UD5: INFERENCE

Part 1: Distributions in sampling

Part 2: Inference about one population

Comparison of 2 populations

Part 3: ANOVA (Analysis of Variance)

Part 4: Regression

UD 5 part 3

ANOVA

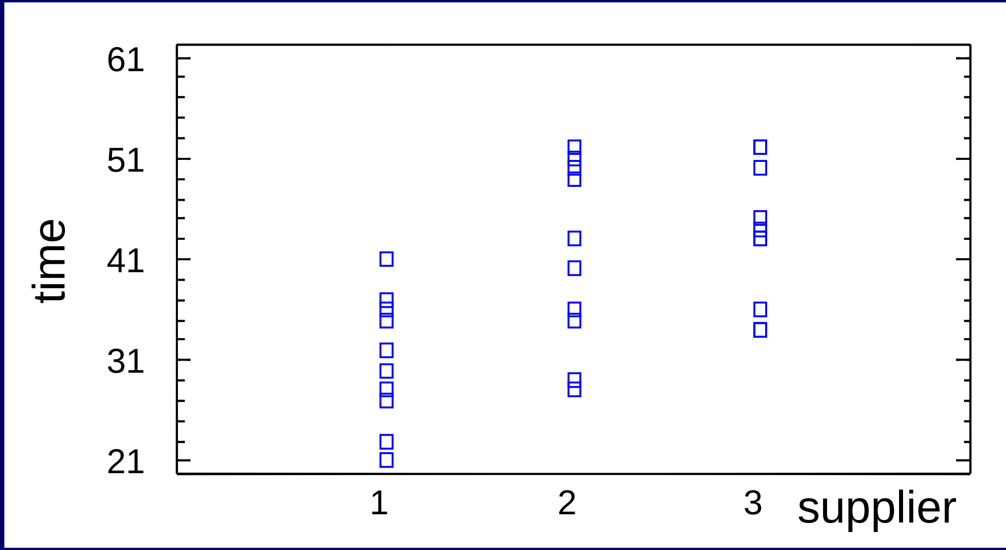
ANALYSIS OF VARIANCE

One computer factory has to purchase the batteries for a new model of laptop. There are three possible battery suppliers: S1, S2 and S3.

In order to determine which one is more convenient, the company purchases 10 batteries from each supplier and determines the following parameter:

1 factor (supplier) with 3 variants:

RESULTS OBTAINED (time of battery operation, months, until the battery lasts 2 hours)	S1	S2	S3
	23	35	50
	28	36	43
	21	29	36
	27	40	34
	35	43	45
	41	49	52
	37	51	52
	30	28	43
	32	50	44
	36	52	34



Which supplier should we choose?

H_0: $m_1 = m_2 = m_3$

Average:	**31**	**41.3**	**43.3**
Price:	**70**	**80**	**85**

Is there enough evidence to affirm that batteries from supplier 3 last longer and therefore would be more appropriate despite their higher price?

Would it be possible to analyze these data by comparing S1 vs S2 ; S1 vs S3 ; S2 vs S3 ?

If we had 5 suppliers, how many pairs should we compare?

THE COMPARISON OF ALL POSSIBLE PAIRS IS NOT RECOMMENDED

ANalysis Of VAriance (ANOVA)

Developed in ~1930 by R. A. Fisher

POWERFUL TOOL TO STUDY OF THE EFFECT OF ONE OR MORE FACTORS ON THE MEAN OF ONE VARIABLE

INTUITIVE IDEA OF ANOVA

Residual = $X_{observed} - X_{predicted}$ → **$X_{observed} = X_{predicted}$ + residual**

$$\mathbf{x_{obs}} - \bar{\mathbf{x}} = \mathbf{x_{pred}} - \bar{\mathbf{x}} + \text{resid}$$

Average of all data

$$\sum^{n} (\mathbf{x_{obs}} - \bar{\mathbf{x}})^2 = \sum^{n} (\mathbf{x_{pred}} - \bar{\mathbf{x}})^2 + \sum (\text{resid})^2$$

