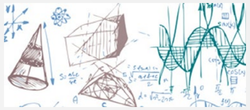

Introduction to probability, statistics and data handling

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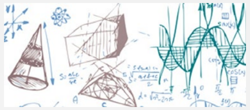
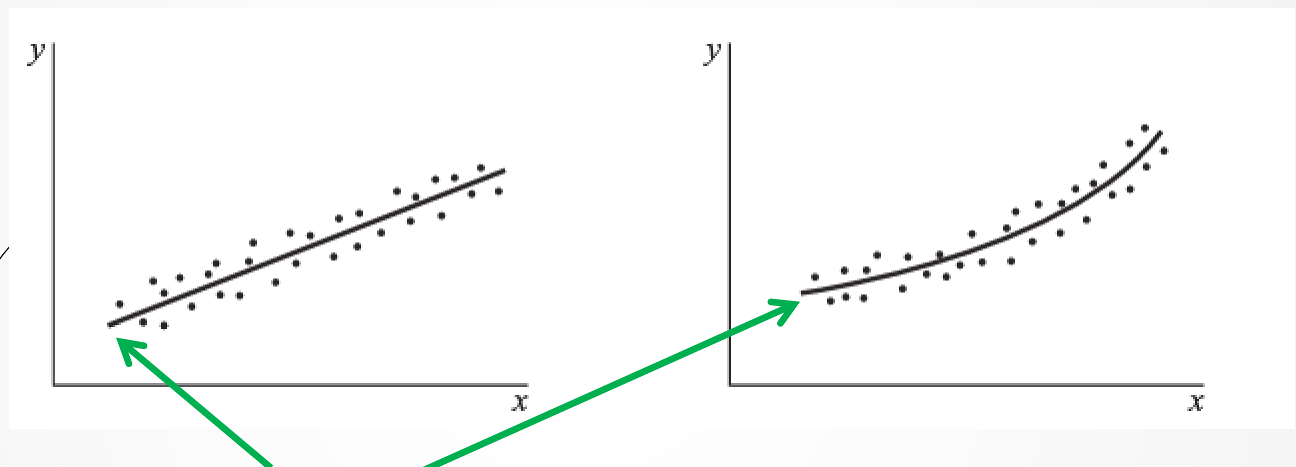


Curve fitting and regression

- 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)
- 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
- Let's get started then – what comes is real life, learn it!

First steps

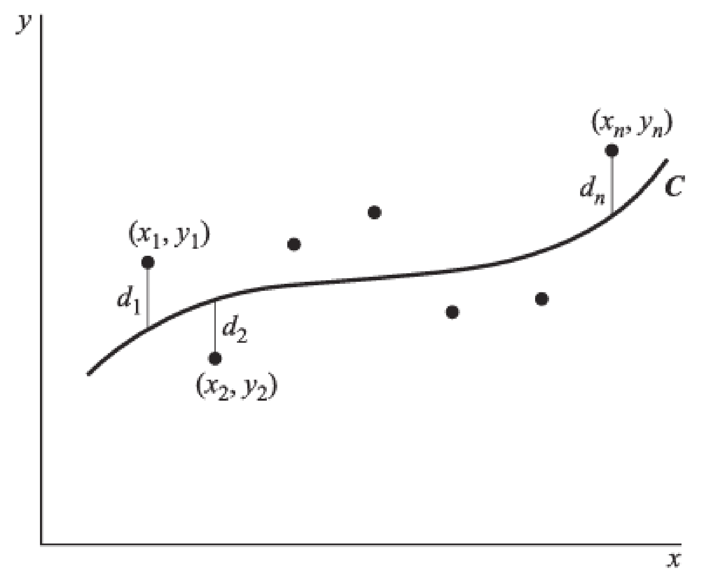
- Usually we make first the **scatter plot** using collected data and take a look…



- The solid lines above are called approximating curves
- What we need to work out is the **equation of this curve**
- That task is called **curve fitting**
- Often to understand the relation, we may need to apply some transformation(s) to the variables
- NOTE. This is related to the approximation of parameters

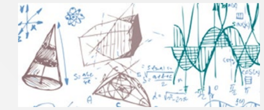
Least squares again!

