Predictive Methods

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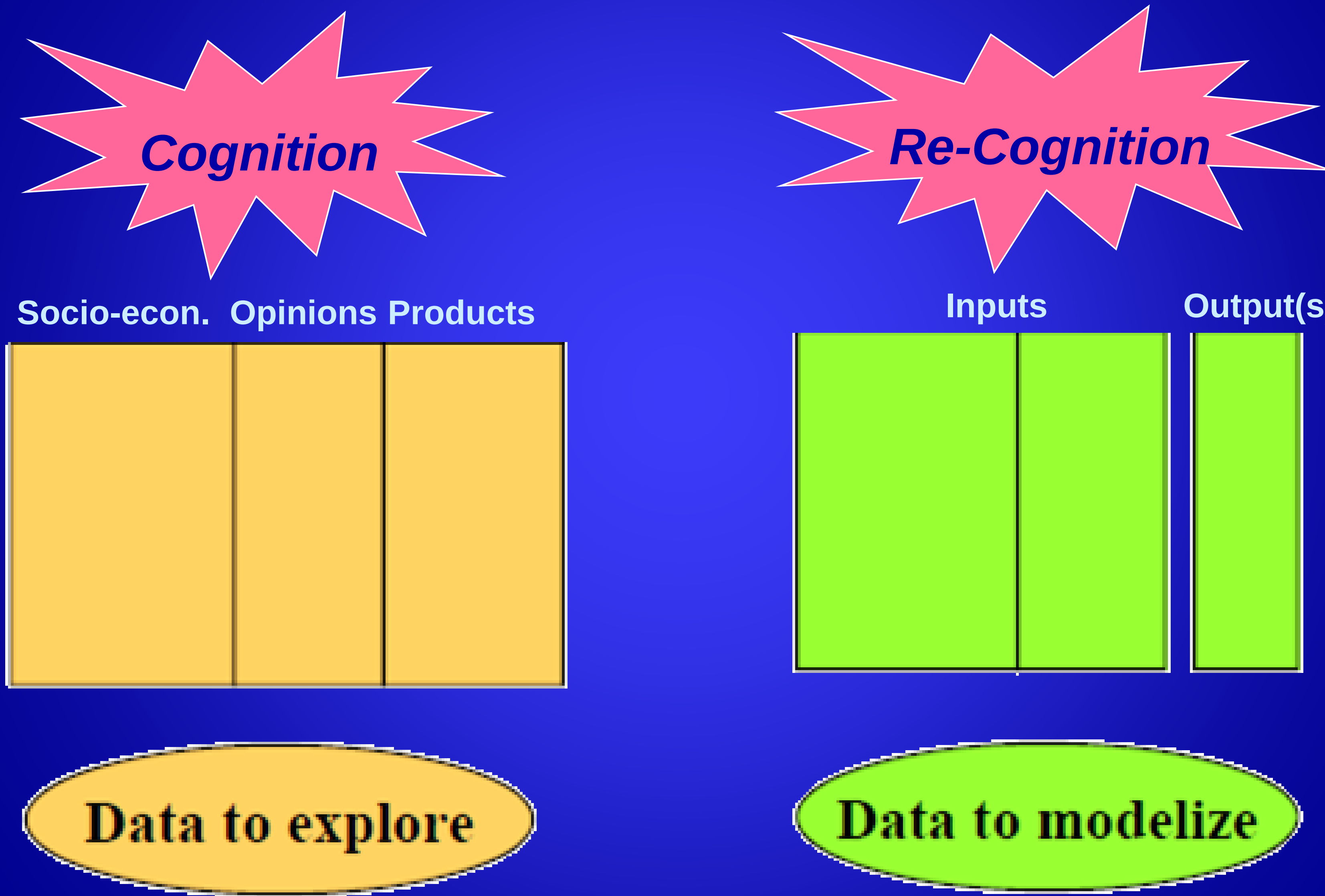
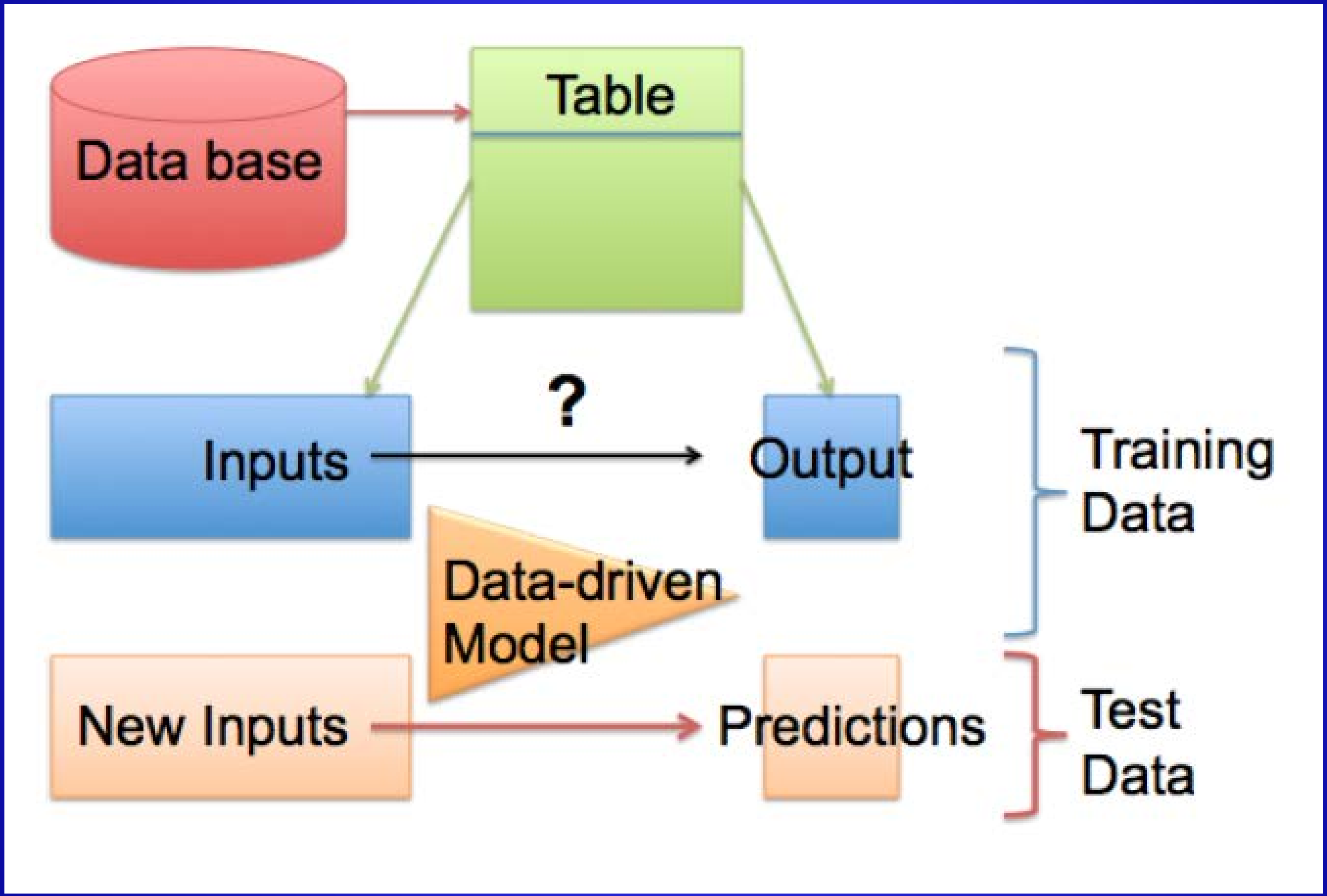
Modelling


Cognition
Re-Cognition
Socio-econ.
Opinions
Products
Inputs
Output(s)
Data to explore
Data to modelize

Supervised Learning



Supervised learning tasks

DM goals [Fayyad et al., 1996]

- **Classification** – labeling a data item into one of several predefined classes (e.g. classify the type of credit client, "good" or "bad", given the status of her/his bank account, credit purpose and amount);
- **Regression** – estimate a real-value (the *dependent variable*) from several (*independent*) attributes (e.g. predict the price of a house based on its number of rooms, age and other characteristics);

- **Classification**: Decision Tree, Random Forest, Classification Rules, Linear Discriminant Analysis, Naive Bayes, Logistic Regression, Neural Networks (MLP, RBF), SVM, ...
- **Regression**: Regression Tree, Random Forest, Multiple Regression, Neural Networks (MLP, RBF), SVM, ...

Statistical Modelling

Data= Fit+Error

- Fit:
  - Structural
  - Law governing the phenomenon
  - Analytic Function

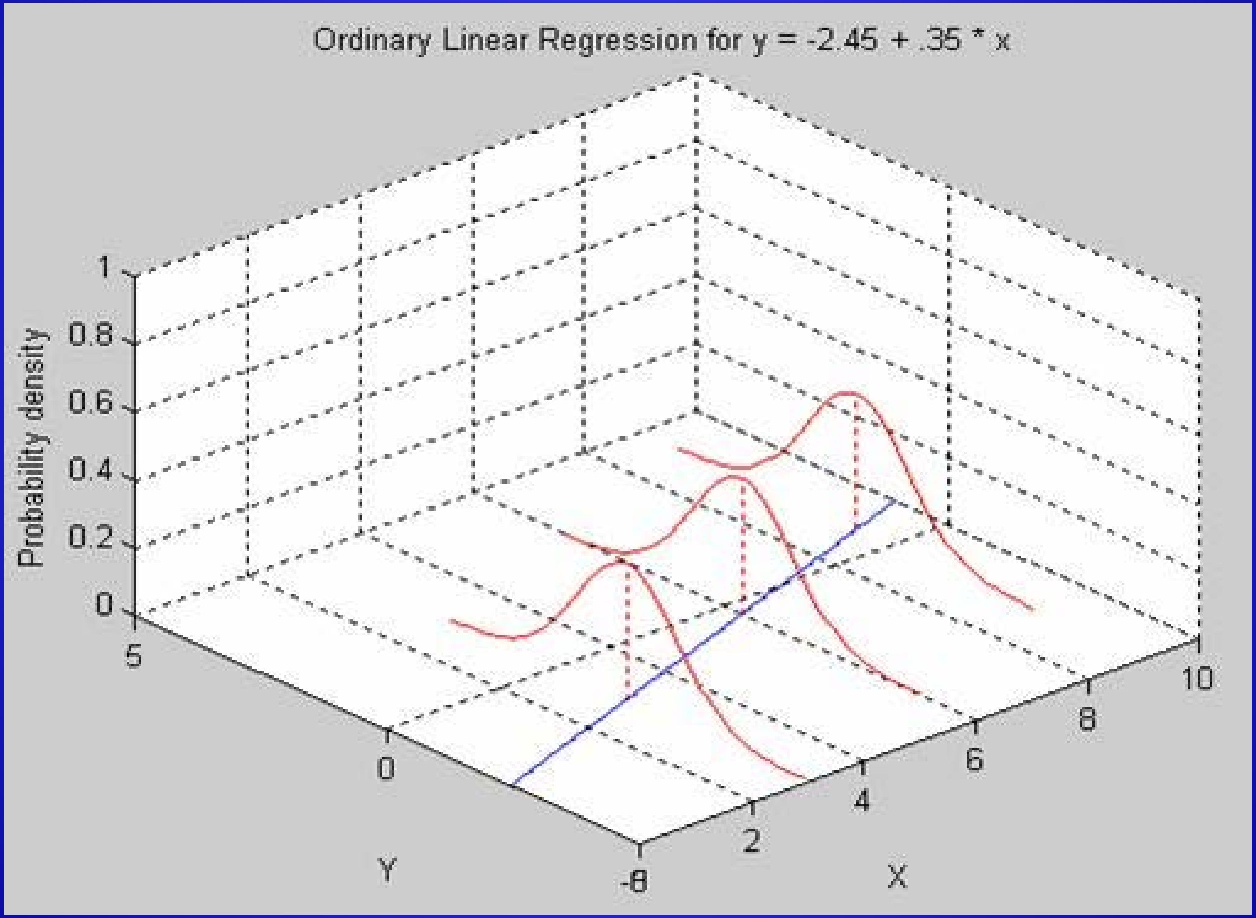
- Error:
  - Random
  - Variability arround Fit (null expectation)
  - Probabilistic model

Statistical models

- Determine the family of fits:
  - Linear
  - Quadratic
  - Exponential
  - .....

