#### UNIVERSIDADE FEDERAL FLUMINENSE

Programa de Mestrado e Doutorado em Engenharia de Produção

Multivariate Data Analysis

Multiple Linear Regression

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### **Outline**

- 1. Definition
  - 2. MLR
- 3. Residuals
- 4. Bibliography

The purpose of MLR (Multiple Linear Regression) to analyze the relationship between metric (or binary) independent variables (predictors) and a metric the dependent variable (response variable), with the following formulation:

$$Y = B_0 + B_1 X_1 + \dots + B_i X_i$$

Where:

Y= Dependent Variable;

 $X_i$ = Independent Variable;

 $B_0$ = Intercept;

 $B_i$ = Slopes.

What is the optimal number of predictors? The suggested rules are:

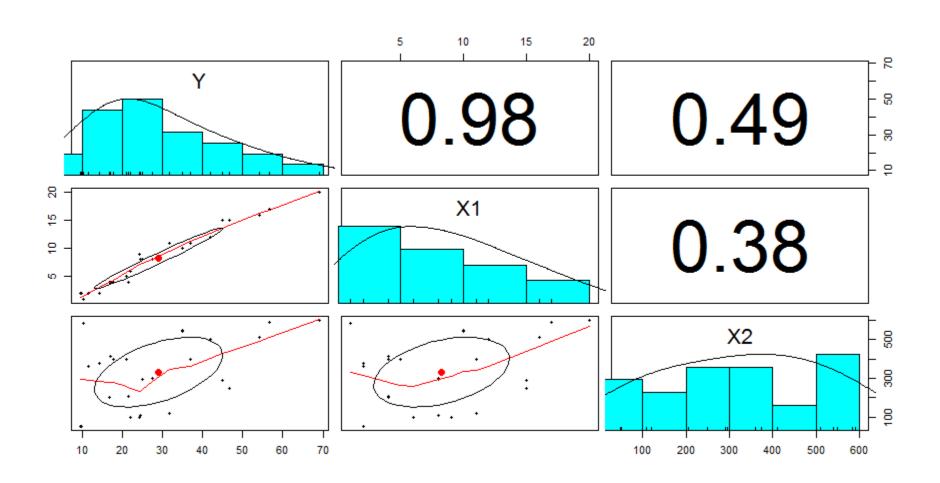
- Evan rule (conservative):  $\frac{n}{k} \ge 10 \to \text{at}$  least 10 observations (n) for predictor (k)
- Doane rule (relaxed):  $\frac{n}{k} \ge 5 \rightarrow \text{at least 5 observations } (n) \text{ for predictor } (k)$

Categorical variables can be included as dummy variables (1 = one belongs to category; 0 = it does not belong to category). It is not necessary to encode all categories because the last one is identified when all the others have a zero value. This method prevents the occurrence of collinearity, and allows the design matrix to be invertible. Dummy variables have the same statistical treatment of the independent variables.

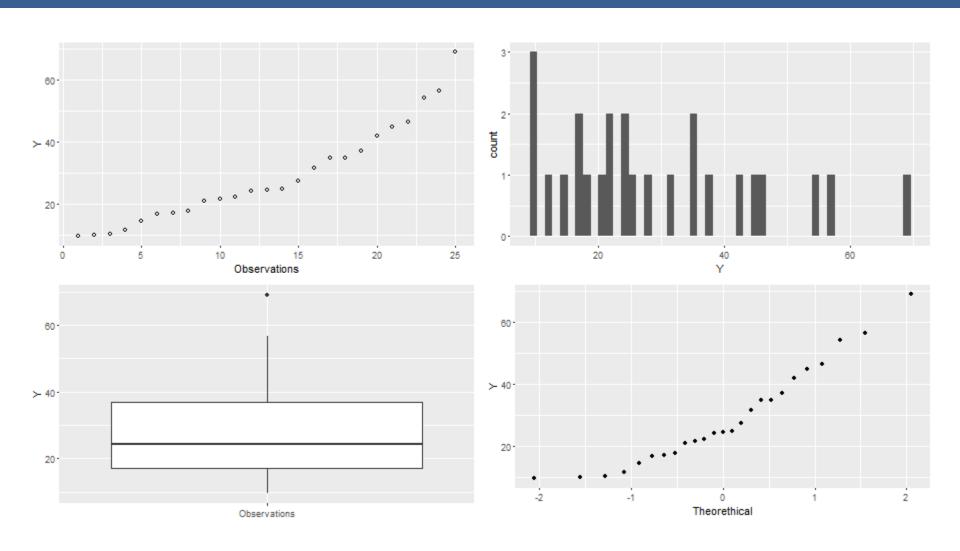
Observation	Y	X1	X2
1	9.6	2	52
2	9.95	2	50
3	10.3	1	585
4	11.66	2	360
5	14.38	2	375
6	16.86	4	200
7	17.08	4	412
8	17.89	4	400
9	21.15	5	400
10	21.65	4	205
11	22.13	6	100
12	24.35	9	100
13	24.45	8	110
14	25.02	8	295
15	27.5	8	300
16	31.75	11	120
17	34.93	10	540
18	35	10	550
19	37	11	400
20	41.95	12	500
21	44.88	15	290
22	46.59	15	250
23	54.12	16	510
24	56.63	17	590
25	69	20	600