Sum of Squares (SS): $SS_{TOTAL} = SS_{FACTOR} + SS_{RESIDUAL}$

$$\frac{\text{sum of squares}}{\text{degrees of freedom}} = \text{Mean Square}$$

SS / d.f. = MS

$d.f._{TOTAL} = d.f._{FACTOR} + d.f._{RESIDUAL}$

MS = SS / d.f.

$$MS_{TOTAL} = \frac{SS_{TOTAL}}{N-1} = \frac{\sum (x_i - \bar{x})^2}{N-1} = s^2$$

Total degrees of freedom = total number of data - 1

$$MS_{RESIDUAL} = \frac{SS_{RESID}}{d.f._{residual}} \qquad MS_{FACTOR} = \frac{SS_{FACTOR}}{d.f._{FACTOR}}$$

Degrees Fr.$_{FACTOR}$ = Number of variants - 1

Comparison of variance of two Normal populations:

$$\frac{s_1^2 / \sigma_1^2}{s_2^2 / \sigma_2^2} \sim F_{N_1-1, N_2-1}$$

Assuming $\sigma^2_1 = \sigma^2_2$:

$$s_1^2 / s_2^2 \approx F_{n_1-1, n_2-1}$$

Mean Square is more or less a variance:

(a measure of data variability)

$$\frac{MS_1}{MS_2} \cong \frac{s_1^2}{s_2^2} \approx F$$

F - TEST

Are there differences between the mean time of battery operation in the batteries from the 3 suppliers?

NULL HYPOTHESIS: $\mathbf{H_0 : m_1 = m_2 = m_3}$ (there are no differences)

IF THE NULL HYPOTHESIS IS TRUE:

1) SAMPLE AVERAGES $\bar{x}_1$, $\bar{x}_2$ AND $\bar{x}_3$ WILL BE "SIMILAR" (AND THEREFORE "SIMILAR" ALSO TO THE GRAND MEAN) $\bar{\bar{X}}$

2) SUM OF SQUARES OF THE FACTOR WILL BE "SMALL", BUT... WHAT SHOULD BE CONSIDER AS "SMALL" ?

3) $MS_{residual}$ IS AN ESTIMATION OF σ^2 ($\sigma^2_1 = \sigma^2_2 = \sigma^2_3$)

4) MS_{factor} IS ALSO AN ESTIMATOR OF σ^2, INDEPENDENT FROM MS_{RESID}, AND CONSEQUENTLY:

$$\text{F-ratio} = (MS_{factor} / MS_{residual}) = S_f^{\,2} / S_r^{\,2} \sim F_{2\,,\,27}$$

T: time of battery operation

$T_1 \sim N(m_1, \sigma^2)$	$T_2 \sim N(m_2, \sigma^2)$	$T_3 \sim N(m_3, \sigma^2)$

$$S_r^2 = \frac{SS_{RES}}{d.f._{res}} = MS_{RES} \quad (\text{estimation of } \sigma^2)$$

$$\frac{MS_{FACTOR}}{MS_{RESID}} = \text{F-ratio}$$

- IF THERE ARE **NO** DIFFERENCES AMONG SUPPLIERS ($m_1 = m_2 = m_3$)

