*

Proof. See literature. □

We can then test the hypothesis $H_0 : \rho_{X,Y} = 0$ and reject it in favor of $H_A : \rho_{X,Y} \neq 0$ on level of significance α if $|T| > t_{\alpha/2,n-2}$, i.e., if the standardised sample correlation coefficient differs significantly from zero.

Is there a significant correlation between the heights of fathers and their sons? Test on $\alpha = 5\%$.

We obtain

$$T = \frac{r_{X,Y}}{\sqrt{1 - r_{X,Y}^2}}\sqrt{n-2} \doteq \frac{0.883}{\sqrt{1 - 0.883^2}}\sqrt{3} \doteq 3.267.$$

The critical value $t_{\alpha/2,n-2} = t_{0.025,3} = 3.182$, thus

$$3.267 = |T| > t_{0.025,3} = 3.182.$$

We reject the null hypothesis that there is no correlation on level of significance 5%. We say that there is a *statistically significant* positive correlation between the heights of fathers and the heights of their sons.

Testing for zero correlation – example

Example 12.5 (– comparing heights of fathers and sons, continued)**.** We can test the non-correlation of the previous example in `R` using `cor.test`:

```
> cor.test(height_father,height_son)

        Pearson's product-moment correlation

data:  height_father and height_son
t = 3.267, df = 3, p-value = 0.04688
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
 0.00564631 0.99229297
sample estimates:
      cor
0.8835115
```

The p-value is smaller than $\alpha = 5\%$, thus we reject the hypothesis that there is no correlation on level of significance 5%. Alternatively we can decide based on the t-statistic $T = 3.267$.

12.2 Regression model

We are often also interested in observing and evaluating the *dependence* of a random variable Y *on* an *explanatory variable* x, which *is not random.*

Examples 12.6.

- The number of cars passing a bridge during various times of the day.
- Body height depending on the age of a person.
- Body weight depending on the height of a person.
- The wind speed depending on the altitude.

Suppose there is a linear dependence of a random variable $Y = Y(x)$ on an explanatory variable x. We measure n *independent observations* $Y_i = Y(x_i)$ at points $x_1, \ldots, x_n$ and thus we obtain pairs $(x_1, Y_1), \ldots, (x_n, Y_n)$.

Based on these pairs we want to *analyze the linear dependence* of $Y = Y(x)$ on x.
For the description of the linear dependence we can use the *linear regression model*

$$Y_i = \alpha + \beta x_i + \varepsilon_i \qquad i = 1, \ldots, n,$$

where:

- x_i are given values – not all equal,
- ε_i are i.i.d. zero mean random variables (experimental errors, often $\mathrm{N}(0, \sigma^2)$),
- α and β are unknown parameters.

It follows that:

$$\mathrm{E}\, Y_i = \alpha + \beta x_i, \qquad \operatorname{var} Y_i = \operatorname{var} \varepsilon_i = \sigma^2.$$

We want to find estimators a and b of the *parameters* α and β such that the values

$$\hat{Y}_i = a + b x_i$$

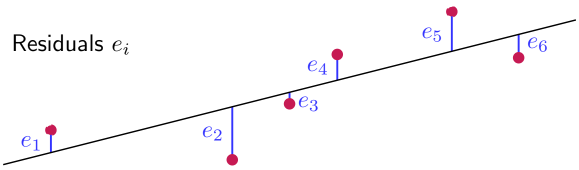
are the best approximations of Y_i.

12.2.1 Least squares method

Parameters α and β are estimated using the *least squares method*.

Good estimators a and b are such values which minimize the *residual sum of squares* S_e:

$$S_e = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} (Y_i - (a + b x_i))^2.$$



The estimated regression line $a + bx$ has the *minimal* sum of the second powers (squares) of the *vertical* distance from the measured values.

Theorem 12.7. *Point estimators of the regression parameters obtained by the least squares method are*

$$b = \frac{\sum_{i=1}^{n} (x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{\sum_{i=1}^{n} (x_i - \bar{x}_n)^2} \quad \textit{and} \quad a = \bar{Y}_n - b\,\bar{x}_n,$$

where $\bar{x}_n = \frac{1}{n} \sum_{i=1}^{n} x_i$ *and* $\bar{Y}_n = \frac{1}{n} \sum_{i=1}^{n} Y_i$.

An unbiased estimator of the variance $\operatorname{var} Y_i = \sigma^2$ *is*

$$s^2 = \frac{1}{n-2} \sum_{i=1}^{n} (Y_i - a - b x_i)^2 = \frac{1}{n-2}\, S_e$$

and is called the residual variance*.*

Proof. We proceed for concrete observations $y_1, \dots, y_n$: By differentiating S_e with respect to a and b we find the minimum:

$$\frac{\partial S_e}{\partial a} = 0, \qquad \frac{\partial S_e}{\partial b} = 0.$$

$$-2 \sum_{i=1}^{n} (y_i - a - b \cdot x_i) = 0 \quad \rightarrow \quad a = \bar{y}_n - b\,\bar{x}_n$$

$$-2 \sum_{i=1}^{n} (y_i - a - b x_i)\, x_i = 0$$

$$
\begin{aligned}
0 &= \sum_{i=1}^{n} x_i y_i - \bar{y}_n \sum_{i=1}^{n} x_i - b \sum_{i=1}^{n} x_i^2 + b\,\bar{x}_n \sum_{i=1}^{n} x_i \\
b &= \frac{\sum_{i=1}^{n} x_i y_i - n\bar{y}_n\bar{x}_n}{\sum_{i=1}^{n} x_i^2 - n\bar{x}_n^2} = \frac{\sum_{i=1}^{n}(y_i - \bar{y}_n)(x_i - \bar{x}_n)}{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2}
\end{aligned}
$$