- We have already encounter 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



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

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

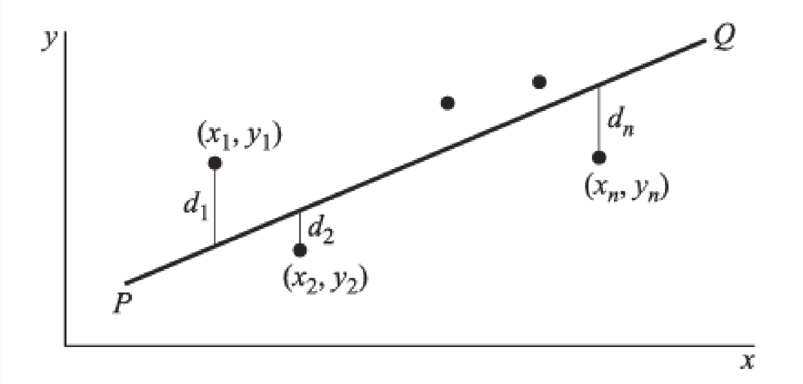


Least squares

- 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

LS line

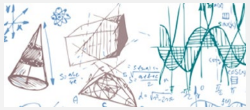
- Here, we consider that our data set show linear dependency, which we denote as: $y = a_0 + a_1 x$ (we will call a_0 the intercept and a_1 slope or gradient)
- To determine the parameters we need to solve



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

$$\Delta = \sum_i d_i^2 = \sum_i (a_0 + a_1 x_i - y_i)^2$$

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



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

$$\boldsymbol{a_0} = \frac{\sum y \cdot \sum x^2 - \sum x \cdot \sum xy}{n \cdot \sum x^2 - (\sum x)^2} \qquad \boldsymbol{a_1} = \frac{n \cdot \sum xy - \sum x \cdot \sum y}{n \cdot \sum x^2 - (\sum x)^2}$$

$$\sum x \equiv \sum_i x_i \,, etc.$$

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 (numerator)

This „looks like" variance (denominator)

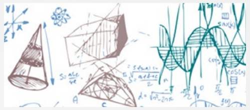
- We can divide the first normal equation by n

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

- And, we can write the LS line as:

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

- This is an interesting result, since it shows clearly that the LS line goes through the point $(\bar{x}, \bar{y})$ - 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

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

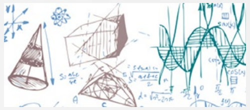
$$y - \bar{y} = \frac{s_{xy}}{s_x^2}(x - \bar{x}) \qquad x - \bar{x} = \frac{s_{xy}}{s_y^2}(y - \bar{y})$$

- And with the sample correlation coefficient $r = \frac{s_{xy}}{s_x s_y}$

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

$$z_y = r z_x$$

- 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 $r = \pm 1$



SL parabola

- Following the same idea we can get employ more complicated model, for instance if we use the parabola equation: $y = a_0 + a_1 x + a_2 x^2$
- Now the sum of the square of residuals will lead to three normal equations for each of the parameters a_i