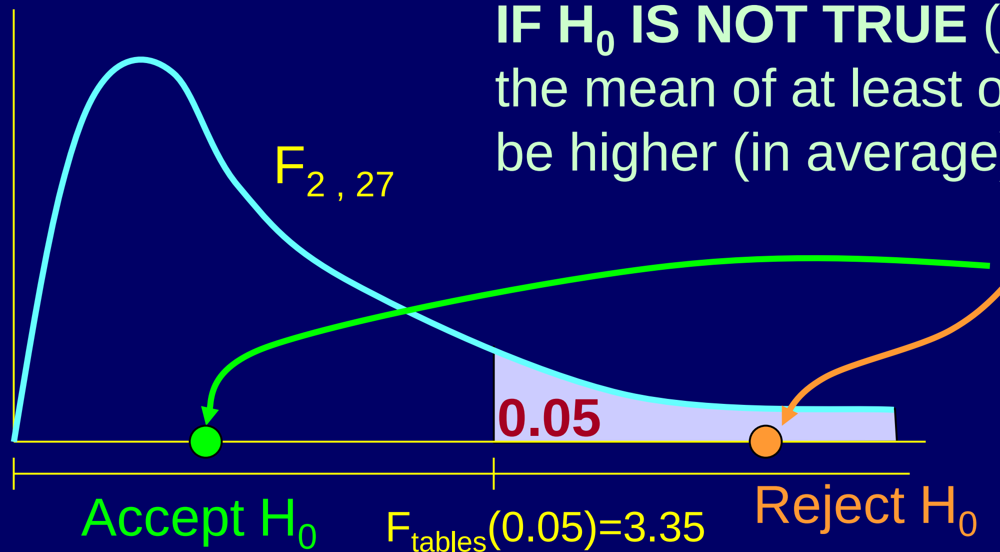
$$\frac{SS_{factor}}{d.f._{factor}} = MS_{FACTOR} = S_f^2 \quad (\text{estimation of } \sigma^2) \longrightarrow \frac{MS_{FACTOR}}{MS_{RESID}} \approx 1$$

- IF THERE ARE DIFFERENCES AMONG SUPPLIERS:

$$\frac{SS_{factor}}{d.f._{factor}} = MS_{FACT} = S_f^2 \text{ will tend to be higher than } \sigma^2 \longrightarrow$$

F-ratio tends to be > 1

IF H_0 IS NOT TRUE (if there are differences in the mean of at least one supplier): F-ratio will be higher (in average) than $F_{2, 27}$



$$\text{F-ratio} = \frac{MS_{factor}}{MS_{residual}}$$

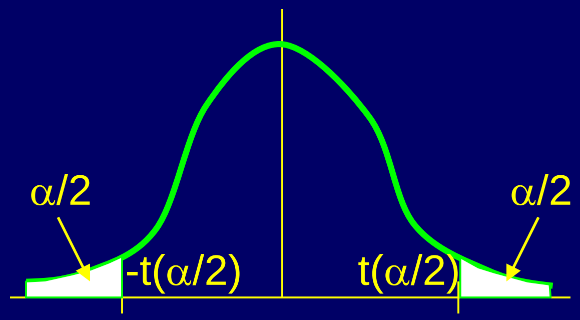
LSD INTERVALS FOR MEAN COMPARISON

IF THE F-TEST HAD RESULTED STATISTICALLY SIGNIFICANT:

Reject H_0 ($m_1 = m_2 = m_3$) → Accept H_1 (at least one m_i is different from the rest)

WHICH ONE IS DIFFERENT ? → OBTAIN LSD INTERVALS ("LEAST SIGNIFICANCE DIFFERENCE") FOR THE SAMPLE AVERAGE OF EACH SUPPLIER

$$\bar{x}_i \pm \frac{\sqrt{2}}{2} \cdot t^{\alpha/2}_{d.f.resid} \sqrt{\frac{MS_{resid}}{K_i}}$$



K: Number of repetitions from supplier i

$t^{\alpha/2}_{dfres}$: critical value from t- table

THE DIFFERENCE BETWEEN TWO MEANS WILL BE SIGNIFICANT IF THEIR LSD INTERVALS **DO NOT OVERLAP...**

... OTHERWISE, THERE IS ENOUGH EVIDENCE TO SAY THAT THE DIFFERENCE IS STATISTICALLY SIGNIFICANT

ATTENTION: LSD INTERVALS **ARE NOT** CONFIDENCE INTERVALS FOR THE MEAN !!

ANOVA with 1 Factor (3 variants)

(example of laptop batteries) T: time of battery operation

3 possible battery suppliers: S_A, S_B and S_C.