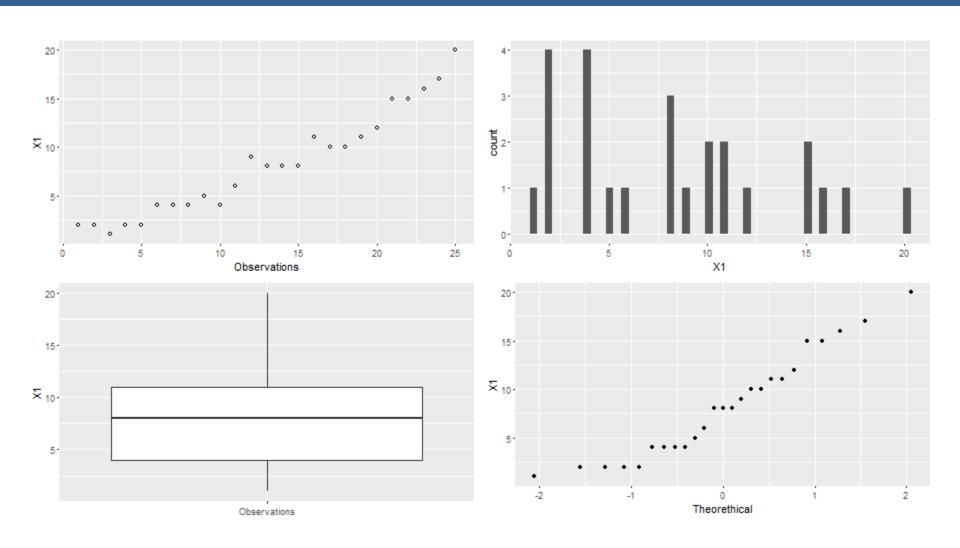
In order to explain a MLR approach, the following dataset will be used: The simulated dataset of 25 observations and 2 independent Variables  $X_1$  and  $X_2$ .

