



# Introduction to probability, statistics and data handling

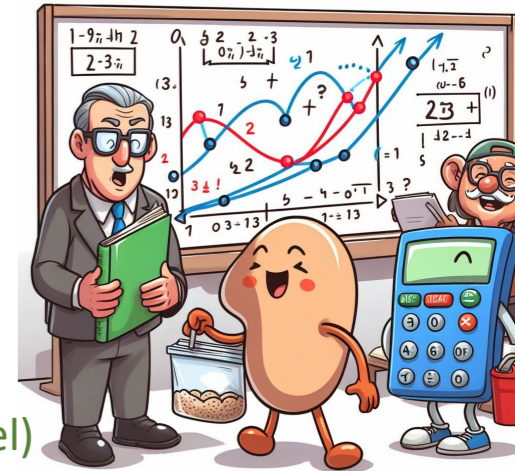
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# Curve fitting and regression

- In many practical problems, when collecting data, we may find that two (or more) R.V.s may **exhibit a relationship**
- It seems so natural to exploit this and express this fact using a mathematical function (model)
- The trick here would be to find the model that **FITS the best** our data (we also say that it connects the R.V.s)



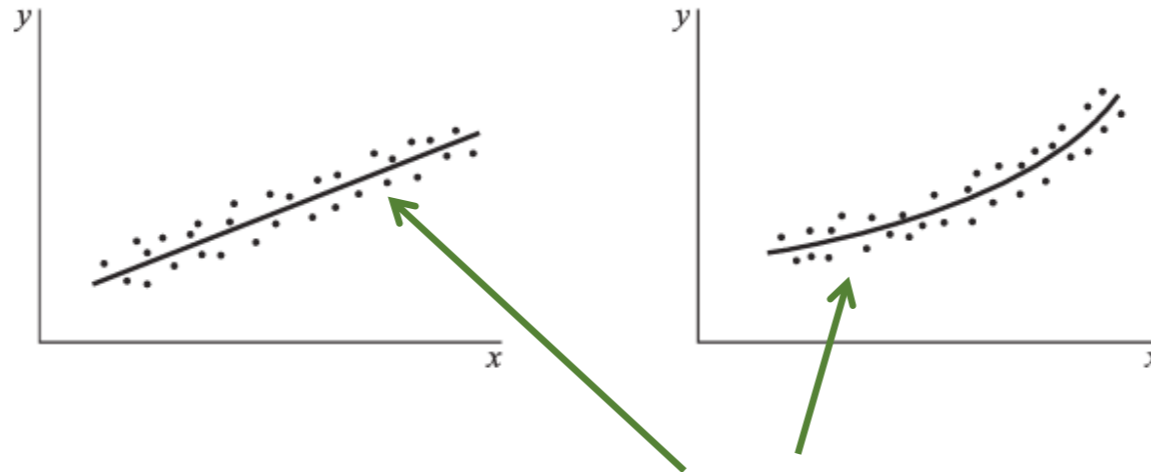
Regression is a statistical approach used to analyze the relationship between a dependent variable (target variable) and one or more independent variables (predictor variables). The objective is to determine the most suitable function that characterizes the connection between these variables. It seeks to find the best-fitting model, which can be utilized to make predictions or draw conclusions.

- Although this technique is well established and used, still **some experience is needed** when we want to choose the right model (this also may be driven by the physics of the phenomena, e.g., radioactive decay)
- NOTE, we may sometimes, when the relation is very complicated, or we are dealing with many dimensions, use the **machine learning approach** – in fact the linear regression can also be treated as machine learning.



# Regression - first steps

- Usually, we make first the **scatter plot** using collected data and take a look...