Time - batteries from S_A:	14	11	15	12	13	$\bar{x}_A = 13$
Time - batteries from S_B:	16	13	17	15	14	$\bar{x}_B = 15$
Time - batteries from S_C:	18	16	19	20	17	$\bar{x}_C = 18$

Are the differences statistically significant (α=0.05)?

H_0: $m_A = m_B = m_C$

Grand mean: $\bar{\bar{x}} = 15.33$

$$SS_{TOTAL} = \sum_{i=1}^{i=15} (x_i - 15.33)^2 = (14 - 15.33)^2 + \ldots + (17 - 15.33)^2 = 93.33$$

$SS_{RESIDUAL} = SS_{TOTAL} - SS_{FACTOR}$

ANOVA with 1 Factor (3 variants)

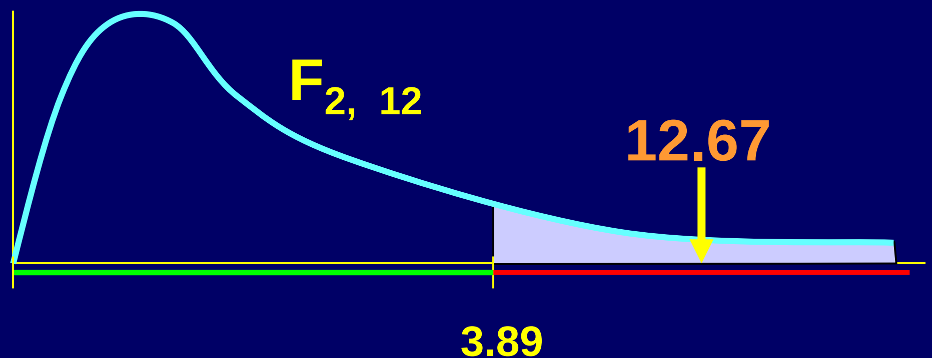
factor	X_{obs}	X_{pred}	$(x_{pred} - \bar{\bar{x}})^2$
A	14 11 15 12 13	13	$5 \cdot (13 - 15.33)^2$
B	16 13 17 15 14	15	$5 \cdot (15 - 15.33)^2$
C	18 16 19 20 17	18	$5 \cdot (18 - 15.33)^2$

$\bar{\bar{x}} = 15.33$

sum:

$63.33 = SS_{FACTOR}$

Source	S.S.	D.F.	M.S.	F_{ratio}
FACTOR	63.33	2	31.67	12.67
RESIDUAL	30	12	2.5	
TOTAL	93.33	14		



* Critical value from table:

$F_{2\ ,12}(0.05) = 3.89 < 12.67$

Reject H_0

ANOVA with 1 Factor (3 variants)

Reject H_0

$H_0: m_A = m_B = m_C$

$H_1: m_A \neq m_B \neq m_C$

$H_1: (m_A = m_B) \neq m_C$

$H_1: (m_A = m_C) \neq m_B$

$H_1: (m_B = m_C) \neq m_A$

At least one mean is significantly different from the rest

Least Significant Differences (LSD) intervals:

$$\bar{x}_i \pm \frac{\sqrt{2}}{2} \cdot t_{d.f.resid}^{\alpha/2} \sqrt{\frac{MS_{resid}}{K}}$$

K: number of data used to calculate $\bar{x}_i$

D.F.res: Residual degrees of freedom

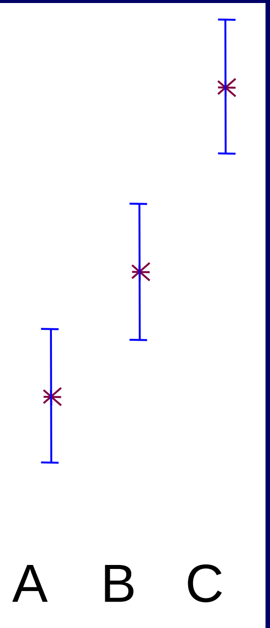
$$t_{12}^{0.025} = 2.179$$

LSD_A: $13 \pm (\sqrt{2}/2) \cdot 2.179 \cdot \sqrt{2.5/5}$

13 ± 1.09 → [11.91, 14.09]

LSD_B: 15 ± 1.09 [13.91, 16.09]

LSD_C: 18 ± 1.09 [16.91, 19.09]



Solution:

$(m_A = m_B) < m_C$

ANALYSIS OF RESIDUALS

This is an important part of ANOVA and regression.