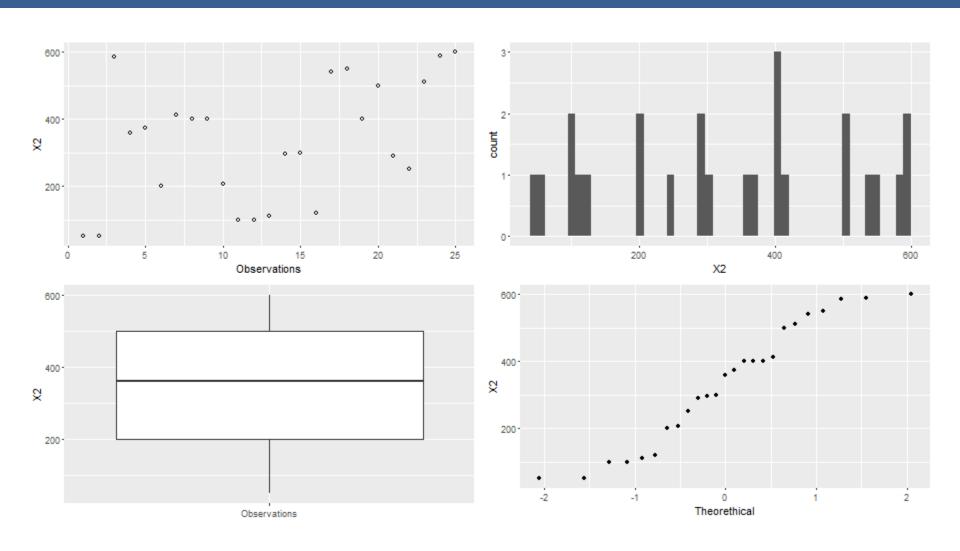
```
# Graph
library (psych)
pairs.panels(my_data)
```



```
library(ggplot2)
ggplot(data = my_data, aes(x = 1:25, y = my_data$Y)) + geom_point(shape = 1) + labs(x = "Observations", y = 1:25, y = my_data$Y)) + geom_point(shape = 1) + labs(x = "Observations", y = 1:25, y = my_data$Y))
ggplot(data = my_data, aes(x = "Observations", y = my_data$Y)) + geom_boxplot() + theme(axis.title.x =
element blank()) + labs(y = "Y")
ggplot(my_data, aes(my_data$Y)) + geom_histogram(bins = 50) + labs(x = "Y")
ggplot(data = my_data, aes(x = 1:25, y = my_data$X1)) + geom_point(shape = 1) + labs(x = "Observations", y =
"X1")
ggplot(data = my_data, aes(x = "Observations", y = my_data$X1)) + geom_boxplot() + theme(axis.title.x = my_data, aes(x = my
element_blank()) + labs(y = "X1")
ggplot(my_data, aes(my_data$X1)) + geom_histogram(bins = 50) + labs(x = "X1")
ggplot(data = my data, aes( sample = my data$X1)) + stat gg()+ xlab("Theorethical") + ylab("X1")
ggplot(data = my_data, aes(x = 1:25 y = my_data$X2)) + geom_point(shape = 1) + labs(x = "Observations", y = 1:25 y = my_data$X2)) + geom_point(shape = 1) + labs(x = "Observations", y = 1:25 y = my_data$X2))
"X2")
ggplot(data = my_data, aes(x = "Observations", y = my_data$X2)) + geom_boxplot() + theme(axis.title.x =
element_blank()) + labs(y = "X2")
ggplot(my_data, aes(my_data$X2)) + geom_histogram(bins = 50) + labs(x = "X2")
ggplot(data = my_data, aes( sample = my_data$X2)) + stat_qq()+ xlab("Theorethical") + ylab("X2")
```







# Multiple Linear Regression

```
# MLR
mlr <- lm(Y \sim ., data = my_data)
summary(mlr)
Call:
Im(formula = Y \sim .., data = my_data)
Residuals:
                       Median
 Min
               1Q
                                      3Q
                                                Max
                        -0.362
                                    1.196
-3.865
            -1.542
                                                5.841
Coefficients:
            Estimate
                           Std. Error
                                           t value
                                                      Pr(>|t|)
                                            2.136
                                                    0.044099 *
(Intercept)
            2.263791
                            1.060066
            2.744270
                           0.093524
                                           29.343
                                                      < 2e-16 ***
X1
X2
            0.012528
                                           4.477
                                                    0.000188 ***
                           0.002798
                                   *** 0.01
                                                 '*' 0.05
                                                             '.' 0.1
Signif. codes: 0
                    '***' 0.001
Residual standard error: 2.288 on 22 degrees of freedom
```