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

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

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

- 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

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

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

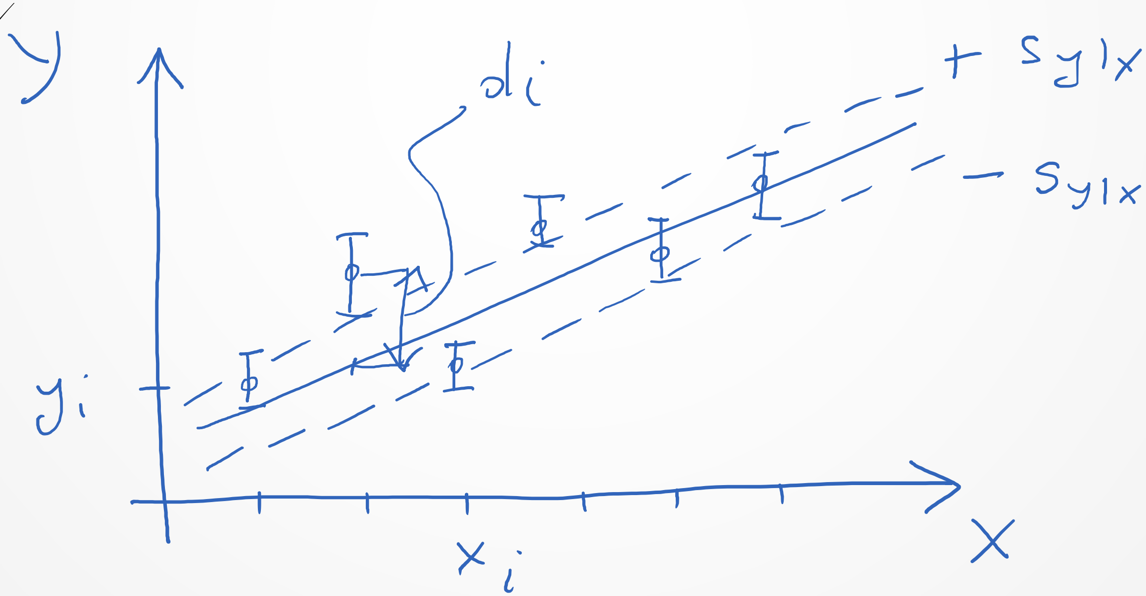
- Where y_{th} ($\hat{y}$) denotes the value calculated using the estimated line (sometimes it is called theory point)
- We see immediately that the LS curve will have the smallest standard error of estimate

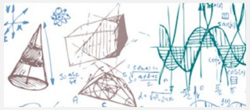
$$s_{y|x}^2 = \frac{\sum y^2 - a_0 \sum y - a_1 \sum xy}{n-1}$$

- 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:

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

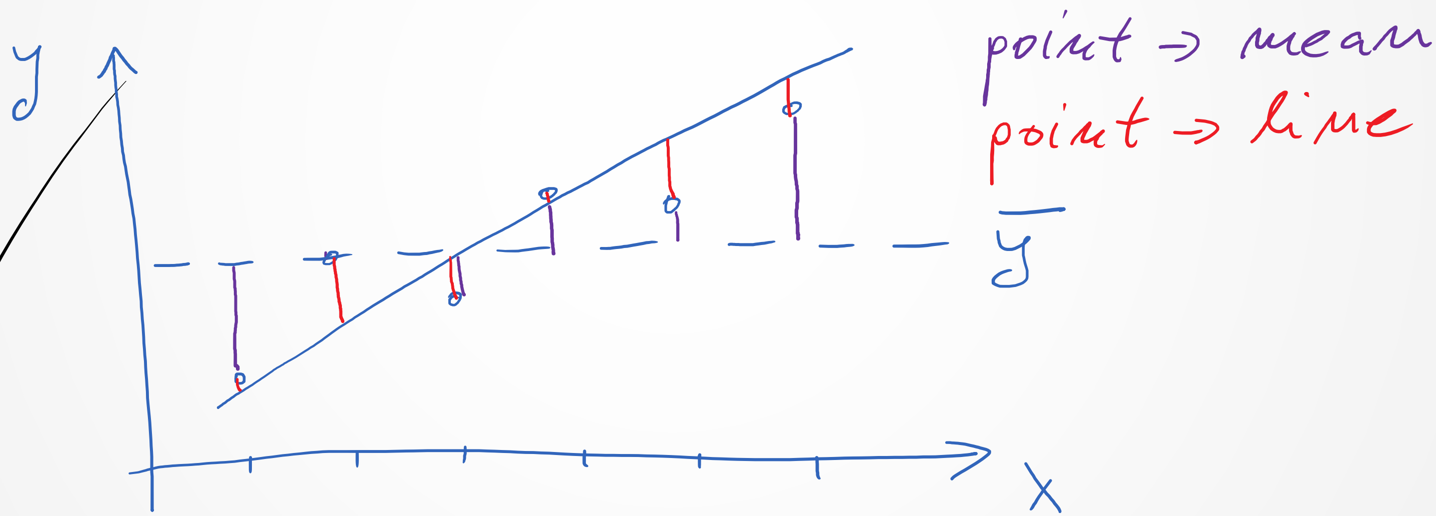
- Also: $\sum(y-\bar{y})^2 = \sum(y-y_{th})^2 + \sum(y_{th}-\bar{y})^2$, and combining with the above we get