Any statistical analysis with real data has to be always completed with the analysis of residuals.

RESIDUAL of observation ij = $X_{ij} - \overline{X}_i$

Residuals reflect the effect in the response variable of all factors not controlled in the experiment.

In ANOVA, studying the residuals allows us to check if:

- Data are normally distributed (with no outliers)

- The population variance of all suppliers is the same

STUDY OF EFFECTS OVER VARIANCES

Is the variance of data from all suppliers the same?

$T_1 = N(m_1 , \sigma_1^2)$	$T_2 = N(m_2 , \sigma_2^2)$	$T_3 = N(m_3 , \sigma_3^2)$

$H_0: \sigma_1^2 = \sigma_2^2 = \sigma_3^2$

QUESTION:

$$s^2_{supplier} \propto \sum_j \frac{e_{ij}^2}{N_i} = \frac{SSresid_i}{N_i}$$

Is there any relationship between the average of squared residuals from one supplier and the variance obtained for that supplier?

ANOVA is very powerful to study differences in the mean of a variable among different populations

EASY WAY TO STUDY EFFECTS OVER DISPERSION:

1.- **Conduct one ANOVA to study effects over the mean.**

2.- **Calculate the residual of each observation.**

3.- **Save the squared residuals**

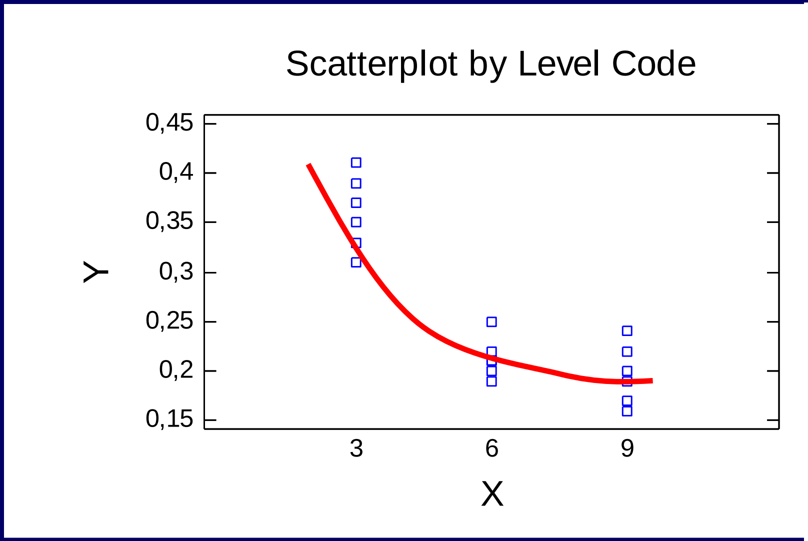
4.- **Conduct one ANOVA considering as response variable: SQUARED RESIDUALS**