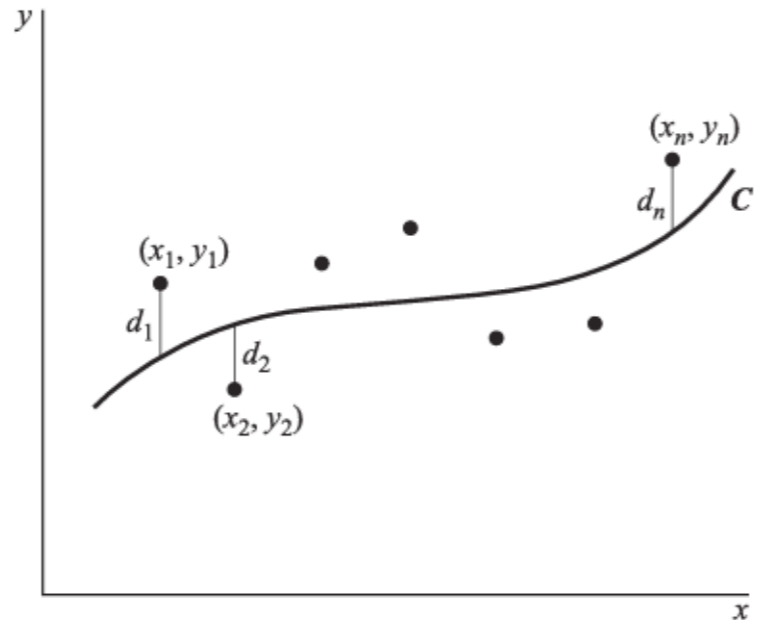


- The solid lines above are called approximating curves and **the approximation of parameters**
- What we need to work out is the **equation of this curve**, ex.  $y = a + bx$ , the variable **x is the independent variable**, and **y is the dependent variable**.
- That task is called **curve fitting**.
- Often to understand the relation, we may need to apply some transformation(s) to the variables



# Least squares again!

- We have already encountered that technique when discussed general estimation theory. The idea is again the same we are going to minimise squares of residuals
- Again, the goal is to estimate a bunch of parameters but this time this is going to lead us to bit different result
- Lets define the data as pairs:  $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$ , next we make the scatter plot

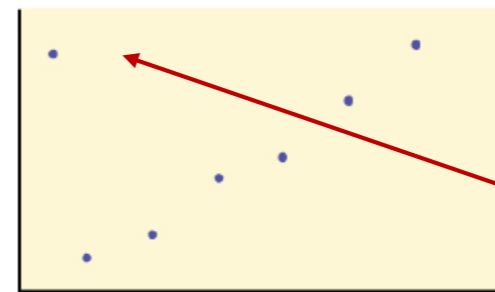
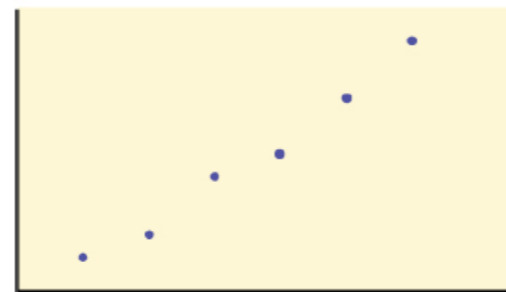


- $(x_1, y_1) \rightarrow d_1$
- $(x_2, y_2) \rightarrow d_2$
- $\vdots$
- $(x_i, y_i) \rightarrow d_i$

$$\Delta = \min \left\{ \sum_i d_i^2 \right\}$$

# Least squares

- So, if we pick-up a given family of approximating curves the one with the property  $\Delta = \min\{\sum_i d_i^2\}$  will be **the best fitting or least-squares curve**
- Certainly, we can also discriminate between families (for instance the linear model or parabola)
- Silently, we assume that the uncertainties of the independent (x) variable is much smaller than on (y) variable
- Formally we can also switch the axes (treat the y variable as independent)
- Let's start discussing the linear model fit

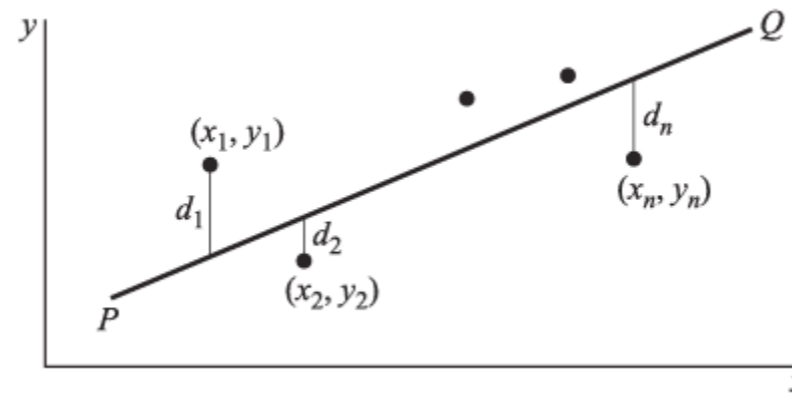


**overall pattern,  
with deviations** from the pattern

# LS line



- Here, we consider that our data set show linear dependency, which we denote as:  
 $y = a_0 + a_1x$  (we will call  $a_0$  the intercept and  $a_1$  slope or gradient)
- To determine the parameters, we need to solve



regression line from the sample is our best estimate of this line in the population

$$d_i = a_0 + a_1x_i - y_i$$

$$\Delta = \sum_i d_i^2 = \sum_i (a_0 + a_1x_i - y_i)^2$$

$$\Delta = \Delta(a_0, a_1) \rightarrow \frac{\partial \Delta}{\partial a_0} = 0, \frac{\partial \Delta}{\partial a_1} = 0$$