- Determine the law of error:
  - Normal
  - Poisson
  - Binomial....

E1 Normally Distributed Error



Linear Multiple regression

- *Fit= linear; Error=Normal and centered*
- *Formalization: I=i:n observations*

  Y: Response variable

  $X_1 \ldots\ldots X_K$ *: ExplanatoryVariables*

  Find $\beta_{0\ldots}\ \beta_K$ such that

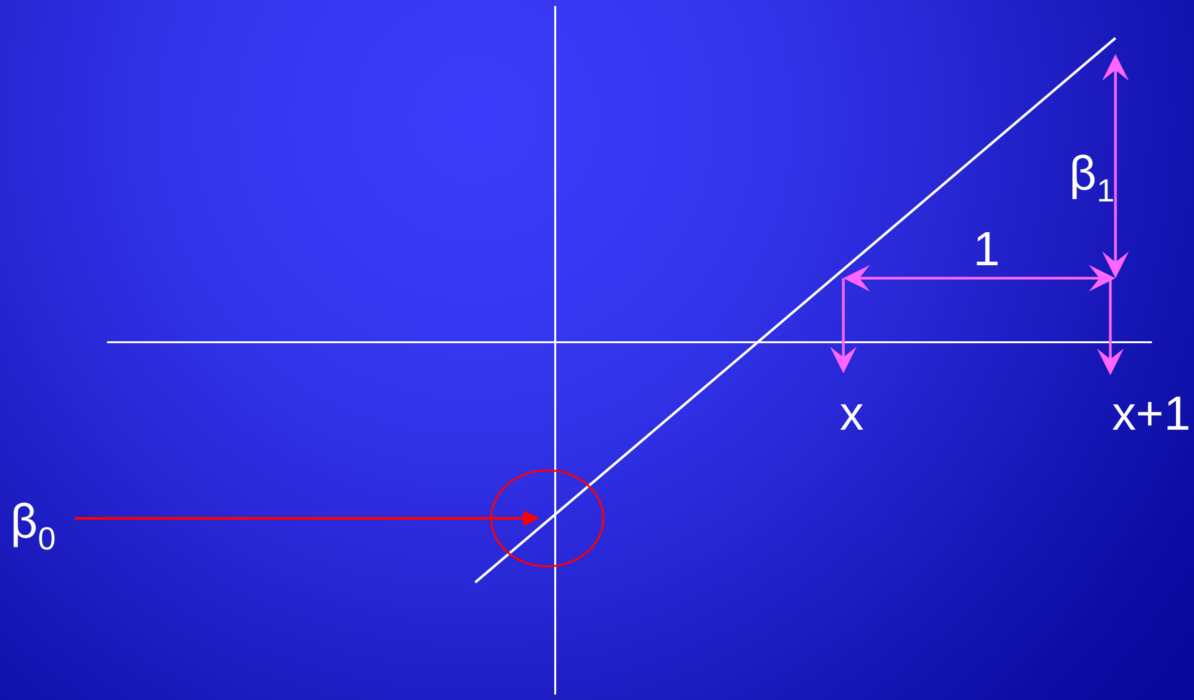
$$Y= \beta_0+\beta_1 X_1+\beta_2 X_2+..+\beta_K X_K+\varepsilon$$

- *Assumptions:*
  - *Linearity:* $E(Y \mid X=x) = \mu_{y|X} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + .. + \beta_K X_K$; $E[\varepsilon] = 0$

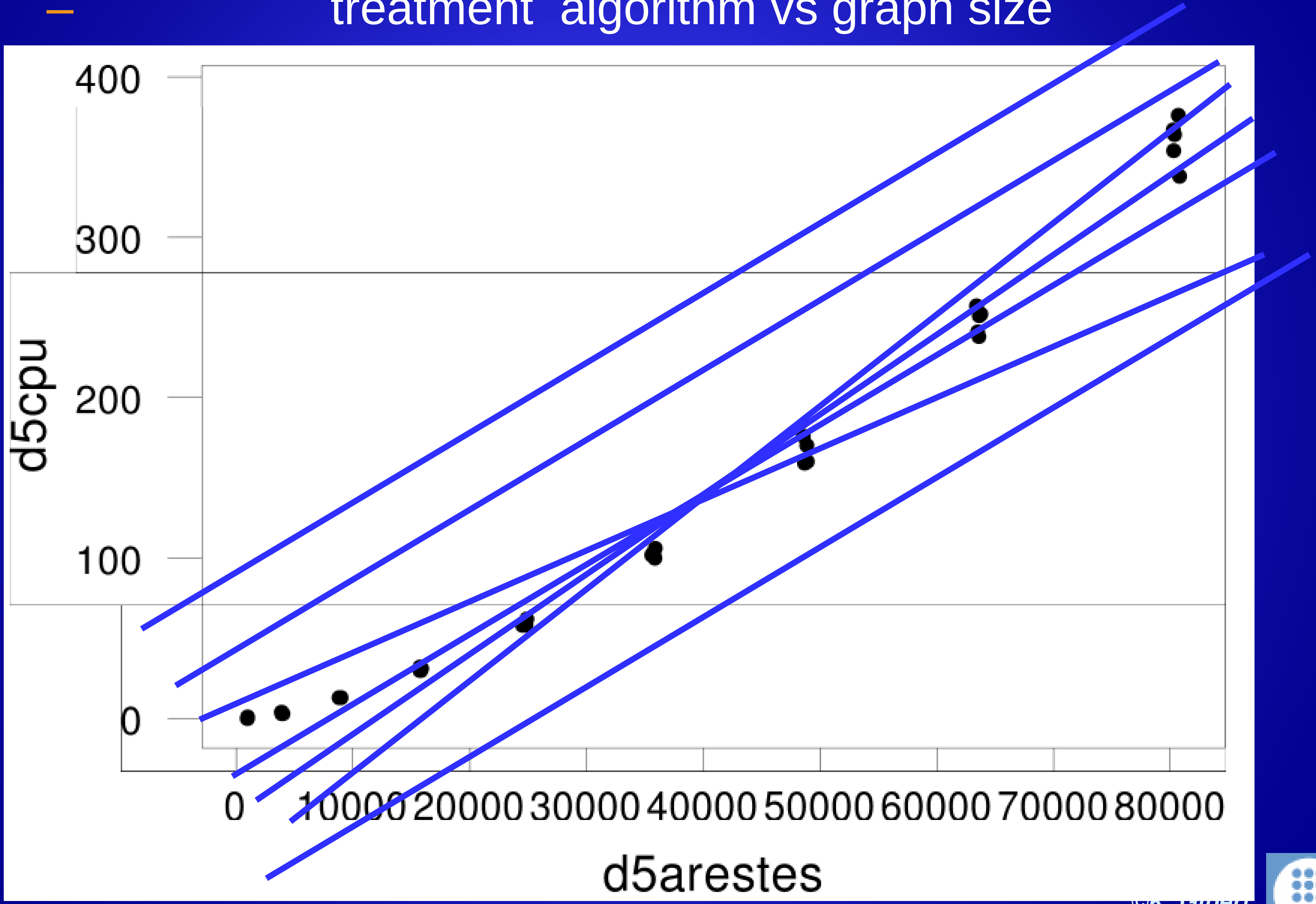
    Population regression line
  - *Normality:* $\varepsilon_1,\ldots,\varepsilon_n \sim \mathcal{N}(0,\sigma_i)$, i=1:n
  - *Homokedasticity:* $Var[\varepsilon_i] = \sigma^2$ forall i
  - *Independence:* $Cov(\varepsilon_i, \varepsilon_j)=0$ forall i,,j

What is “Linear”?

- Remember this:
- $Y = \beta_0 + \beta_1 X$



- Real case: Experimental CPU time of a graph
- treatment algorithm vs graph size



– Real case: Experimental CPU time of a graph
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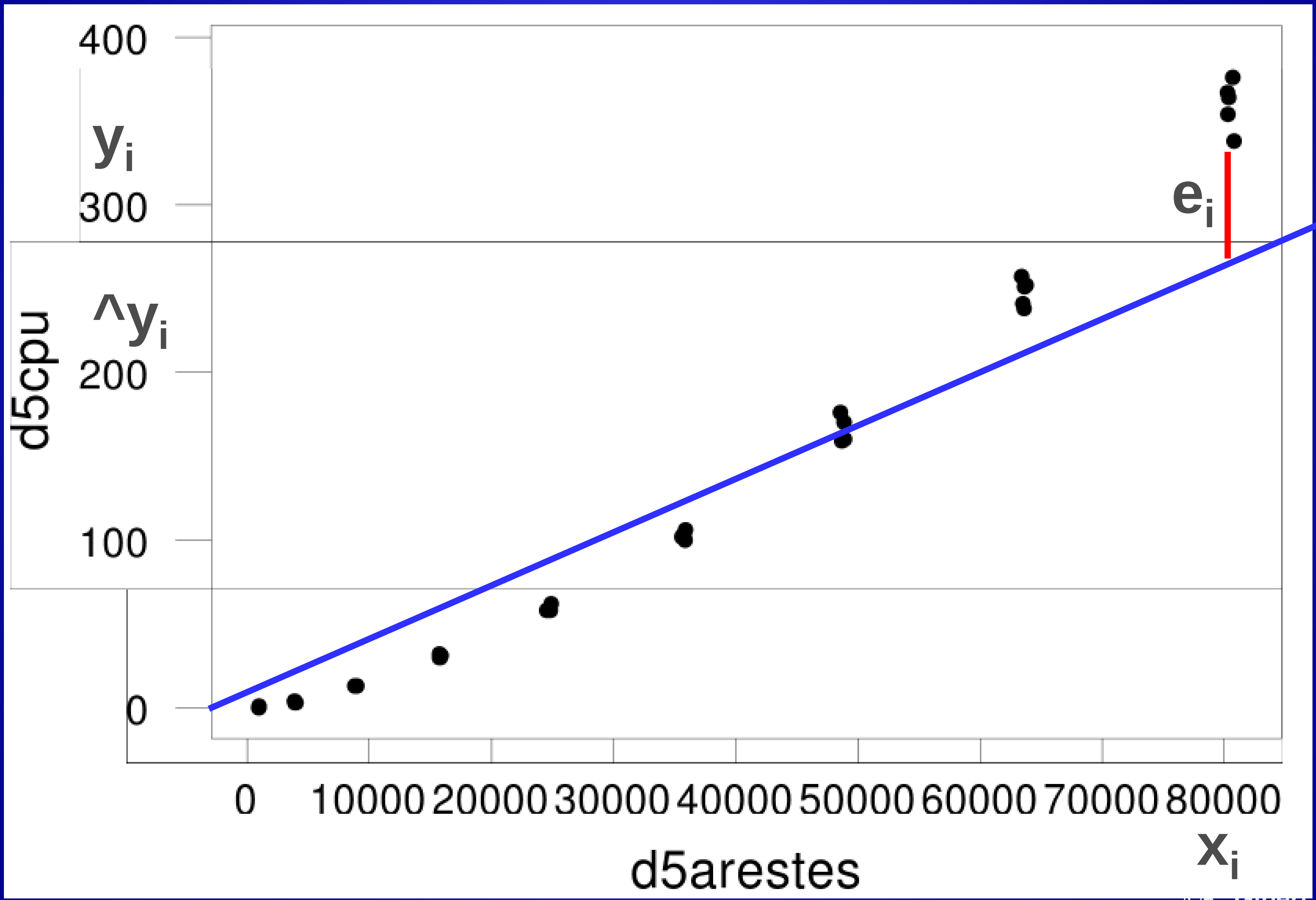