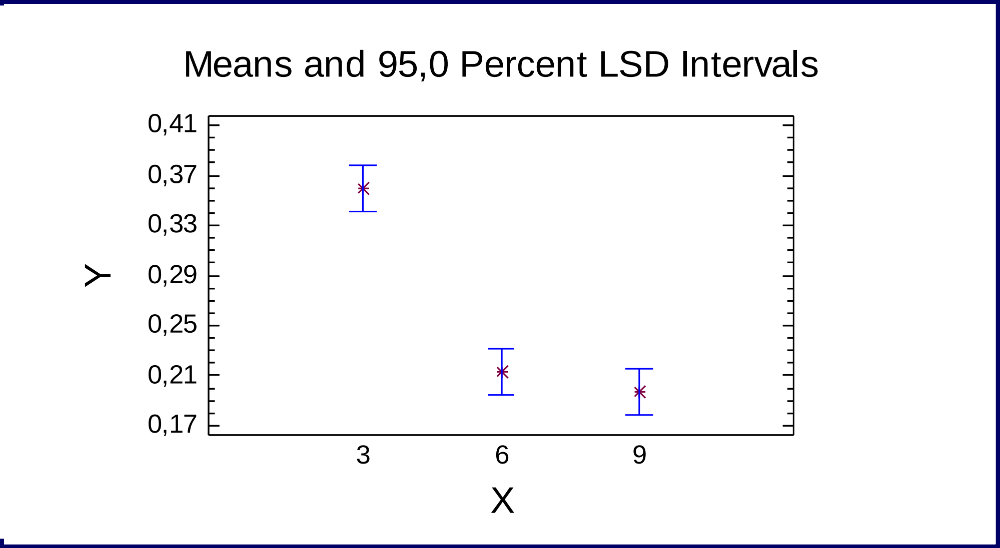
ANOVA WITH A QUANTITATIVE FACTOR

One experiment has been conducted to obtain the optimum pesticide dose (tested at 3 levels) for the control of a certain insect. The response variable measured is related to the pest population. RESULTS:

Dose = 3	Dose = 6	Dose = 9
0.31	0.20	0.20
0.35	0.22	0.19
0.39	0.21	0.22
0.37	0.25	0.16
0.33	0.21	0.17
0.41	0.19	0.24

What dose would you recommend to minimize Y?





What dose would you recommend to minimize Y?

Based on the LSD intervals, dose = 6 OR dose = 9 (the difference between both doses is not statistically significant)

BUT if the factor is quantitative, the interest is to study if there is a "relationship" between X and Y (and not the comparison between tested levels)

ANOVA => H_0: $m_{dose3} = m_{dose6} = m_{dose9}$

REGRESSION => $Y = a + b \cdot X + c \cdot X^2$ H_0: $b = 0$ H_0: $c = 0$

It makes more sense to analyze data with regression !!

ANOVA

with >1 factors

ANOVA WITH 3 FACTORS

One experiment has been carried out to determine the optimum conditions that maximize the quality parameter (Y) of a chemical product. Three experimental factors are considered:

- **Catalyst (two types tested: A or B)**
- **Supplier of the raw material (s1 or s2)**
- **Temperature of the reaction (two levels tested: 70ºC and 80ºC)**

catalyst	supplier	temperature	Y
A	**s1**	**70**	15
B	**s1**	**70**	20
A	**s2**	**70**	16
B	**s2**	**70**	14
A	**s1**	**80**	17
B	**s1**	**80**	23
A	**s2**	**80**	10
B	**s2**	**80**	13

What operative conditions should be adopted to maximize Y?

One engineer thinks that, since the highest value is 23, the optimum conditions would be: Catalyst B, suppler s1, Tª = 80

Is this the "best" operative condition?

NO: the effect of all factors may not be statistically significant !

catalyst	X_{obs}	$(x_{obs} - \bar{\bar{x}})^2$	X_{pred}	$(x_{pred} - \bar{\bar{x}})^2$
A	15	$(15 - 16)^2$	14.5	$(14.5 - 16)^2$
A	16	$(16 - 16)^2$	14.5	$(14.5 - 16)^2$
A	17	$(17 - 16)^2$	14.5	$(14.5 - 16)^2$
A	10	$(10 - 16)^2$	14.5	$(14.5 - 16)^2$
B	20	$(20 - 16)^2$	17.5	$(17.5 - 16)^2$
B	14	$(14 - 16)^2$	17.5	$(17.5 - 16)^2$
B	23	$(23 - 16)^2$	17.5	$(17.5 - 16)^2$
B	13	$(13 - 16)^2$	17.5	$(17.5 - 16)^2$
sum:		$116 = SS_{TOTAL}$		$18 = SS_{CATALYST}$