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

Explained variation

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

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



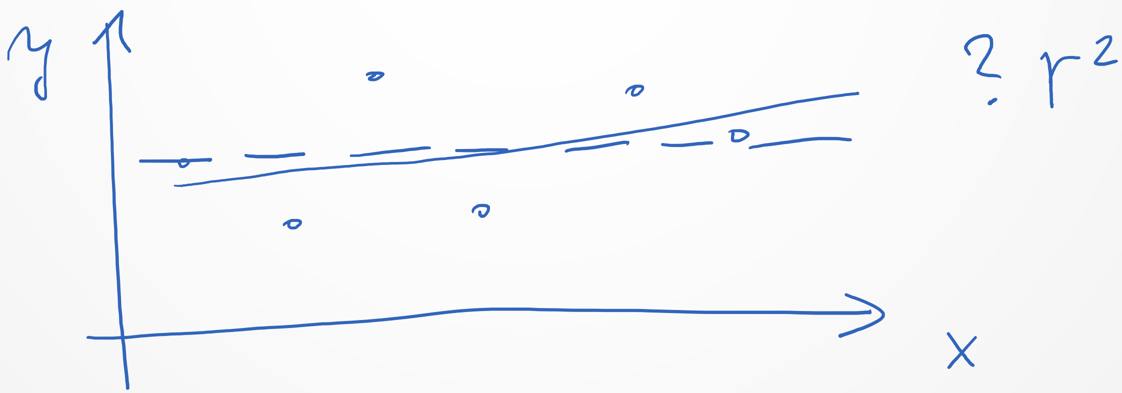
- The „red residuals" will never be larger than the „purple residuals", so the r-squared will be always between 0 and 1 or we can measure it in percents

Explained variation

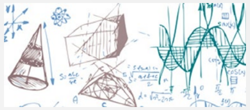
- Say, for the previous example we obtained: $V[mean] = 36$ and $V[line] = 8$, thus

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

- 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…



Sampling properties of LS

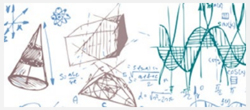
- The complete treatment of the estimated parameters' uncertainty is out of the scope of this lecture. I just give you somewhat simplified version – but still important and perfectly usable in practice!
- Assume that our model can be written as follow:

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

- 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 $(0,0)$), from slide 9 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, $\boldsymbol{E[\hat{a}_1] = a_1}$ and its variance $\boldsymbol{V[\hat{a}_1] = \frac{\sigma^2}{\sum x^2}}$



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 σ^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:

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

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

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

Sampling properties of LS

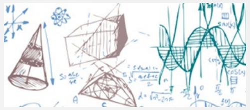
- We are familiar with this estimator already! It follows the χ^2 distribution:

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

- 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:

$$C.I._{90\%}^{t}(\hat{a}_1) = \left(\hat{a}_1 - t_{0.9}\frac{s_{y|x}}{\sqrt{\sum_i x_i^2}}, \hat{a}_1 + t_{0.9}\frac{s_{y|x}}{\sqrt{\sum_i x_i^2}}\right) =$$

$$= \left(1.289 - 1.729\frac{\sqrt{5.647}}{\sqrt{6226.38}}, \hat{a}_1 + 1.729\frac{\sqrt{5.647}}{\sqrt{6226.38}}\right) =$$

$$= (1.237, 1.341)$$