# LS line – normal equations



- Searching for the extremum we get:

$$\frac{\partial \Delta}{\partial a_0} = \sum_i 2 \cdot (a_0 + a_1 x_i - y_i) = 0$$

$$\frac{\partial \Delta}{\partial a_1} = \sum_i 2 \cdot x \cdot (a_0 + a_1 x_i - y_i) = 0$$

$$\sum_i y_i = a_0 n + a_1 \sum_i x_i$$

$$\sum_i x_i y_i = a_0 \sum_i x_i + a_1 \sum_i x_i^2$$

- These two we call the normal equation for the LS line

$$a_0 = \frac{\sum y \cdot \sum x^2 - \sum x \cdot \sum xy}{n \cdot \sum x^2 - (\sum x)^2}$$

$$a_1 = \frac{n \cdot \sum xy - \sum x \cdot \sum y}{n \cdot \sum x^2 - (\sum x)^2}$$

$$\sum x \equiv \sum_i x_i, \text{ etc.}$$

# LS line – normal equations



- The second equation can be written in more convenient way:

$$a_1 = \frac{\sum(x - \bar{x})(y - \bar{y})}{\sum(x - \bar{x})^2}$$

This „looks like” covariance  
 This „looks like” variance

- We can divide the first normal equation by  $n$

$$\frac{1}{n} \sum_i y_i = \frac{1}{n} \left( a_0 n + a_1 \sum_i x_i \right) \rightarrow \bar{y} = a_0 + a_1 \bar{x} \rightarrow a_0 = \bar{y} - a_1 \bar{x}$$

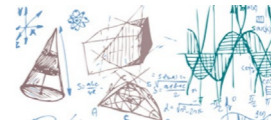
- And, we can write the LS line as:

$$y - \bar{y} = \frac{\sum(x - \bar{x})(y - \bar{y})}{\sum(x - \bar{x})^2} (x - \bar{x})$$

- This is an interesting result, since it shows clearly that the LS line goes through the point  $(\bar{x}, \bar{y})$ - sample means - it is called **the centroid of the data**



# LS line – simple(r) way



- The SL line equation can be simplified using the sample variance and covariance

$$s_x^2 = \frac{\sum_i (x_i - \bar{x})^2}{n - 1}, s_y^2 = \frac{\sum_i (y_i - \bar{y})^2}{n - 1}, s_{xy} = \frac{\sum_{i,j} (x_i - \bar{x})(y_j - \bar{y})}{n - 1}$$

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

- And with the sample correlation coefficient one can express the slope:  $r = \frac{s_{xy}}{s_x s_y}$

$$\frac{y - \bar{y}}{s_y} = r \left( \frac{x - \bar{x}}{s_x} \right) \quad \frac{x - \bar{x}}{s_x} = r \left( \frac{y - \bar{y}}{s_y} \right) \quad z_y = r z_x$$

- This is of outmost interest – the lines that are obtained for  $(x, y)$  pairs will be in general different than for  $(y, x)$  pairs
- The equivalence is possible only when the correlation coefficient is  $r = \pm 1$

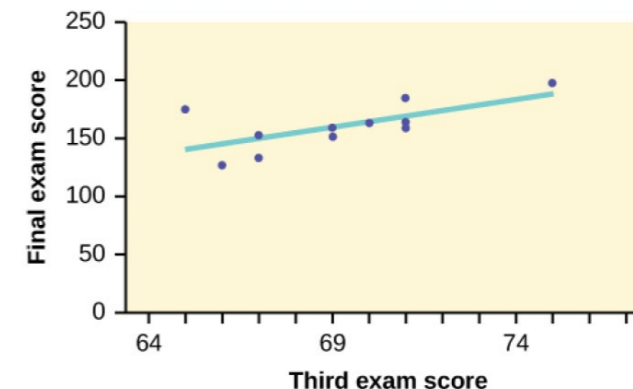
# Correlation Coefficient- interpretation

The variable  $r^2$  is called the coefficient of determination

- $r^2$  , when expressed as a percent, represents the percent of variation in the dependent (predicted) variable  $y$  that can be explained by variation in the independent (explanatory) variable  $x$  using the regression (best-fit) line.
- $1 - r^2$  , when expressed as a percentage, represents the percent of variation in  $y$  that is NOT explained by variation in  $x$  using the regression line

EX: The line of best fit is:  $\hat{y} = -173.51 + 4.83x$

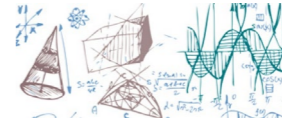
- ✓ The correlation coefficient is  $r = 0.6631$
- ✓ The coefficient of determination is  $r^2 = 0.6631^2 = 0.4397$



Approximately 44% of the variation (0.4397 is approximately 0.44) in the final-exam grades can be explained by the variation in the grades on the third exam, using the best-fit regression line.