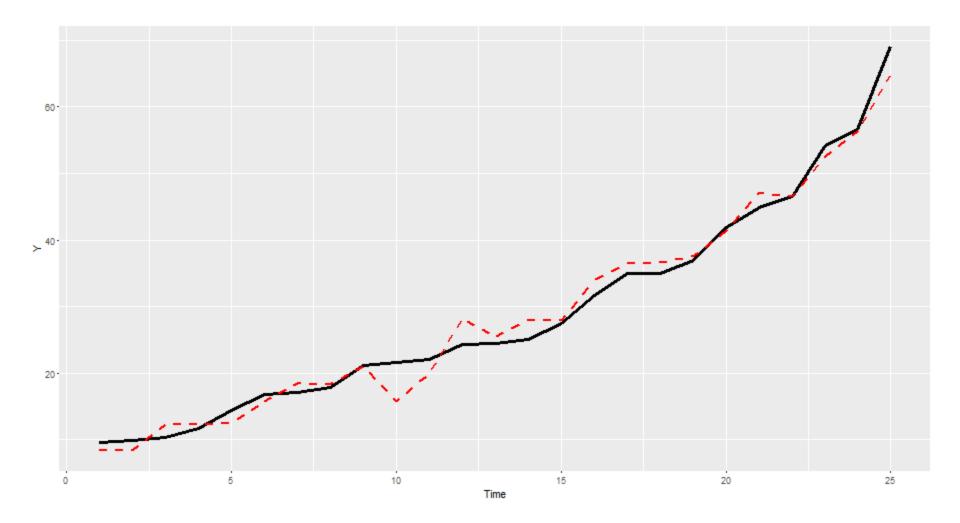
Multiple R-squared: 0.9811 Adjusted R-squared: 0.9794

F-statistic: 572.2 on 2 and 22 DF, p-value: < 2.2e-16

Observation	Y	X1	<b>X2</b>	$\widehat{y}$
1	9.6	2	52	8.40
2	9.95	2	50	8.38
3	10.3	1	585	12.34
4	11.66	2	360	12.26
5	14.38	2	375	12.45
6	16.86	4	200	15.75
7	17.08	4	412	18.40
8	17.89	4	400	18.25
9	21.15	5	400	21.00
10	21.65	4	205	15.81
11	22.13	6	100	19.98
12	24.35	9	100	28.21
13	24.45	8	110	25.60
14	25.02	8	295	27.91
15	27.5	8	300	27.98
16	31.75	11	120	33.95
17	34.93	10	540	36.47
18	35	10	550	36.60
19	37	11	400	37.46
20	41.95	12	500	41.46
21	44.88	15	290	47.06
22	46.59	15	250	46.56
23	54.12	16	510	52.56
24	56.63	17	590	56.31
25	69	20	600	64.67

```
# Predicted Y
mlr$fitted.values

ggplot() + geom_line(data = my_data, aes(x = 1:25, y = Y), colour =
"black", size = 1.2) + xlab("Time") + ylab("Y") + geom_line(data =
my_data, aes(x = 1:25, y = mlr$fitted.values), colour = "red", size = 1,
linetype = 2)
```



The model standard error is calculated by.

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n - (k+1)}; \hat{\sigma}^2 = 5.235$$

$$\hat{\sigma} = 2.288$$

Where:

k = Total number of independent variables;

 $\hat{y}$  = Estimated value of the dependent variable;

summary(mlr)

Residual standard error: 2.288 on 22 degrees of freedom

Multiple R-squared: 0.9811 Adjusted R-squared: 0.9794

F-statistic: 572.2 on 2 and 22 DF, p-value: < 2.2e-16

The following hypothesis test for  $B_i$  can then be done:

```
H_0: B_i = 0 (There is not a linear relation between x_i e y)

H_1: B_i \neq 0 (There is a linear relation between x_i e y)
```

```
summary(mlr)
Call:
Coefficients:
          Estimate
                       Std. Error
                                   t value
                                             Pr(>|t|)
                                   2.136
(Intercept) 2.263791
                       1.060066
                                           0.044099 *
    2.744270
                                   29.343 < 2e-16 ***
X1
                      0.093524
X2
                      0.002798 4.477
                                           0.000188 ***
   0.012528
```

Signif. codes: **0** '\*\*\*' 0.001 '\*\*' 0.05 '.' 0.1

To evaluate the adequacy of the model with the data, the following hypothesis is made to test the model adequacy:

 $H_0$ : The model is not adequate  $H_1$ : The model is adequate

#### summary(mlr)

Residual standard error: 2.288 on 22 degrees of freedom

Multiple R-squared: 0.9811 Adjusted R-squared: 0.9794

F-statistic: 572.2 on 2 and 22 DF, p-value: < 2.2e-16

The  $r^2$  (r-squared or coefficient of determination) measures the strength of the relationship, indicating that the model explains a percentage of the variance of the dependent variable. For example, a  $r^2$  equal to 0.80 means that 80% of the variance of the dependent variable comes from its relation with the independent variables. The  $(r^2)_a$  - adjusted  $r^2$  - is na indicator that adjusts the  $r^2$  based on the number of k independent variables and it is useful to penalize models that uses too many independent variables.

summary(mlr)

Residual standard error: 2.288 on 22 degrees of freedom

Multiple R-squared: 0.9811 Adjusted R-squared: 0.9794

F-statistic: 572.2 on 2 and 22 DF, p-value: < 2.2e-16

The collinearity (correlation between two predictors) or multicollinearity (correlation between multiple predictors) can be harmful for the model because:

- Estimates may be unstable;
- Standard errors can be unreliable;
- Confidence intervals can become very large;
- The coefficient of determination can be high, even though the T-tests are insignificant.

To detect this problem is necessary to calculate the **VIF** (*Variance Inflator Factor*) for each predictor. If its value is > 5 the predictor is highly correlated indicating collinearity:

```
# VIF (Variance Inflation Factors)
library("car")
vif(mlr)

X1 X2
1.167128 1.167128
```

#### Suggest interpretation:

VIF	Interpretation	
$VIF_j = 1.00$	Insignifiant	
$VIF_j = 2.00$	Medium	
$VIF_j = 10.00$	Strong	
$VIF_j = 100.00$	Severe	

### Residuals

Once verified the adequacy of the estimated model, it is also necessary to validate the errors (residuals) of the model. Supposedly, the residuals must be:

- Normally distributed;
- Homoscedastic;
- Independent (uncorrelated within a series of time).

The studentized residuals are most indicated approach to proceed with the evaluation. The studentized residual is the quotient resulting from the division of a residual by an estimate of its standard deviation, usually ranging from -3 to +3.

# Studentized Residuals library("MASS") sresid <- studres(mlr)

#### Normally Distributed

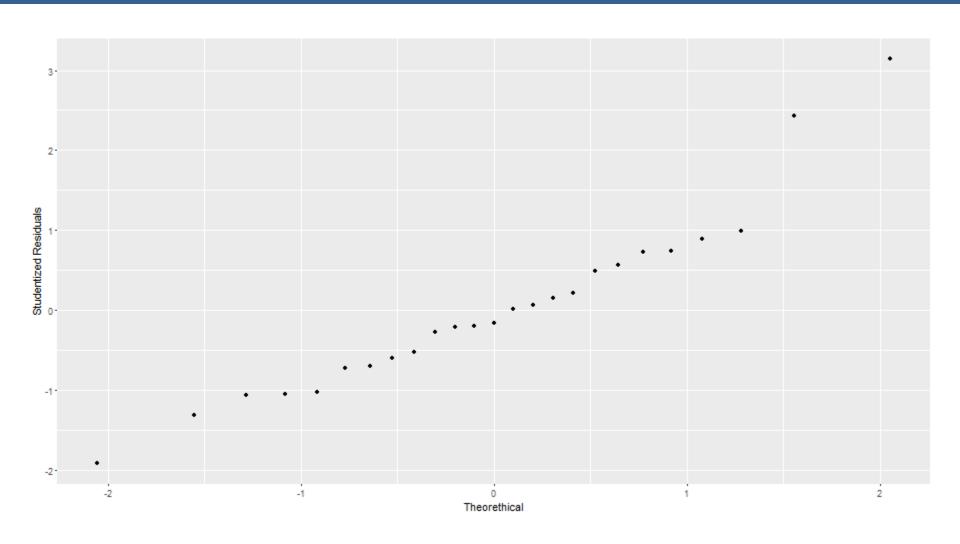
Violation of this assumption is considered mild and can make the confidence intervals unreliable. Large samples, logarithmic transformations in the dependent and independent variables or removal of outliers, can avoid this violation.

```
# QQ Plot
ggplot(data = my_data, aes( sample = sresid)) + stat_qq()+ xlab("Theorethical") + ylab("Studentized Residuals")

# Univariate Normality
shapiro.test(sresid)

Shapiro-Wilk normality test
```