Minimum Least Squares solution

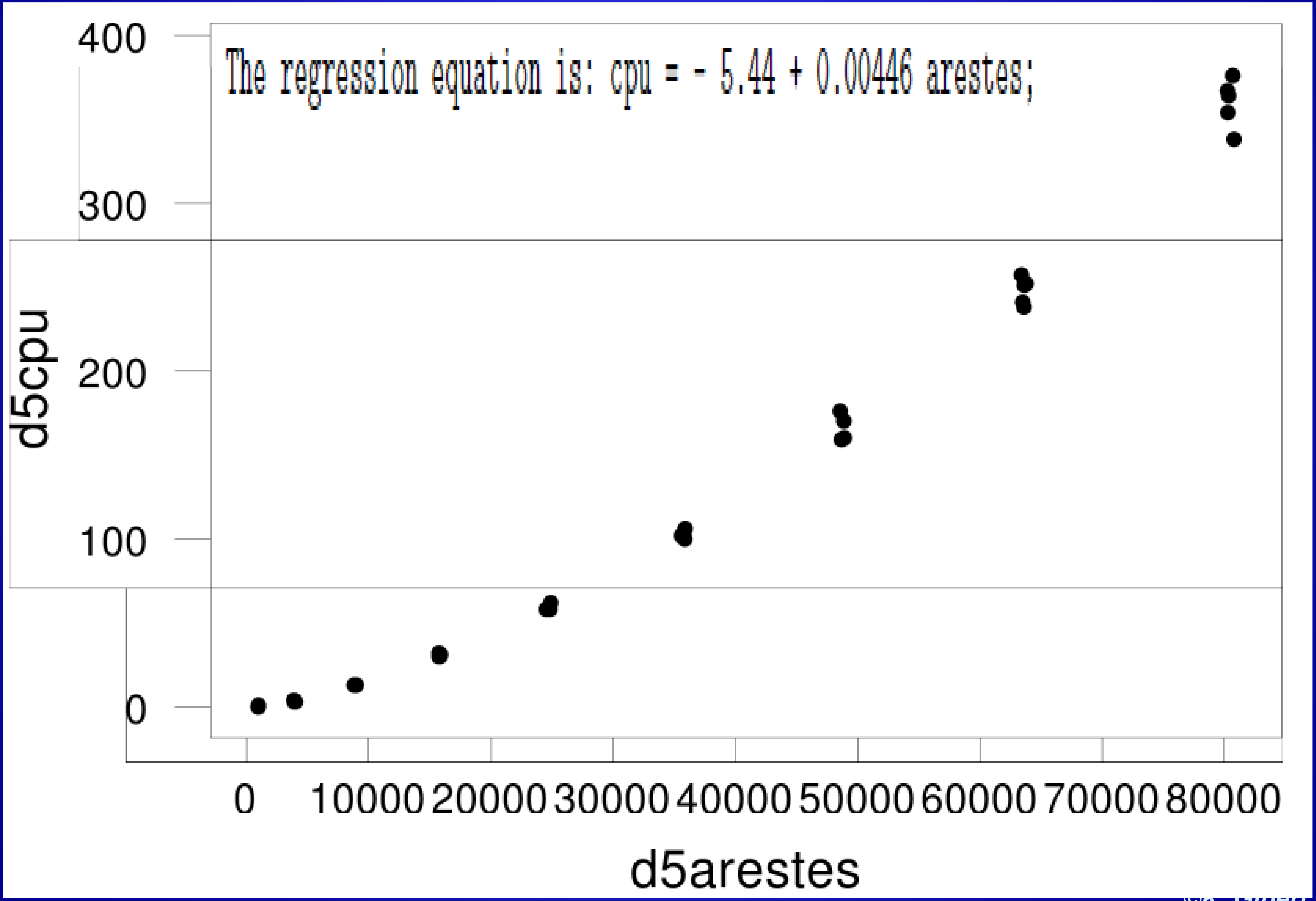
Find $\widehat{\beta}_0, \widehat{\beta}_1$ such that $\min_{\widehat{\beta}_0, \widehat{\beta}_1} \sum_{\forall i} (y_i - \widehat{\beta}_0 - \widehat{\beta}_1 x_i)^2$

$$\hat{\beta}_1 = \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sum_i (x_i - \overline{x})^2}$$

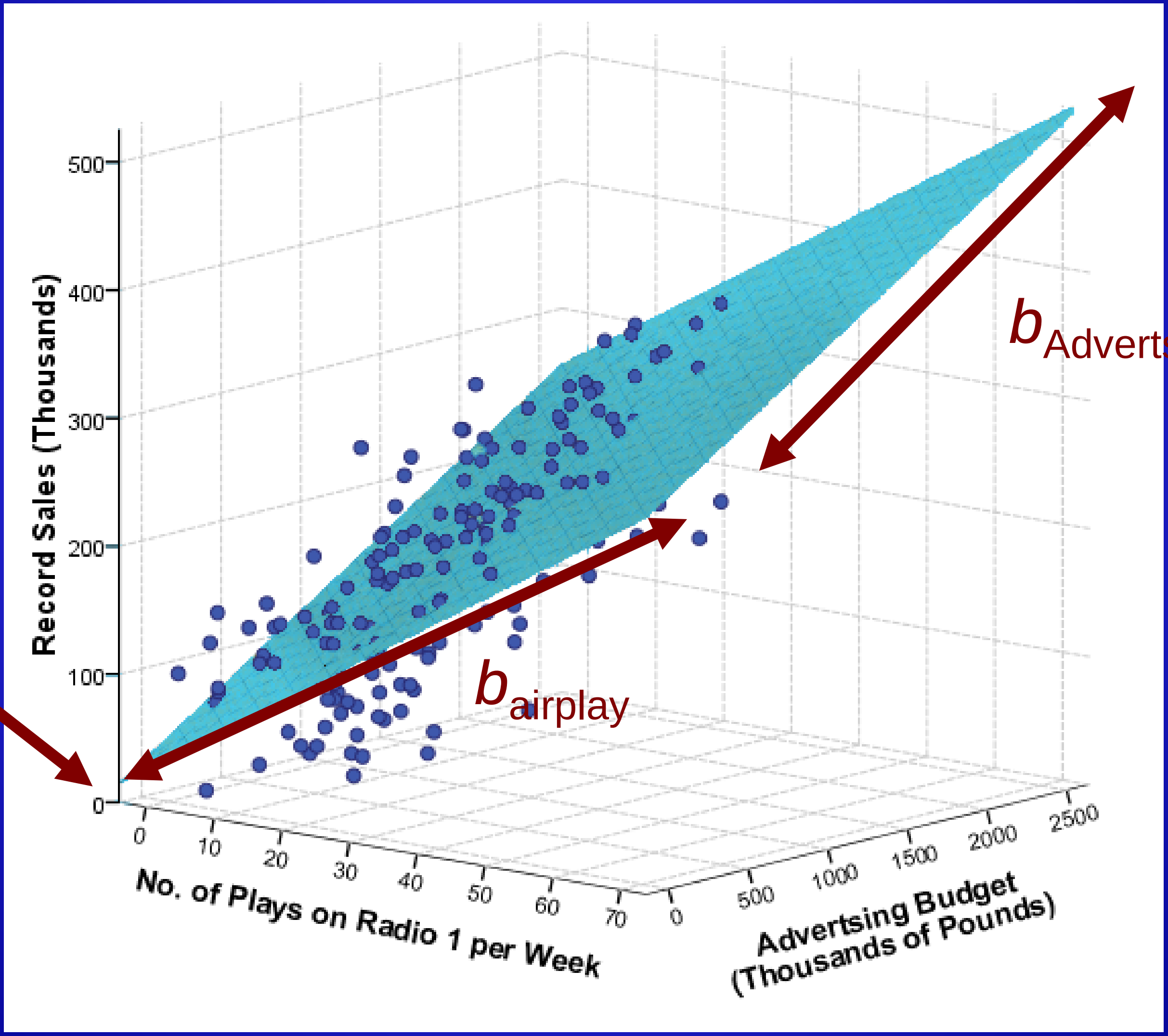
$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}$$

– Real case: Experimental CPU time of a graph

– treatment algorithm vs graph size



The Model with Two Predictors



b_0

Matricial formulation

Regression fit criterion: $\min_r E\left[\left(y_i - r(x_{i1},\cdots,x_{ip})\right)^2\right]$

$$r(x_{i1},\cdots,x_{ip}) = E\left[\,y_i \,\middle|\, x_{i1},\cdots,x_{ip}\right]$$

$$E\left[\,y_i \,\middle|\, x_{i1},\cdots,x_{ip}\right] = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}$$

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \varepsilon_i$$

Estimation of coefficients

$$y_i = b_0 + b_1 x_{i1} + \cdots + b_p x_{ip} + e_i$$

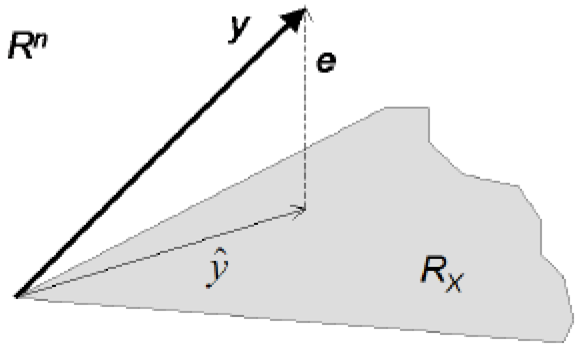
In matrix notation

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_p \end{bmatrix} + \begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix} \equiv \quad y = Xb + e = \hat{y} + e$$

Geometric interpretation

$$y_i = \hat{y}_i + e$$

$$\begin{array}{ccccc} y & & \hat{y} & & e \\ \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} & = & \begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_n \end{bmatrix} & + & \begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix} \end{array}$$



$$\hat{y}_i = b_0 + b_1 x_{i1} + \cdots + b_p x_{ip}$$

Criterion: $\min\limits_{b_0,\ldots,b_p} \sum_{i=1}^{n} (e_i)^2 = \|e\|^2$

$$\langle \hat{y}, e \rangle = \langle \hat{y}, y - \hat{y} \rangle = 0$$

$$\hat{y} = Xb,\ \ b'X'y - b'X'Xb = 0$$

$$b = (X'X)^{-1} X'y$$

Validation

- Technical Assumptions
  - normality, linearity, independence, homokedasticity
  - Tools
    - Graphical residuals analysis
    - Influence-point indicators (hi)
- Quality:
  - R2 (determination coeficient): goodness, reliability
  - s-2: noise, precision
  - Both guarantee generalizability (only interpolation)

Quantify Goodnes of model

$$s^2 = \hat{\sigma}^2 = \frac{\sum_{i=1}^{n} (e_i)^2}{n-2}$$

Estimates the variance of residuals

The biggest, the worst the model, more impresice predictions

Non-standardized

Quantify Goodnes of fit

R^2 : proportion of explained variance

SStotal = V(Y) variance of response variable

Decomposition: SStotal = SSexplainedByModel + SSerrror

Dividing all sides by SStotal:

$$R^2 = \frac{SSexplainedByModel}{SSTotal} = 1 - \frac{SSError}{SSTotal}$$

Quantify Goodnes of model

SSTotal= V(Y) = $\frac{\sum_{i=1}^{n}(y_i - \bar{y})^2}{n-1}$

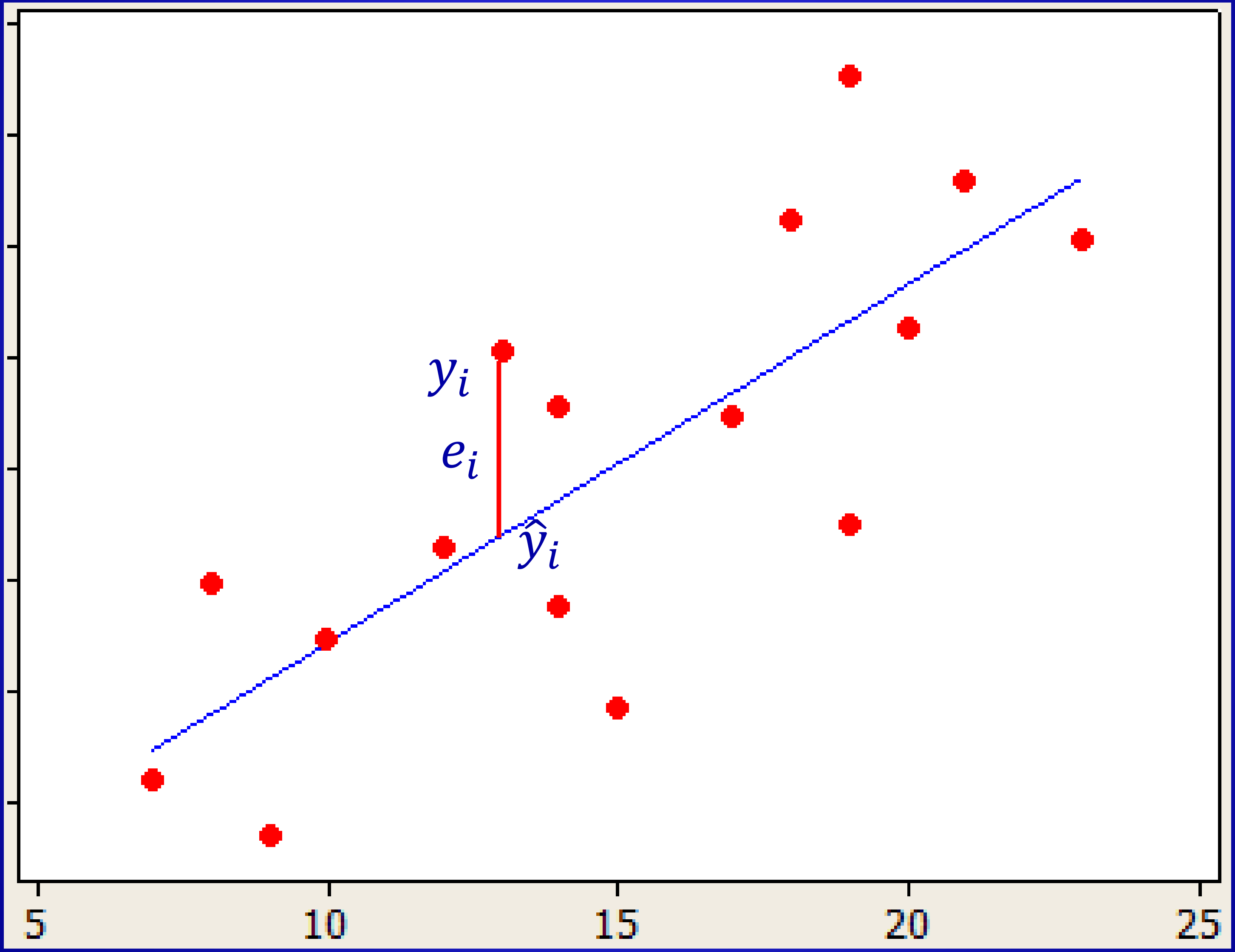
SSExplainedByModel= $\frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{k-1}$

SSError= $\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n-k}$

$$\hat{y}_i = \widehat{\beta}_0 + \widehat{\beta}_1\ x_{1i} + \widehat{\beta}_2\ x_{2i} + .. + \widehat{\beta}_k\ x_{Ki}$$

$$\bar{y} = \frac{\sum_{i=1}^{n} y_i}{n}$$

The residuals



Quantify Goodnes of model

SSTotal= V(Y) = $\frac{\sum_{i=1}^{n}(y_i - \bar{y})^2}{n-1}$

SSExplainedByModel= $\frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{k-1}$

SSError= $\frac{\sum_{i=1}^{n}(e_i)^2}{n-k}$

$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{1i} + \hat{\beta}_2 x_{2i} + .. + \hat{\beta}_k x_{Ki}$

$\bar{y} = \frac{\sum_{i=1}^{n} y_i}{n}$

Quantify Goodnes of model

assume linearity

R^2 = proportion of explained variance

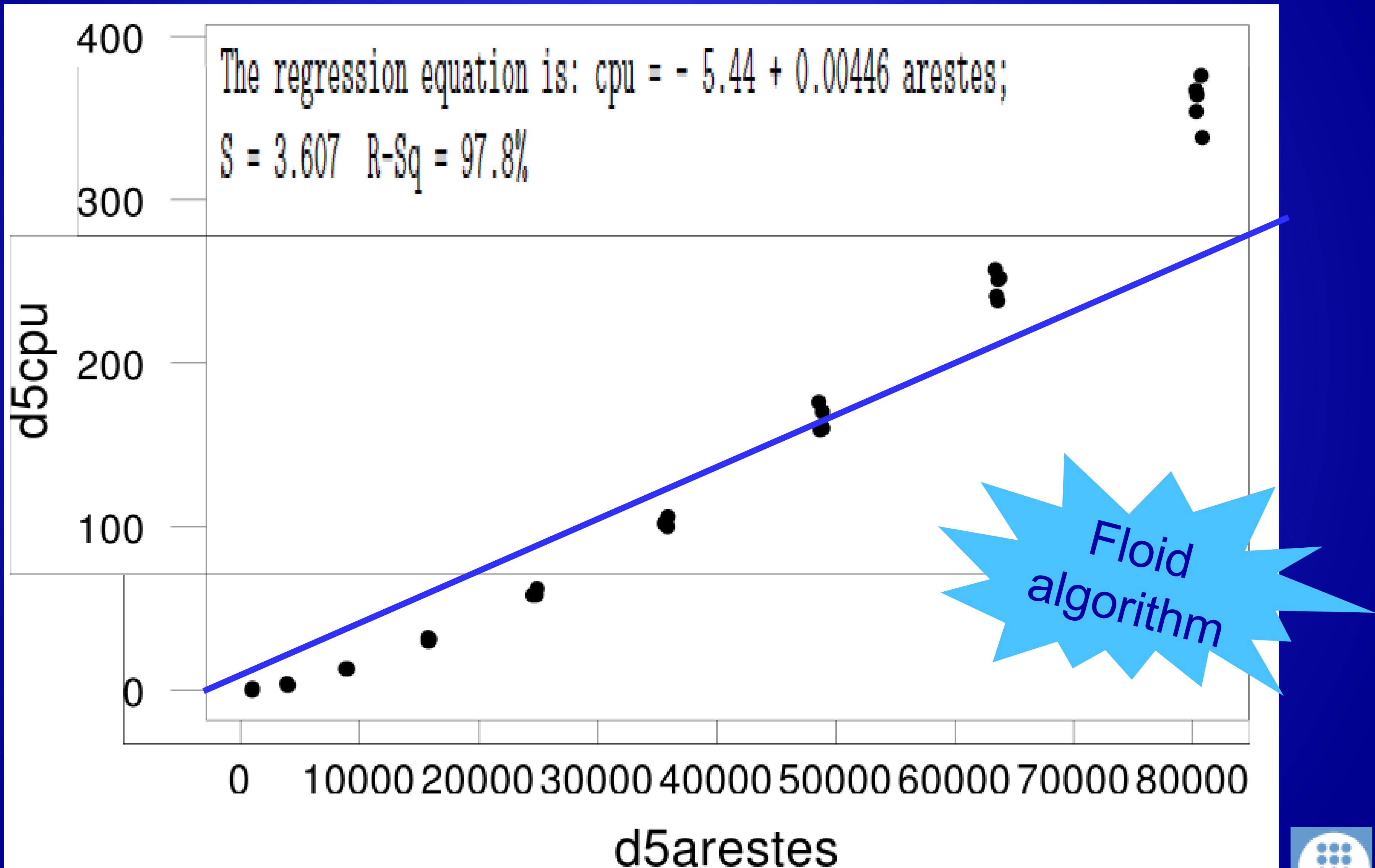
$$R^2 = 1 - \frac{SSError}{SSTotal}$$

$0 < R^2 < 1$

The biggest R^2, the better the model explains Y

For simple linear regression R2=Corr(Y, X)^2

– Real case: Experimental CPU time of a graph
– treatment algorithm vs graph size



Model inference

To test significance of the model

$$F = \frac{SSExplainedByModel}{SSError} \sim F_{(k-1,n-k)}$$

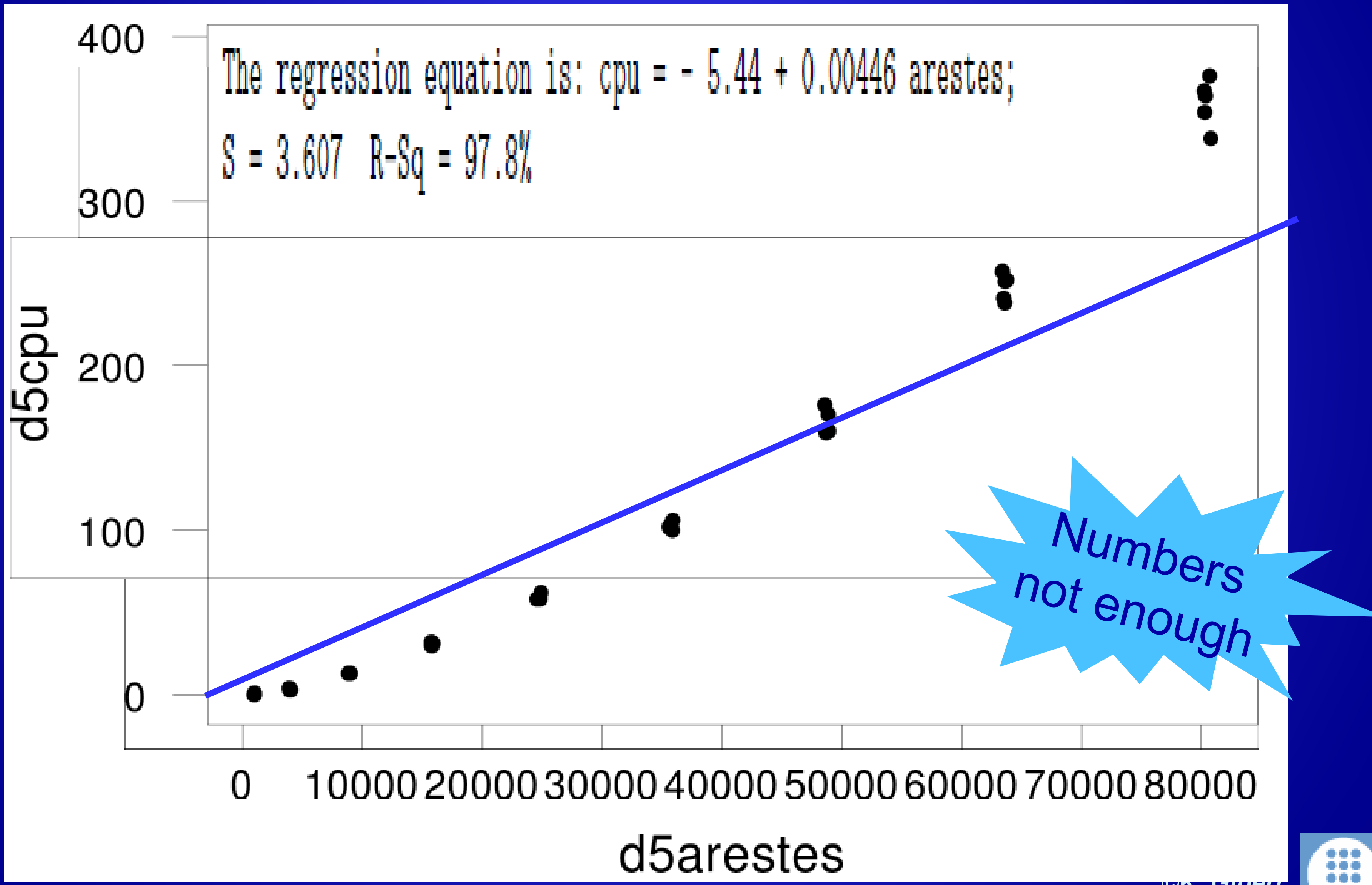
To test significance of a model term $\widehat{\beta}_k$

$$t_k = \frac{\widehat{\beta}_k}{S_{\widehat{\beta}_k}} \sim t_{n-K}$$

To test significance of a model term

Both assume normality

- Real case: Experimental CPU time of a graph
- treatment algorithm vs graph size



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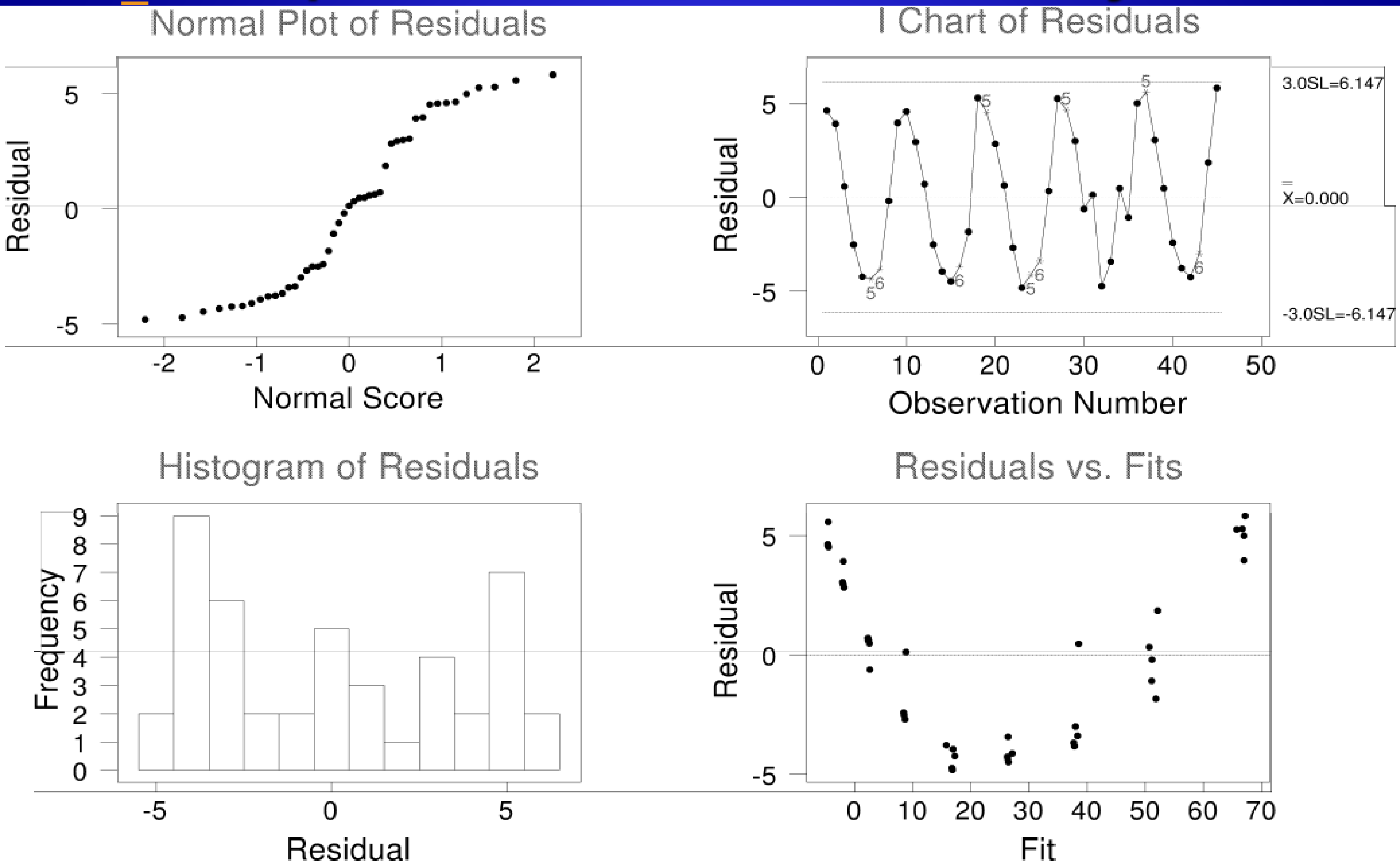
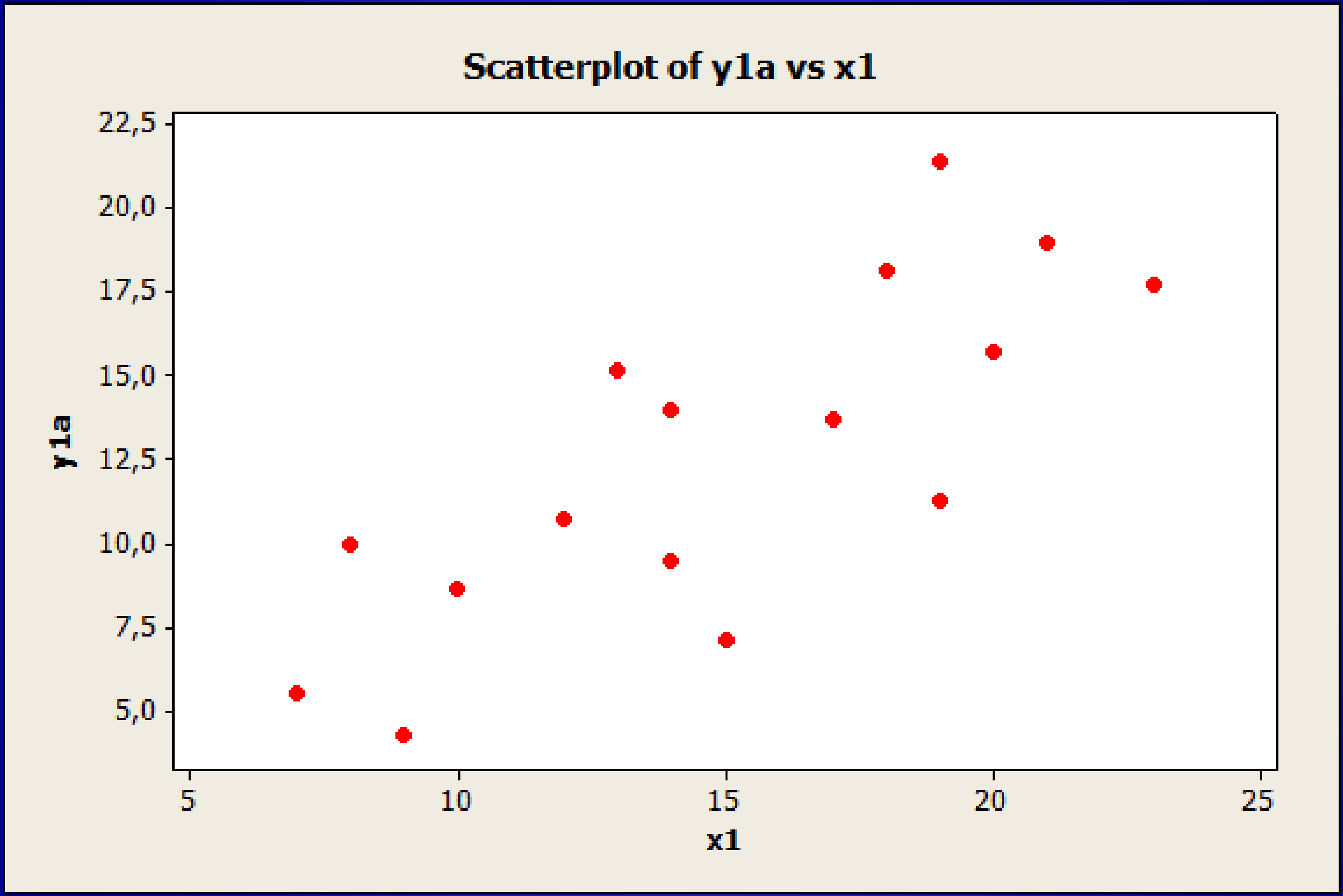
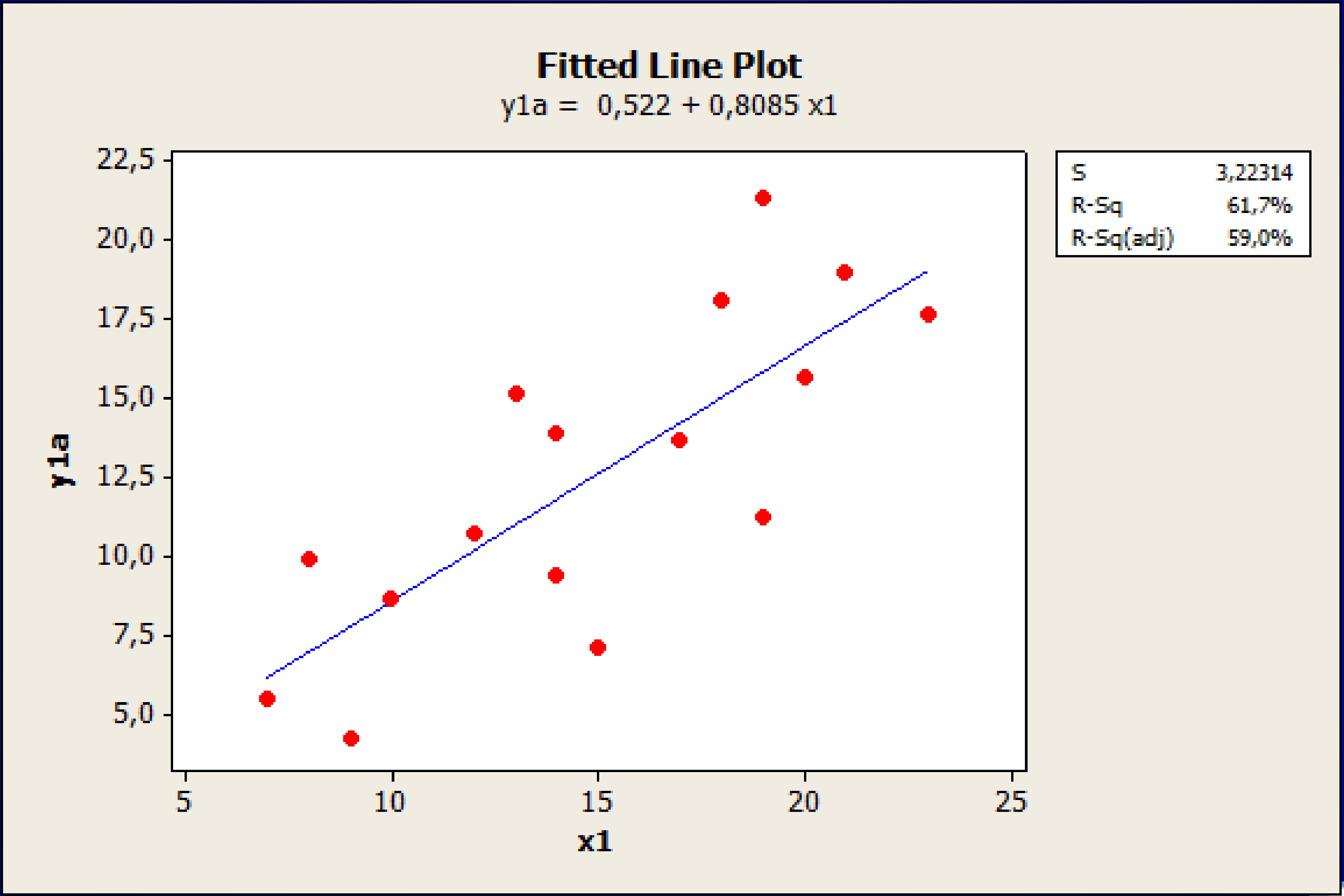
Graphical residuals analysis



Regression

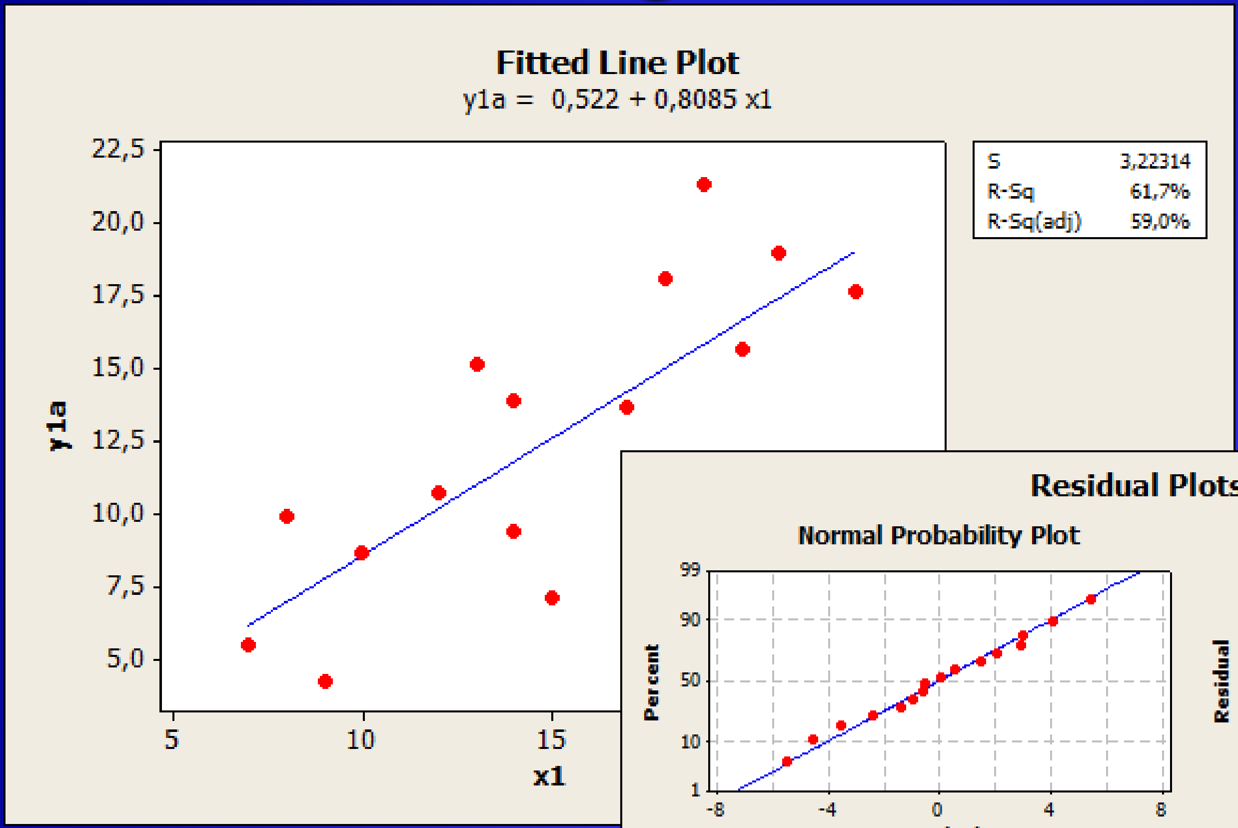
[Tomassone 56]