Therefore, approximately 56% of the variation ( $1 - 0.44 = 0.56$ ) in the final exam grades can NOT be explained by the variation in the grades on the third exam, using the best-fit regression line. (This is seen as the scattering of the points about the line.)

# SL parabola



- Following the same idea we can get employ more complicated model, for instance if we use the parabola equation:  $y = a_0 + a_1x + a_2x^2$
- Now the sum of the square of residuals will lead to three normal equations for each of the parameters  $a_i$

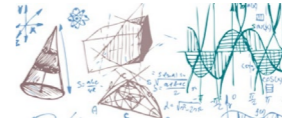
$$\sum y = na_0 + a_1 \sum x + a_2 \sum x^2$$

$$\sum xy = a_0 \sum x + a_1 \sum x^2 + a_2 \sum x^3$$

$$\sum x^2y = a_0 \sum x^2 + a_1 \sum x^3 + a_2 \sum x^4$$

- Usually, for more complicated models we use computer libraries to make the calculations for us or machine learning approach

# Multiple regression



- It is just as easy to extend this idea to higher dimensions, for instance the dependence between 3 R.V.s

$$z = a + a_x x + a_y y, \text{ or } x_3 = a_0 + a_1 x_1 + a_2 x_2$$

- Formally, this is a **plane equation**, thus, we call it **the regression plane**. Again we can use the least-squares principle to find our normal equations

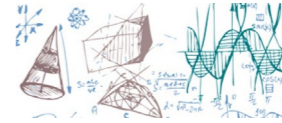
$$\sum z = na + a_x \sum x + a_y \sum y$$

$$\sum xz = n \sum x + a_x \sum x^2 + a_y \sum xy$$

$$\sum yz = n \sum y + a_x \sum xy + a_y \sum y^2$$

- It is quite popular in the domain of machine learning

# Estimate error



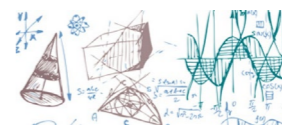
- As usual, we should take into account that the job is not yet done if we do not give error on the estimated parameters
- We can define the „standard” error of the estimate

$$s_{y|x} = \sqrt{\frac{\sum(y - y_{th})^2}{n - 1}} = \sqrt{\frac{\sum(y - \hat{y})^2}{n - 1}}$$

- Where  $y_{th} (\hat{y})$  denotes the value calculated using the estimated line (sometimes it is called theory point)
- We see immediately that the LS curve will have the smallest standard error of estimate

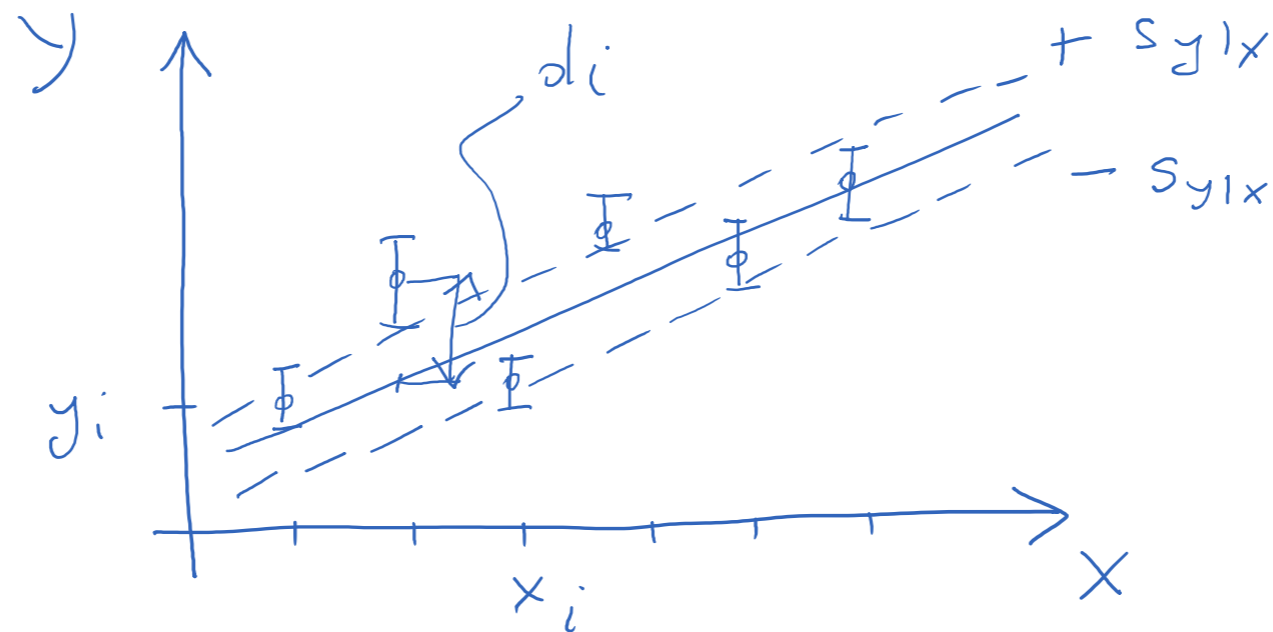
$$s_{y|x}^2 = \frac{\sum y^2 - a_0 \sum y - a_1 \sum xy}{n - 1}$$