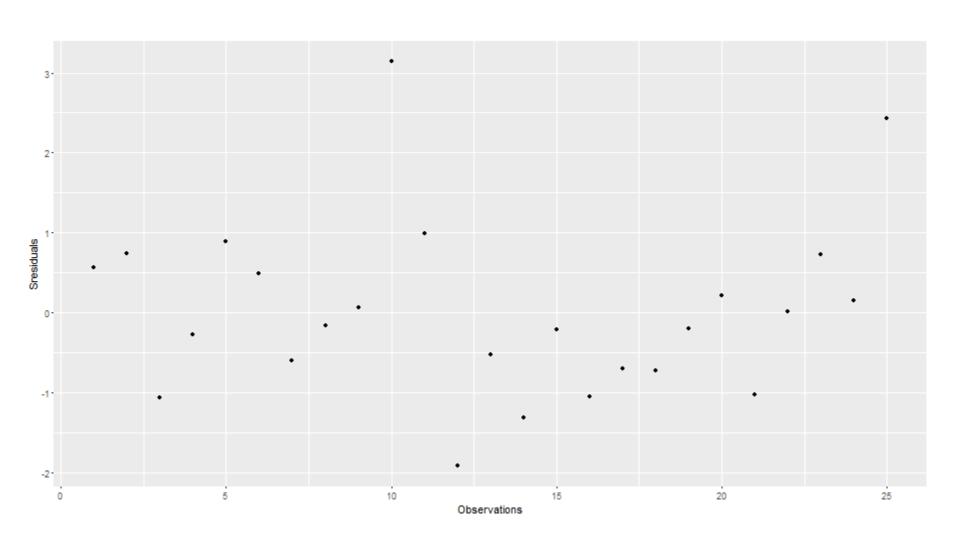
data: sresid W = 0.93094, p-value = 0.09136



#### Homocedastic

Violation of this assumption is considered severe and can increase the range of confidence intervals and make the model unfeasible. Large samples, logarithmic transformations in the dependent and independent variables or removal of outliers, can avoid this violation. To verify that the errors are homoscedastic (constant variance) the residual graphic, ideally, will have no patterns.

```
# Homoscedascity
ggplot(data = my_data, aes(x = 1:25, y = sresid)) + geom_point() + labs(x = "Observations", y = "Sresiduals")
```



The Breusch-Pagan Test can be done to verify the homoscedasticity, with the following hypothesis:

 $H_0$ : The model is homoscedastic  $H_1$ : The model is not homoscedastic

```
# Breusch-pagan test
library("car")
ncvTest(mlr)
```

```
Non-constant Variance Score Test
Variance formula: ~ fitted.values
Chisquare = 0.04524206 Df = 1 p = 0.8315596
```

Independency

Violation of this assumption is considered mild and can increase the range of the confidence intervals. This assumption is only considered in time series.

A differentiation of the first order or the removal of outliers, can avoid this violation.

# Prediction

```
# Prediction
new_data <- as.data.frame(cbind(2, 50))
colnames(new_data) <- c("X1", "X2")
predict(mlr, new_data)</pre>
```

#### **MVDA**

#### https://github.com/Valdecy/Multivariate\_Data\_Analysis

```
# Created by: Prof. Valdecy Pereira. D.Sc.
```

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- # Course: Multivariate Data Analysis
- # Lesson: Multiple Linear Regression

#### Citation:

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repository: <a href="https://github.com/Valdecy/Multivariate\_Data\_Analysis">https://github.com/Valdecy/Multivariate\_Data\_Analysis</a>

#### Bibliography

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- FÁVERO, L. P.; BELFIORE, P.; SILVA, F. L.; CHAN, B. **Análise de Dados: Modelagem Multivariada** para **Tomada de Decisões**. CAMPUS, 2009.
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- LATTIN, J.; CARROLL, J. D.; GREEN, P. E. **Análise de Dados Multivariados**. CENGAGE Learning, 2011.
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