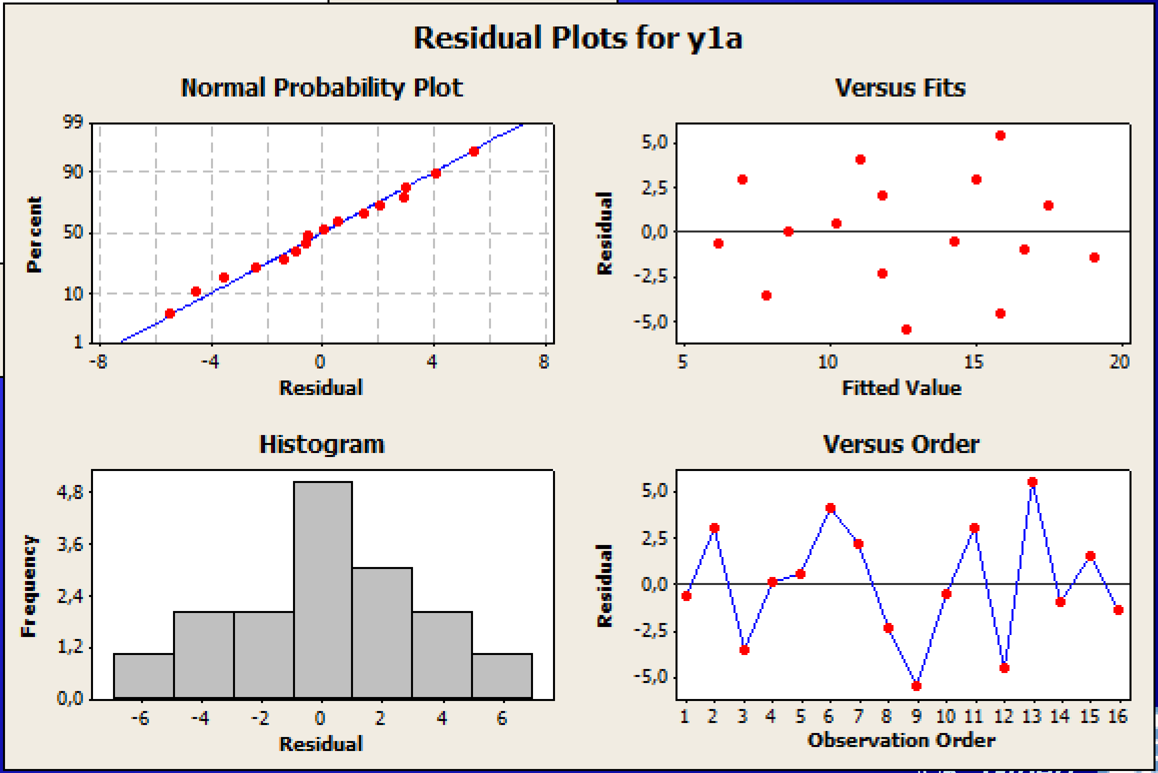


Fitted Line Plot
y1a = 0,522 + 0,8085 x1
S 3,22314
R-Sq 61,7%
R-Sq(adj) 59,0%
22,5
20,0
17,5
15,0
12,5
10,0
7,5
5,0
y1a
5
10
15
20
25
x1

Regression

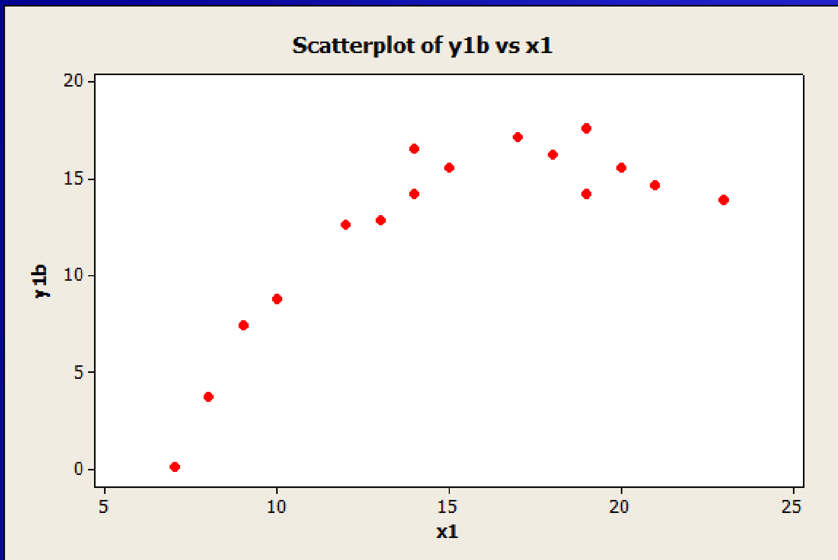


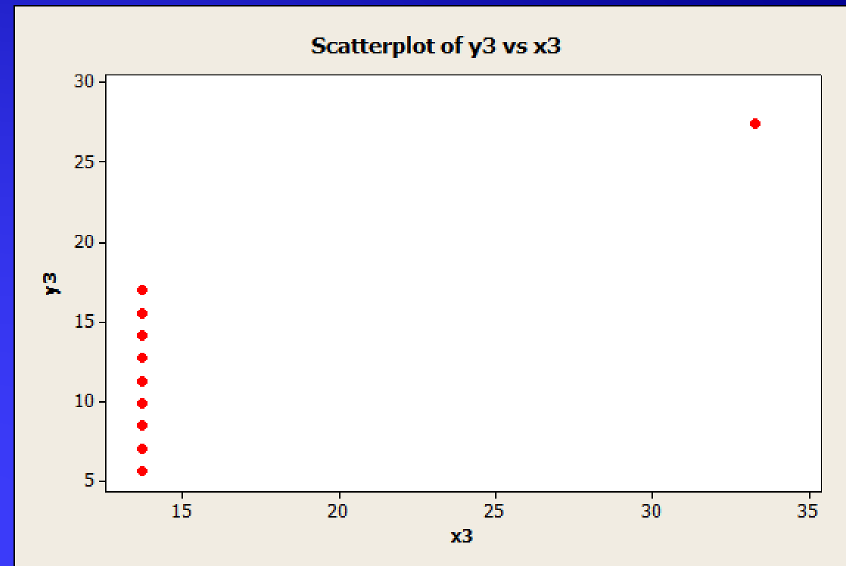
Fitted Line Plot
y1a = 0,522 + 0,8085 x1
S 3,22314
R-Sq 61,7%
R-Sq(adj) 59,0%
y1a
x1

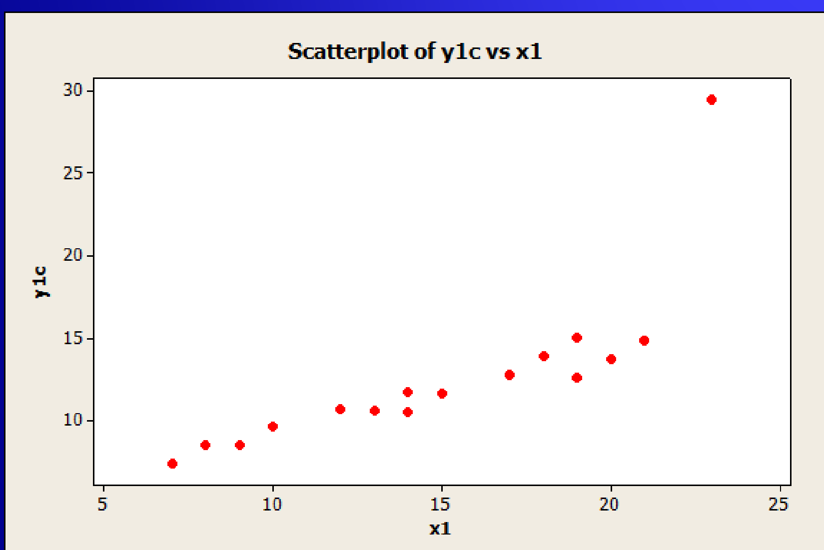


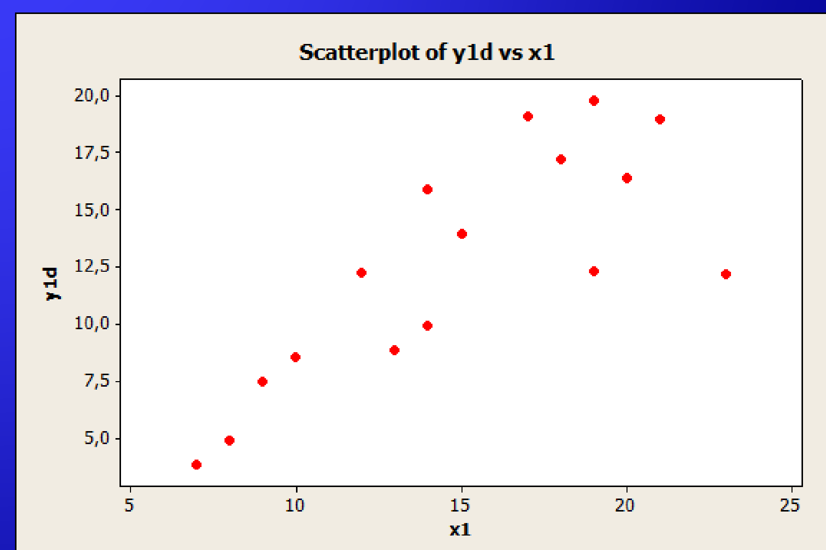
Residual Plots for y1a
Normal Probability Plot
Percent
Residual
Versus Fits
Residual
Fitted Value
Histogram
Frequency
Residual
Versus Order
Residual
Observation Order

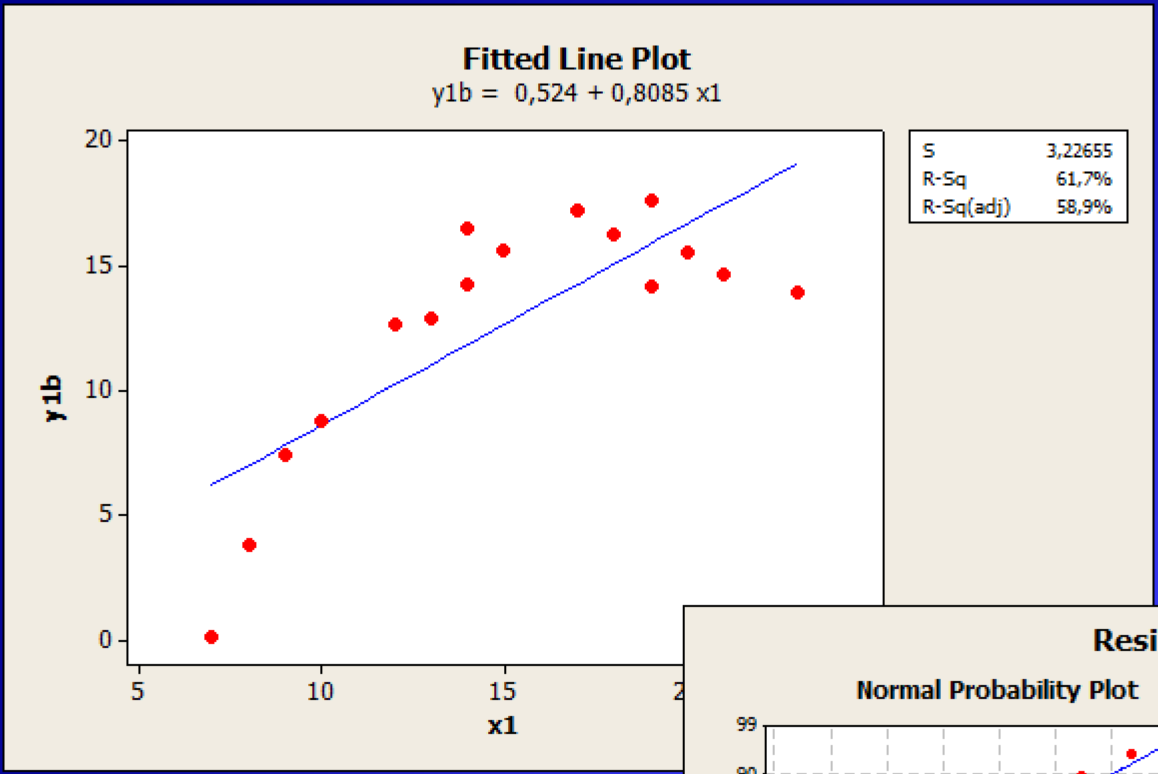
Regression

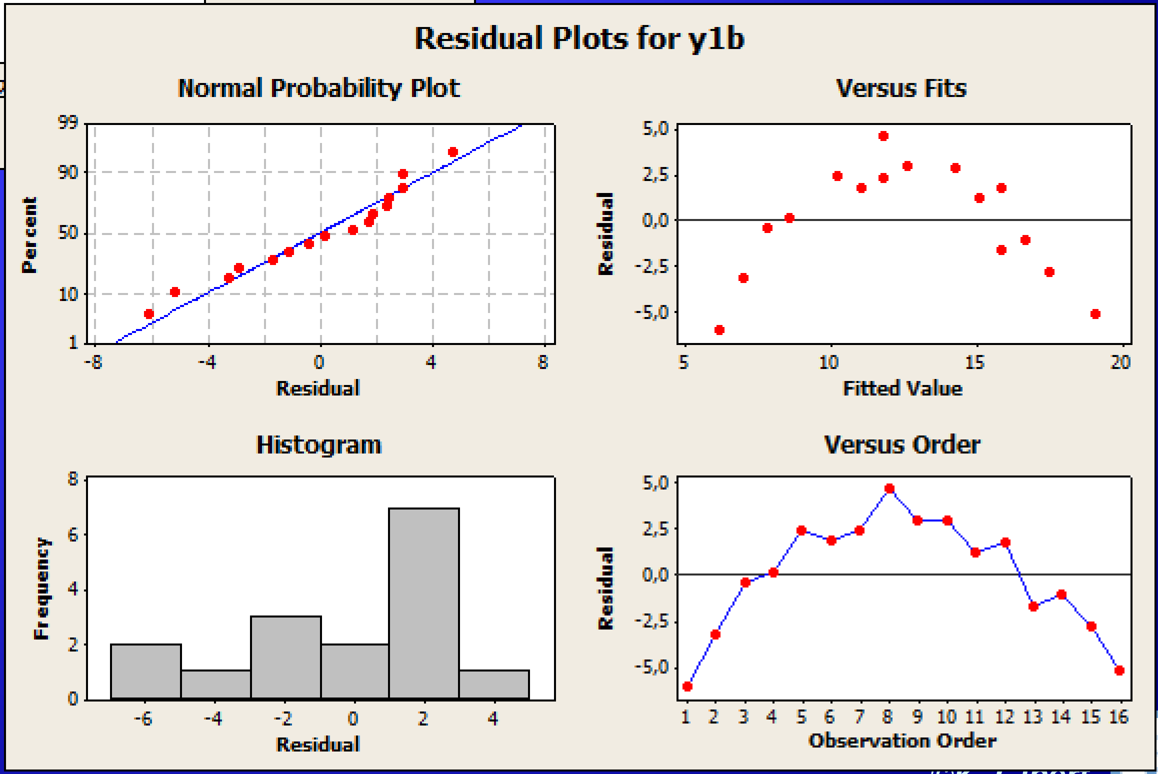

Scatterplot of y1b vs x1
y1b
20
15
10
5
0
5
10
15
20
25
x1

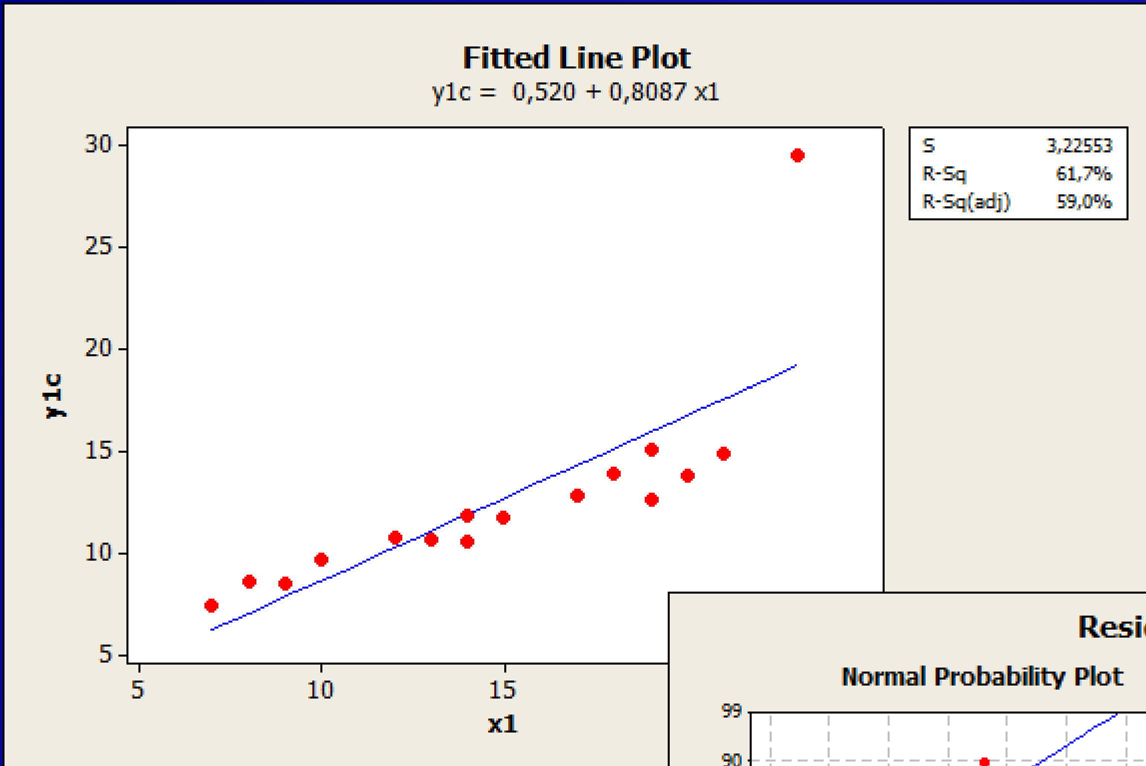

Scatterplot of y3 vs x3
y3
30
25
20
15
10
5
15
20
25
30
35
x3

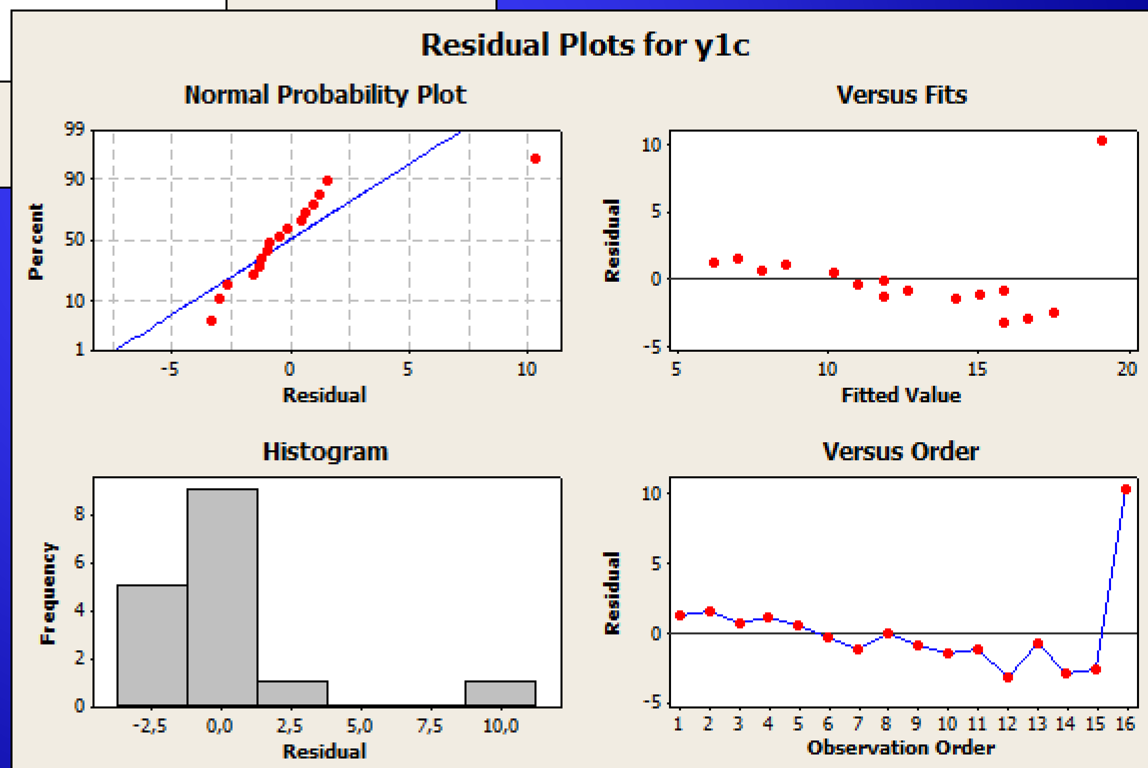

Scatterplot of y1c vs x1
y1c
30
25
20
15
10
5
10
15
20
25
x1

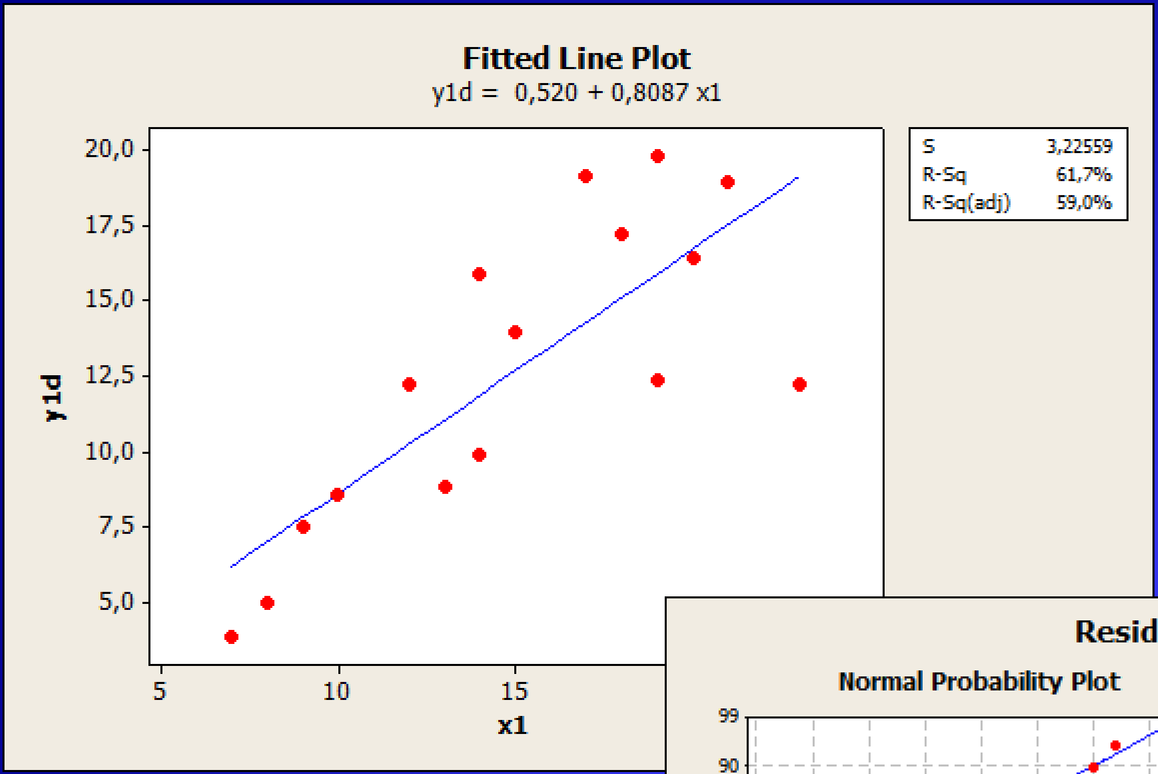

Scatterplot of y1d vs x1
y1d
20,0
17,5
15,0
12,5
10,0
7,5
5,0
5
10
15
20
25
x1


Fitted Line Plot
y1b = 0,524 + 0,8085 x1
S 3,22655
R-Sq 61,7%
R-Sq(adj) 58,9%
y1b
x1