- This estimator, has properties similar to those of standard deviation



# Estimate error

- This analogy can be made a bit more intuitive: if we draw a pair of lines parallel to the LS line at respective vertical distances of  $\pm s_{y|x}$  then we should expect that about 68% of the sampling point will be between them
- It is then easy to extend this for distances of  $\pm 2s_{y|x}$  and  $\pm 3s_{y|x}$





# Linear correlation coefficient

- The square of the standard error of estimate can be written as:

$$s_{y|x}^2 = \frac{\sum(y - \bar{y})^2 - a_1 \sum(x - \bar{x})(y - \bar{y})}{n}$$

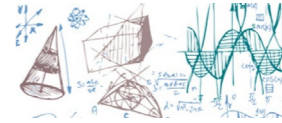
- And using the variance and correlation coefficient  $s_{y|x}^2 = s_y^2(1 - r^2)$
- Combining these definitions we have:

$$r^2 = 1 - \frac{\sum(y - y_{th})^2}{\sum(y - \bar{y})^2} = \frac{\sum(y - \bar{y})^2 - \sum(y - y_{th})^2}{\sum(y - \bar{y})^2}$$

- Also:  $\sum(y - \bar{y})^2 = \sum(y - y_{th})^2 + \sum(y_{th} - \bar{y})^2$ , and combining with the above we get

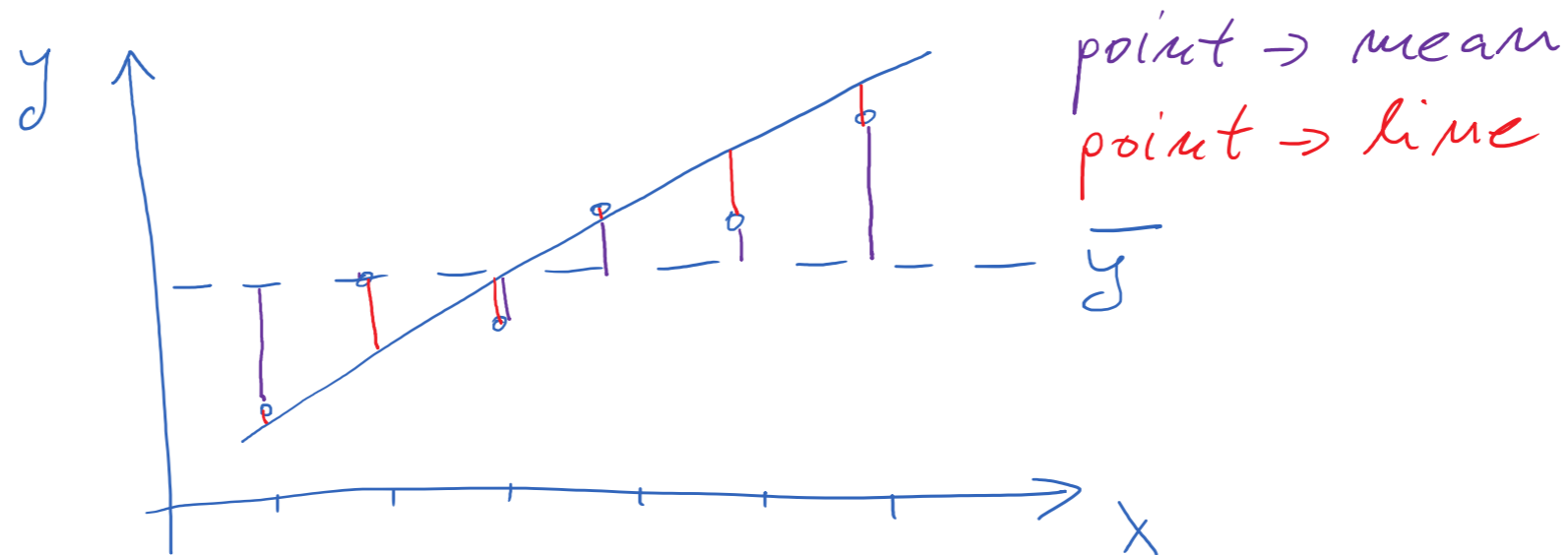
$$r^2 = \frac{\sum(y_{th} - \bar{y})^2}{\sum(y - \bar{y})^2} = \frac{\text{explained variation}}{\text{total variation}}$$