By computing the matrix of second derivatives and showing that it is positive definite it can be proven that this point is indeed the minimum. For the proof of the unbiasedness of the estimator of the variance see literature. □

✓ *It can be shown that the above mentioned estimators are the best unbiased estimators of the regression parameters.*

If we treated the explanatory variables as random, $X_1, \ldots, X_n$, the estimator of the regression parameter β can be given by means of estimators of variances and the covariance:

$$
b = \frac{\sum_{i=1}^{n}(X_i - \bar{X}_n)(Y_i - \bar{Y}_n)}{\sum_{i=1}^{n}(X_i - \bar{X}_n)^2} = \frac{s_{X,Y}}{s_X^2} = r_{X,Y}\frac{s_Y}{s_X}\,,
$$

where $s_{X,Y}$ is the sample covariance and $r_{X,Y}$ is the sample correlation coefficient

$$
s_{X,Y} = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)(Y_i - \bar{Y}_n), \qquad r_{X,Y} = \frac{s_{X,Y}}{s_X s_Y}
$$

and s_X and s_Y are the sample standard deviations – square roots of sample variances

$$
s_X^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2, \qquad s_Y^2 = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \bar{Y}_n)^2.
$$

Example 12.8 (– dependence of the heights of sons on the heights of their fathers)**.** Suppose we want to model the linear dependence of the heights of sons on the heights of their fathers from the previous example. Their height was measured as follows:

height of father [cm]	x_i	172	176	180	184	186
height of son [cm]	Y_i	178	183	180	188	190

We find the sample variance and covariance as follows:

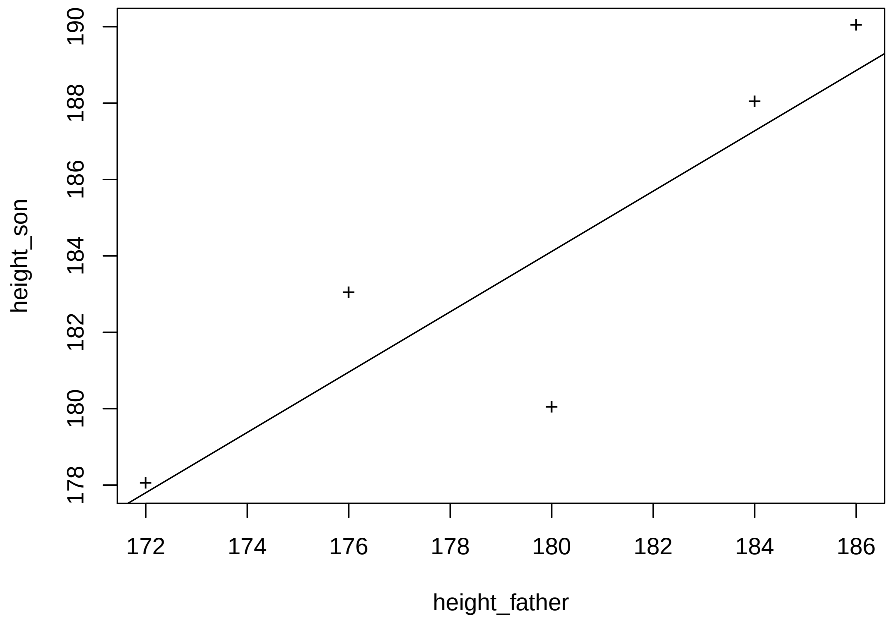
$$
s_X^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2 = 32.8, \qquad s_{X,Y} = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)(Y_i - \bar{Y}_n) = 25.9.
$$

The parameters of the regression line are then estimated as

$$
\begin{aligned}
b &= \frac{s_{X,Y}}{s_X^2} = \frac{25.9}{32.8} \doteq 0.79 \\
a &= \bar{Y}_n - b\cdot\bar{X}_n \doteq 183.8 - \frac{25.9}{32.8}\cdot 179.6 \doteq 41.98.
\end{aligned}
$$

For every centimeter of difference between the fathers' height, we expect an average difference of 0.79 centimeters between their sons.

The estimates can be called in `R` using `lm(height_son height_father)`.



12.2.2 Precision of the regression model

For evaluating the precision of a linear model we can use the *coefficient of determination* R^2*:*

$$R^2 = 1 - \frac{S_e}{S_T},$$

where S_e is the residual sum of squares and $S_T = (n-1)s_Y^2$:

$$S_T = \sum_{i=1}^{n}(Y_i - \bar{Y}_n)^2.$$

The closer R^2 *is to 1 the better the linear model fits the data.* More precisely, it can be compared with the critical values of its proper distribution – see literature.