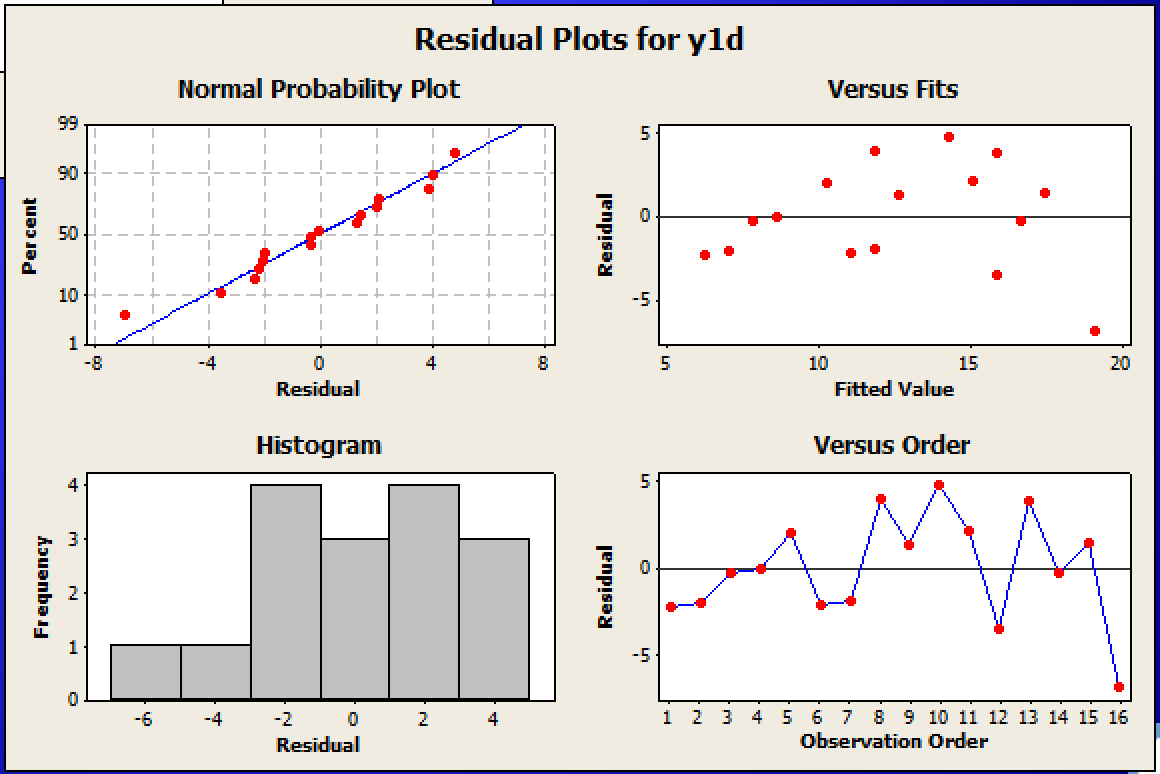

Residual Plots for y1b
Normal Probability Plot
Percent
Residual
Versus Fits
Residual
Fitted Value
Histogram
Frequency
Residual
Versus Order
Residual
Observation Order


Fitted Line Plot
y1c = 0,520 + 0,8087 x1
S 3,22553
R-Sq 61,7%
R-Sq(adj) 59,0%
y1c
x1
30
25
20
15
10
5
5
10
15


Residual Plots for y1c
Normal Probability Plot
Percent
Residual
99
90
50
10
1
-5
0
5
10
Versus Fits
Residual
Fitted Value
10
5
0
-5
5
10
15
20
Histogram
Frequency
Residual
8
6
4
2
0
-2,5
0,0
2,5
5,0
7,5
10,0
Versus Order
Residual
Observation Order
10
5
0
-5
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16

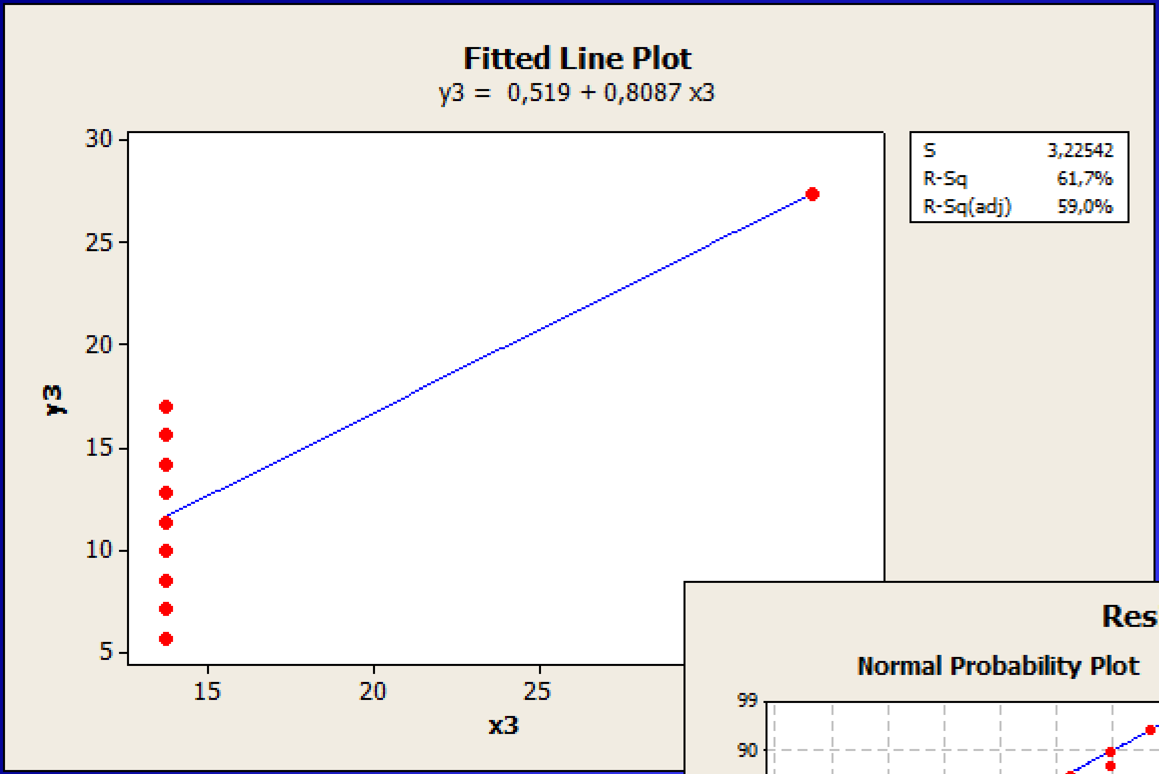


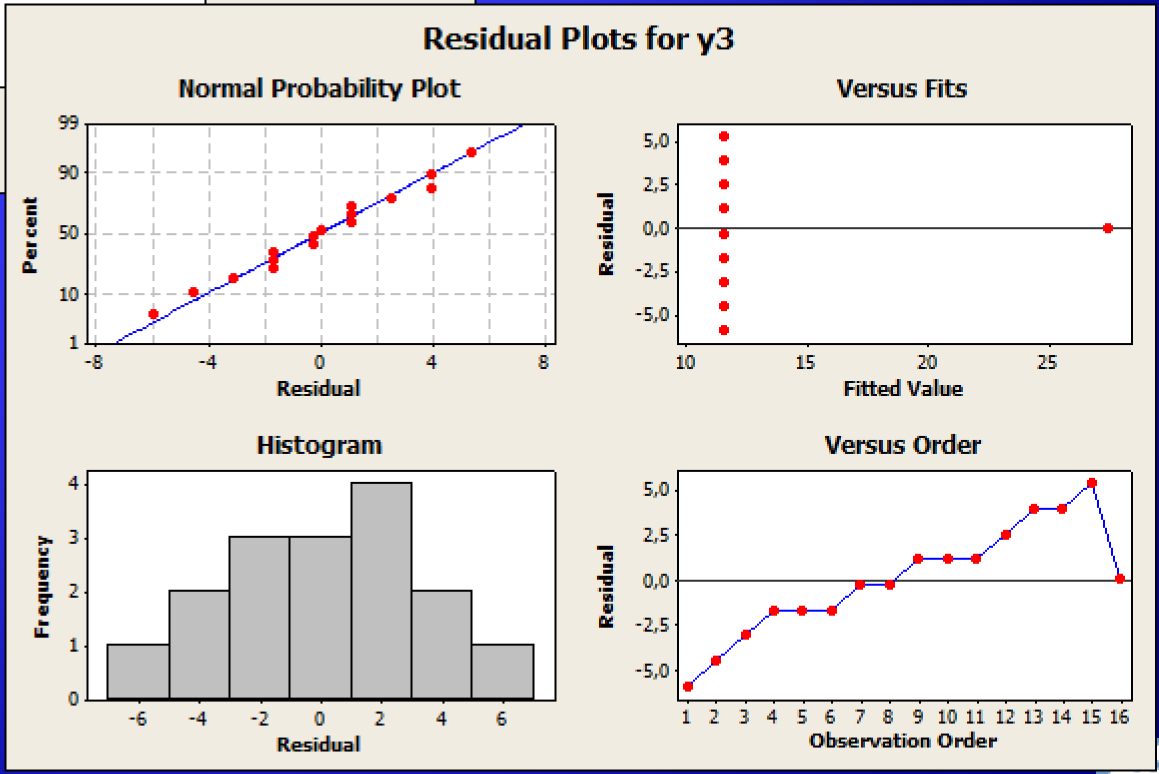
Fitted Line Plot
y1d = 0,520 + 0,8087 x1
S 3,22559
R-Sq 61,7%
R-Sq(adj) 59,0%
y1d
x1



Residual Plots for y1d
Normal Probability Plot
Versus Fits
Histogram
Versus Order
Percent
Residual
Fitted Value
Frequency
Observation Order

4/28/2017


Fitted Line Plot
y3 = 0,519 + 0,8087 x3
S 3,22542
R-Sq 61,7%
R-Sq(adj) 59,0%
y3
x3


Residual Plots for y3
Normal Probability Plot
Percent
Residual
Versus Fits
Residual
Fitted Value
Histogram
Frequency
Residual
Versus Order
Residual
Observation Order

Going further

- ANCOVA: to introduce qualitative variables
- Interaction terms to introduce multiplicative models
- Polynomic regression to estimate higher order polynomial functions
- General Linear Model (common formulation for simple/multiple linear regression, ANOVA and ANCOVA)
- Generalized linear models: common formulation for an extension of families of models:
  - Linear,
  - Poisson
  - Logit.....
- Non linear relationships: LOESS (Locally Weighted Least Squares Regression), uses more local data to estimate the model. It uses a 'nearest neighbors' method to smooth data.
- Complex functions: Artificial Neural Networks