# Explained variation



- Machine learning very often uses the r-squared as a **specific goodness of fit metric**.  
It is also much easier to interpret

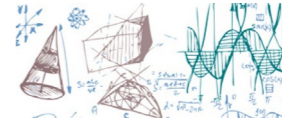
$$r^2 = 1 - \frac{\sum(y - y_{th})^2}{\sum(y - \bar{y})^2} = \frac{\sum(y - \bar{y})^2 - \sum(y - y_{th})^2}{\sum(y - \bar{y})^2} = \frac{V[mean] - V[line]}{V[mean]}$$



- The „red residuals” will never be larger than the „purple residuals”, so the r-squared will be always between 0 and 1 or we can measure it in percents



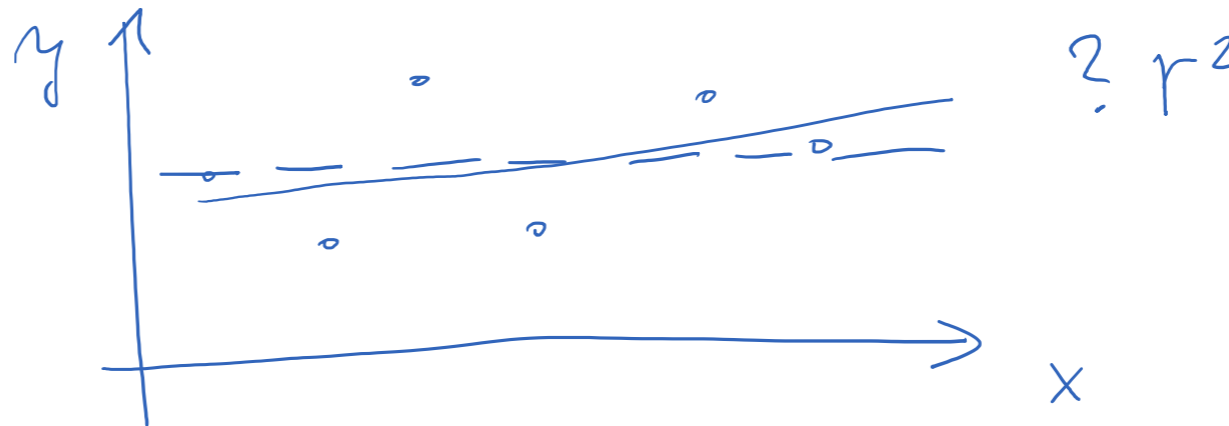
# Explained variation



- Say, for the previous example we obtained:  $V[mean] = 36$  and  $V[line] = 8$ , thus

$$r^2 = \frac{V[mean] - V[line]}{V[mean]} = \frac{36 - 8}{36} = 0.78$$

- We say, that most of the variation (78%) seen in our data can be explained by the line – or by the relationship between our variables. So, applying the model makes sense!



- Here making the fit does not make much sense...

# Correlation Coefficient – test of significance

- The correlation coefficient,  $r$ , tells us about the strength and direction of the linear relationship between  $x$  and  $y$ .
- We perform a hypothesis test of the "**significance of the correlation coefficient**" to decide whether the linear relationship in the sample data is strong enough to use to model the relationship in the population.

$\rho$  = population correlation coefficient (unknown)

$r$  = sample correlation coefficient (known; calculated from sample data)

Null Hypothesis:  $H_0: \rho = 0$ , The population correlation coefficient IS NOT significantly different from zero. There IS NOT a significant linear relationship (correlation) between  $x$  and  $y$  in the population.

Alternate Hypothesis:  $H_a: \rho \neq 0$ , The population correlation coefficient IS significantly DIFFERENT FROM zero. There IS A SIGNIFICANT LINEAR RELATIONSHIP (correlation) between  $x$  and  $y$  in the population.