R^2 can be interpreted as the proportion of variability in the data which is explained by the regression model.

12.2.3 Testing linear independence

Often we want to test the hypothesis

$$H_0 : \beta = 0 \qquad \text{versus} \qquad H_A : \beta \neq 0.$$

Which equivalently means testing

$$H_0 : Y_i = \alpha + \varepsilon_i \qquad \text{versus} \qquad H_A : Y_i = \alpha + \beta x_i + \varepsilon_i.$$

In fact we test whether Y actually does linearly depend on x or not. Testing can be based on the *two-sided confidence interval* for β. When the random errors ε_i are normally distributed, then the corresponding confidence interval can be found as:

$$\left(b - t_{\alpha/2,n-2}\frac{\sqrt{s^2}}{\sqrt{(n-1)s_X^2}}\ ,\ b + t_{\alpha/2,n-2}\frac{\sqrt{s^2}}{\sqrt{(n-1)s_X^2}}\right),$$

where s^2 is the *residual variance* from the last theorem and $t_{\alpha/2,n-2}$ is the critical value of the Student's t-distribution with $n-2$ degrees of freedom. We can then check whether 0 lies in the interval or not. Alternatively we can decide based on the p-value of the test.

Example 12.9 (– heights of fathers and sons, continued)**.** We want to test whether the heights of sons depend significantly on the heights of their fathers. In `R` we can call the properties of a fitted linear model using `summary(lm())`:

```
> summary(lm(height_son~height_father))

Call:
lm(formula = height_son ~ height_father)

Residuals:
      1       2       3       4       5
 0.2012  2.0427 -4.1159  0.7256  1.1463

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)    41.9817    43.4272   0.967   0.4050
height_father   0.7896     0.2417   3.267   0.0469 *
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.769 on 3 degrees of freedom
Multiple R-squared:  0.7806,    Adjusted R-squared:  0.7075
F-statistic: 10.67 on 1 and 3 DF,  p-value: 0.04688
```

The p-value corresponding to $H_0 : \beta = 0$ is 0.0469 and is smaller than $\alpha = 5\%$. On level of significance 5% we can thus reject the hypothesis that there is no dependence.

12.2.4 Prediction intervals

Suppose that we have estimated the parameters of the regression model from obtained data. For a new value x for which we do not know the value Y we may be interested in a *prediction* of Y and the *confidence interval* for the prediction.

Prediction $\hat{Y}$:

$$\hat{Y} = a + b \cdot x.$$

$(1-\alpha)100\%$ confidence interval for the prediction

$$a + b \cdot x \pm t_{\alpha/2,n-2}\sqrt{s^2}\sqrt{\frac{1}{n} + \frac{(x-\bar{x}_n)^2}{\sum_{i=1}^n (x_i - \bar{x}_n)^2}}.$$

If we plot the regression line and the boundaries of the confidence interval of the prediction as a function of x, we obtain the *pointwise confidence intervals*.

We can also construct a band in which the regression line lies with a probability $1-\alpha$. Such band is called the *confidence band for the whole regression line*. The corresponding expression is based on the Fisher's F-distribution (see literature), with $t_{\alpha/2,n-2}$ replaced with $\sqrt{2F_{\alpha/2,2,n-2}}$.

Example 12.10 (– dependence of the heights of sons on the heights of their fathers)**.** *Suppose we want to estimate the expected height of a son whose father is 175 centimeters tall.* For given $x = 175$ cm, we want to predict $\hat{Y}$:

$$\begin{aligned}\hat{Y} &= a + b \cdot x \\ &\doteq 41.98 + 0.79 \cdot 175 \\ &\doteq 180.2 \text{ cm.}\end{aligned}$$

The 95% confidence interval for the prediction is then

$$(174.9, 185.5).$$

Example 12.11 (– concentration of lactic acid)**.** It was studied how much lactic acid there is in 100 ml of new mothers' blood (values x_i) and their newborn children (values Y_i) directly after birth.

x_i	40	64	34	15	57	45
Y_i	33	46	23	12	56	40

We consider a linear dependence between the concentration in mothers' and their children's blood. The estimates of the regression parameters are:

$$\begin{aligned}b &= \frac{\sum_{i=1}^{6}(x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{\sum_{i=1}^{6}(x_i - \bar{x}_n)^2} = 0.8543 \\ a &= \bar{Y}_n - b\bar{x}_n = -1.3082\end{aligned}$$

Let us test the hypothesis that the concentration in mother's blood does not influence the concentration in their children's blood: $H_0 : \beta = 0$ versus $H_A : \beta \neq 0$

The 95% confidence interval for β is

$$0 \notin (0.404, 1.305).$$

This means that we reject the null hypothesis. The dependence is thus significant.

Example 12.11 (– concentration of lactic acid, continued)**.** Let us plot the measured data, the estimated regression line and corresponding confidence bands: