Linear regression

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Probability and Statistics

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Content

- **Probability theory:**
  - Events, probability, conditional probability, Bayes' Theorem, independence of events.
  - Random variables, distribution function, functions of random variables, characteristics of random variables: expected value, variance, moments, generating function, quantiles, critical values, important discrete and continuous distributions.
  - Random vectors, joint and marginal distributions, functions of random vectors, independence of random variables, conditional distribution, conditional expected value, covariance and correlation.
  - Markov's and Chebyshev's inequality, weak law of large numbers, strong law of large numbers, Central limit theorem.
- **Mathematical statistics:**
  - Point estimators, sample mean, sample variance, properties of point estimators, Maximum likelihood method.
  - Interval estimators, hypothesis testing, one-sided vs. two-sided alternatives, linear regression, estimators of regression parameters, testing of linear model.

Recap

Based on a **random sample** of i.i.d. random variables $X_1, \ldots, X_n$ from a parametric distribution F_θ we can:

- Estimate the parameters using **point estimates** – sample mean, sample variance, etc.
- Find **confidence intervals** – regions, where the parameter lies with a large probability:

$$\mathrm{P}(L < \theta < U) = 1 - \alpha.$$

- Test **hypotheses** – verify whether statements about parameters may or may not be true, with a given maximal probability of wrongful rejection.

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

- 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.

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First we model this connection using **correlation**.

Covariance and correlation

The **covariance** of two random variables X and Y is defined as

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

and can be computed as

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

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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.

Covariance and correlation

Theorem

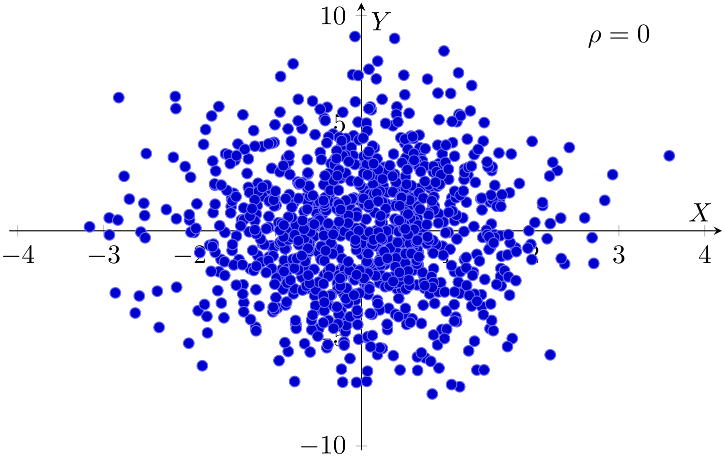
For the correlation coefficient $\rho_{X,Y}$ it holds that

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



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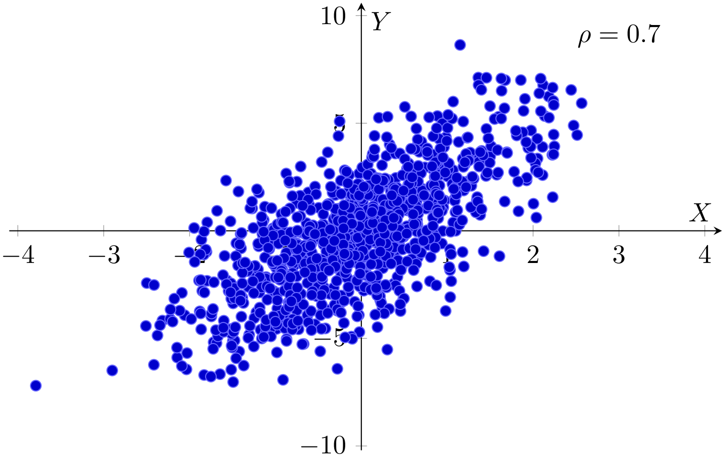

Covariance and correlation – estimation

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**:

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

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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.

Sample covariance and correlation – properties

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.

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

Estimating the correlation – example

Example – 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

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We have computed the following characteristics from the data:

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

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

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

Estimating the correlation – example

Example – comparing heights of fathers and sons, continued

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

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

$$s_X^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i^2 - n\bar{X}_n^2\right) = \frac{1}{4}\left(161412 - 5\cdot 179.6^2\right) = 32.8,$$

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The sample correlation coefficient is obtained as

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

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The sample correlation coefficient can be computed in R using

`cor(height_father,height_son)`.

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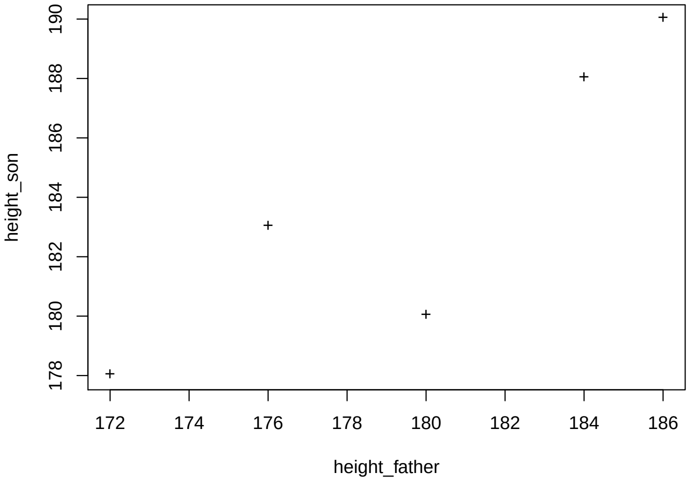

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We want to be able to determine whether the correlation between the variables is **statistically significant**.

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Theorem

*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. □

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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.

Testing for zero correlation – example

Example – comparing heights of fathers and sons, continued

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

We obtain

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

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

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We reject the null hypothesis that there is no correlation on level of significance 5%.

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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 – comparing heights of fathers and sons, continued

We can test the non-correlation 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 $T = 3.267$.

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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 $x_1, \dots, x_n$ and thus we obtain pairs $(x_1, Y_1), \dots, (x_n, Y_n)$.

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Based on these pairs we want to analyze the linear dependence of $Y = Y(x)$ on x.

Regression model

For the description of the linear dependence we can use the **linear regression model**

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

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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.

Least squares method

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

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

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

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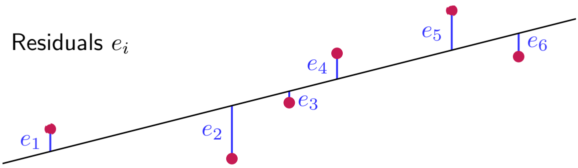

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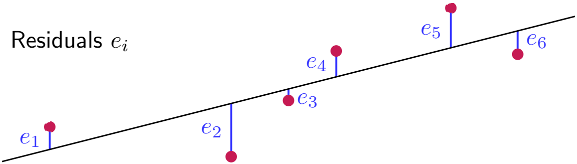

The estimated regression line $a + bx$ has the minimal sum of the second powers (squares) of the vertical distance from the measured values.

Estimating parameters of the regression line

Theorem

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*

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

and is called the ***residual variance****.*

Estimating parameters of the regression line

Proof

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

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$$0 = \sum_{i=1}^{n} x_i y_i - \bar{y}_n \sum_{i=1}^{n} x_i - b\sum_{i=1}^{n} x_i^2 + b\,\bar{x}_n \sum_{i=1}^{n} x_i$$

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$$b = \frac{\sum_{i=1}^{n} x_i y_i - n\bar{y}_n\bar{x}_n}{\sum_{i=1}^{n} x_i^2 - n\bar{x}_n^2}$$

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Estimating parameters of the regression line

Proof

We proceed for concrete observations $y_1, \dots, y_n$:
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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

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

Linear regression – example

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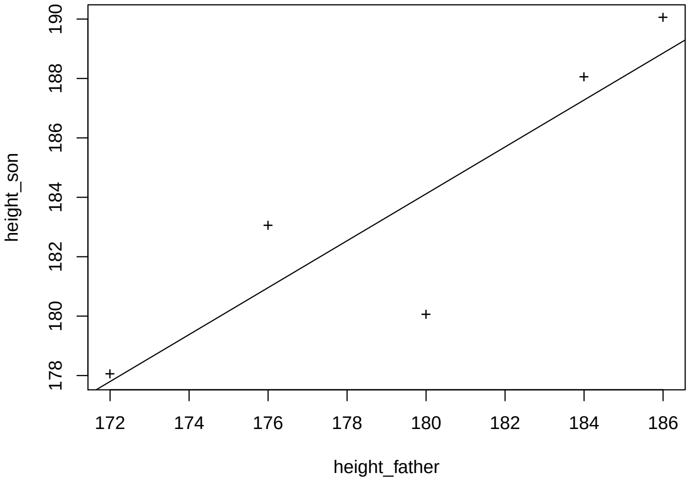
The estimates can be called in R using `lm(height_son height_father)`.

Linear regression – example



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 $S_T = (n-1)s_Y^2$:

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

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

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

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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.

Testing linear independence – example

Example – 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.

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.

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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 $\sqrt{2F_{\alpha/2,2,n-2}}$.

Regression prediction – example

Example – 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.

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For given $x = 175$ cm, we want to predict $\hat{Y}$:

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

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

The 95% confidence interval for the prediction is then

$$(174.9, 185.5).$$

Example – 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.

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$$b = \frac{\sum_{i=1}^{6}(x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{\sum_{i=1}^{6}(x_i - \bar{x}_n)^2} = 0.8543$$

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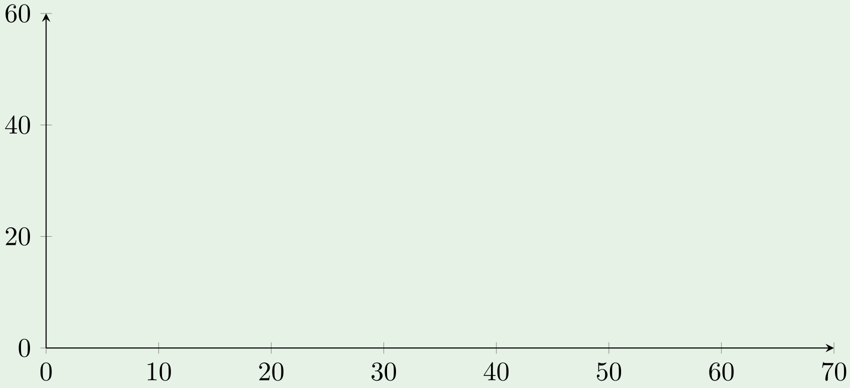
The 95% confidence interval for β is

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

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

Example – concentration of lactic acid, continued

Let us plot the measured data, the estimated regression line and corresponding confidence bands:



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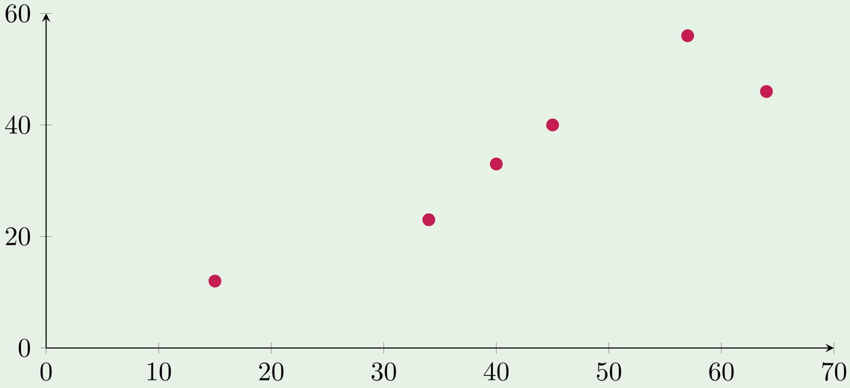

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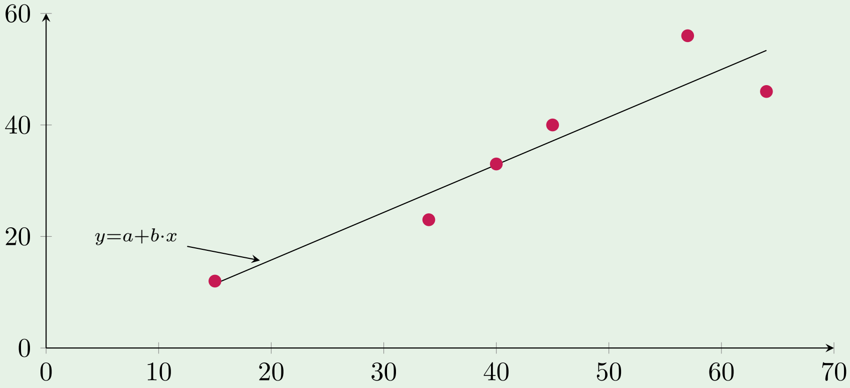

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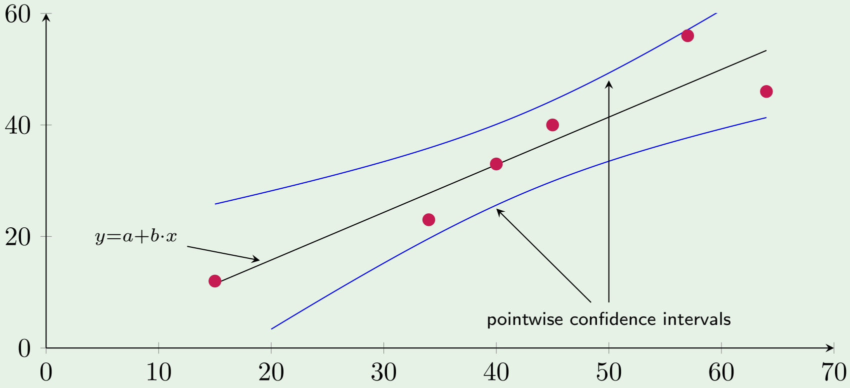

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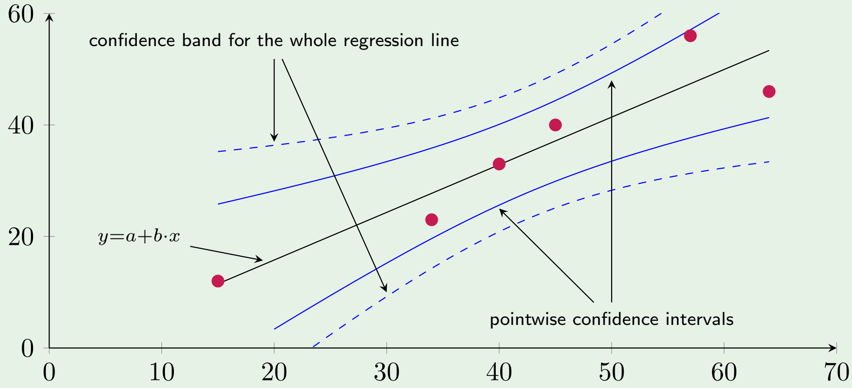

Recap

The **correlation coefficient** gives a measure of linear dependence between two random variables and is defined as

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

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

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

where $s_{X,Y}$ is the **sample covariance**.

If we want to model the dependence of Y on x taken as fixed, we can use **linear regression**. We assume that there is a linear dependence of the form

$$Y_i = \alpha + \beta x_i + \varepsilon_i,$$

where ε_i are independent zero-mean random errors and α and β are parameters which we want to estimate.

Given observed data, we obtain the estimators a and b of the parameters using the **least squares method** as:

$$b = \frac{\sum_{i=1}^{n} x_i y_i - n\bar{x}_n\bar{y}_n}{\sum_{i=1}^{n} x_i^2 - n\bar{x}_n^2} = \frac{s_{X,Y}}{s_X^2} = r_{X,Y}\frac{s_Y}{s_X},$$

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