# Correlation Coefficient – test of significance

**Method 1: Using the  $p$ -value**, we usually take significance level of 5%,  $\alpha = 0.05$

- $p$ -value is calculated with a  $t$ -distribution with  $n-2$  degrees of freedom.
- test statistics is:  $t = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}}$
- If the  $p$ -value is less than the significance level ( $\alpha = 0.05$ ):
  - ✓ Decision: Reject the null hypothesis.
  - ✓ Conclusion: "There is sufficient evidence to conclude that there is a significant linear relationship between  $x$  and  $y$  because the correlation coefficient is significantly different from zero"
- If the  $p$ -value is NOT less than the significance level ( $\alpha = 0.05$ )
  - ✓ Decision: DO NOT REJECT the null hypothesis.
  - ✓ Conclusion: "There is insufficient evidence to conclude that there is a significant linear relationship between  $x$  and  $y$  because the correlation coefficient is NOT significantly different from zero."

EX: The line of best fit is:  $\hat{y} = -173.51 + 4.83x$  with  $r = 0.6631$  and there are  $n = 11$  data points. The  $p$ -value is 0.026, what is the decision?

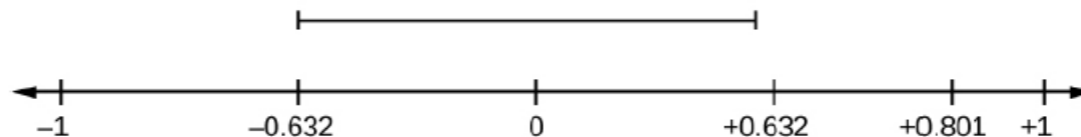
# Correlation Coefficient – test of significance

## Method 2: Using a table of critical values, $\alpha = 0.05$

The **95% Critical Values of the Sample Correlation Coefficient Table** can be used to give you a good idea of whether the computed value of  $r$  is **significant or not**.

If  $r$  is not between the positive and negative critical values, then the correlation coefficient is significant. If  $r$  is significant, then you may want to use the line for prediction.

EX: Suppose you computed  $r = 0.801$  using  $n = 10$  data points.  $df = n - 2 = 10 - 2 = 8$ . The critical values associated with  $df = 8$  are  $-0.632$  and  $+0.632$ . If  $r <$  negative critical value or  $r >$  positive critical value, then  $r$  is **significant**. Since  $r = 0.801$  and  $0.801 > 0.632$ ,  $r$  is significant and the line may be used for prediction.



# Correlation Coefficient – test of significance

## Method 2: Using a table of critical values, $\alpha = 0.05$

### THIRD-EXAM vs FINAL-EXAM EXAMPLE: critical value method

Consider the **third exam/final exam example**. The line of best fit is:  $\hat{y} = -173.51 + 4.83x$  with  $r = 0.6631$  and there are  $n = 11$  data points. Can the regression line be used for prediction? **Given a third-exam score ( $x$  value), can we use the line to predict the final exam score (predicted  $y$  value)?**

$$H_0: \rho = 0$$

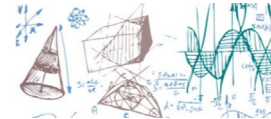
$$H_a: \rho \neq 0$$

$$\alpha = 0.05$$

- Use the "95% Critical Value" table for  $r$  with  $df = n - 2 = 11 - 2 = 9$ .
- The critical values are  $-0.602$  and  $+0.602$
- Since  $0.6631 > 0.602$ ,  $r$  is significant.
- Decision: Reject the null hypothesis.
- Conclusion: There is sufficient evidence to conclude that there is a significant linear relationship between the third exam score ( $x$ ) and the final exam score ( $y$ ) because the correlation coefficient is significantly different from zero.

**Because  $r$  is significant and the scatter plot shows a linear trend, the regression line can be used to predict final exam scores.**

# Sampling properties of LS



- The complete treatment of the estimated parameters' uncertainty is out of the scope of this lecture. I just give you somewhat simplified version – but still important and perfectly usable in practice!
- Assume that our model can be written as follow:

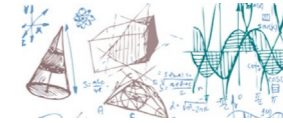
$$y_i = a_0 + a_1 x_i + d_i$$

- We assume that the residuals are independent of one another and are distributed with  $\mu = 0$  and  $V[d_i] = \sigma^2$
- Let's start discussing the constraint fit (with the point (0,0)), we know that the best estimate of the slope in that case is

$$\hat{a}_1 = \frac{\sum xy}{\sum x^2}$$

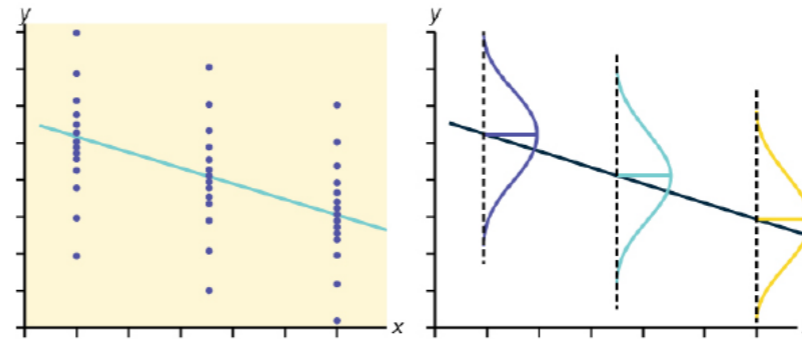
- It is quite easy to show, that this estimator is unbiased,  $E[\hat{a}_1] = a_1$  and its variance  $V[\hat{a}_1] = \frac{\sigma^2}{\sum x^2}$

# Sampling properties of LS



- The variance of the slope estimator says a few interesting things – to improve the estimate, we should take more data, improve the precision of measurement of each data point (expressed as  $\sigma^2$ ) and the most important measurements are done close to the origin point!
- If we assume that the residuals are normally distributed (not too crazy assumption), we find that the slope estimator is also normally distributed

$$\hat{a}_1 \sim \mathcal{N}\left(a_1, \frac{\sigma^2}{\sum_i x_i^2}\right)$$

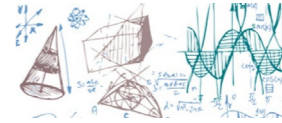


The standard deviations of the population  $y$  values about the line are equal for each value of  $x$ . In other words, each of these normal distributions of  $y$  values has the same shape and spread about the line.

- In case, when the distribution is not Gaussian or the variance is not known one can use the regression estimation variance

$$s_{y|x} = \sqrt{\frac{\sum (y - y_{th})^2}{n - 1}} \rightarrow s_{y|x}^2 = \frac{\sum (y - y_{th})^2}{n - 1} \rightarrow s_{y|x}^2 = \frac{\sum_i (y_i - \hat{y}_i)^2}{n - 1}$$

# Sampling properties of LS



- We are familiar with this estimator already! It follows the  $\chi^2$  distribution:

$$\frac{(n-1)s_{y|x}^2}{\sigma^2} \sim \chi^2(n-1)$$

- And, in that case the distribution of the slope estimator is:

$$\frac{\hat{a}_1 - a_1}{s_{y|x} / \sqrt{\sum_i x_i^2}} \sim t(n-1)$$

- Now we can calculate the C.I. for the slope and even test hypothesis related to estimated slope!



# C.I. for the slope



- Ex. 1 Let's assume that we performed the procedure of LS line estimation and obtained  $\hat{a}_1 = 1.289$ , the sum of residual squares are  $\sum_i (y_i - \hat{y}_i)^2 = 107.30$  and the number of points in our data set was 20.
- The estimate variance:

$$s_{y|x}^2 = \frac{\sum_i (y_i - \hat{y}_i)^2}{n - 1} = \frac{107.30}{19} = 5.647$$

- So, the 90% C.I. for the slope can be constructed as follow:

$$\begin{aligned} C.I._{90\%}^t(\hat{a}_1) &= \left( \hat{a}_1 - t_{0.9} \frac{s_{y|x}}{\sqrt{\sum_i x_i^2}}, \hat{a}_1 + t_{0.9} \frac{s_{y|x}}{\sqrt{\sum_i x_i^2}} \right) = \\ &= \left( 1.289 - 1.729 \frac{\sqrt{5.647}}{\sqrt{6226.38}}, \hat{a}_1 + 1.729 \frac{\sqrt{5.647}}{\sqrt{6226.38}} \right) = (1.237, 1.341) \end{aligned}$$

# Unconstrained fit



- If there is no special points in our fitting procedure we need to proceed with the unconstrained fit. In this case it can be shown

$$E[\hat{a}_0] = a_0 \quad V[\hat{a}_0] = \frac{\sigma^2}{n}$$

$$E[\hat{a}_1] = a_1 \quad V[\hat{a}_1] = \frac{\sigma^2}{\sum_i (x_i - \bar{x}_i)^2}$$

Again, the larger the interval where we measure data the more precise the estimate

- The variance of the estimate

$$s_{y|x}^2 = \frac{\sum_i (y_i - \hat{y}_i)^2}{n - 2}$$

- If we assume that the residuals are normally distributed

$$\hat{a}_1 \sim \mathcal{N}\left(a_1, \frac{\sigma^2}{\sum_i (x_i - \bar{x}_i)^2}\right), \quad \frac{(n - 2)s_{y|x}^2}{\sigma^2} \sim \chi^2(n - 2)$$

- Otherwise

$$\frac{\hat{a}_1 - a_1}{s_{y|x} / \sqrt{\sum_i (x_i - \bar{x}_i)^2}} \sim t(n - 2)$$