$$\bar{\bar{x}} = 16$$

$$\bar{x}_A = 14.5$$

$$\bar{x}_B = 17.5$$

X_{obs}	suppl	X_{pred}	$(x_{pred} - \bar{\bar{x}})^2$	Temp.	X_{pred}	$(x_{pred} - \bar{\bar{x}})^2$
15	s1	18.75	$(18.75 - 16)^2$	70	16.25	$(16.25 - 16)^2$
20	s1	18.75	$(18.75 - 16)^2$	70	16.25	$(16.25 - 16)^2$
17	s1	18.75	$(18.75 - 16)^2$	80	15.75	$(15.75 - 16)^2$
23	s1	18.75	$(18.75 - 16)^2$	80	15.75	$(15.75 - 16)^2$
16	s2	13.25	$(13.25 - 16)^2$	70	16.25	$(16.25 - 16)^2$
14	s2	13.25	$(13.25 - 16)^2$	70	16.25	$(16.25 - 16)^2$
10	s2	13.25	$(13.25 - 16)^2$	80	15.75	$(15.75 - 16)^2$
13	s2	13.25	$(13.25 - 16)^2$	80	15.75	$(15.75 - 16)^2$
	$SS_{SUPPL} = 60.5$			$SS_{TEMP} = 0.5$		

FACTOR	S.S.	D.F.	M.S.	F_{ratio}	
catalyst	18	1	18	1.95	<<7.71
supplier	60.5	1	60.5	6.54	<7.71
temperature	0.5	1	0.5	0.05	<<7.71
RESIDUAL	37	**4**	9.25		
TOTAL	116	7			

$F_{1;4}^{0.05} = 7.71$

ANOVA table after discarding non-significant factors:

FACTOR	S.S.	D.F.	M.S.	F_{ratio}	
supplier	60.5	1	60.5	6.54	>5.99
RESIDUAL	55.5	**6**	9.25		
TOTAL	116	7			$F_{1;6}^{0.05} = 5.99$

Factor supplier is statistically significant (α=0.05)

Optimum conditions to maximize Y: use supplier s1 for the raw material; use either Tª 70 or 80; use either catalyst A or B.

Average value of Y using supplier s1: $\bar{x}_{S1} = 18.75$

Next, we should check that:

- Residuals follow a Normal distributions (no outliers)

- The interaction between supplier and Tª or catalyst is not statistically significant

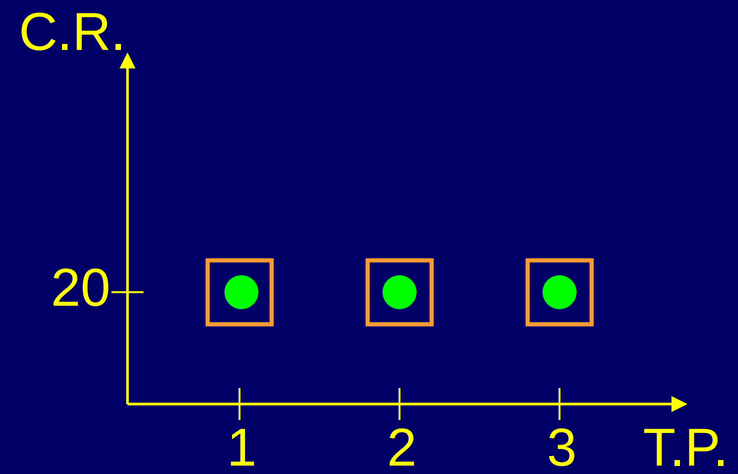
WHAT IS AN INTERACTION ?

INTUITIVE EXAMPLE:

EFFECT OF THE PAINTING LAYER AND METAL TYPE ON THE CORROSION RATE (C.R.) OF 12 PROTOTYPES

CASE A:

		THICKNESS OF PAINTING					
		1		2		3	
METAL TYPE	1	20	20	20	20	20	20
	2	20	20	20	20	20	20



TOTAL SUM OF SQUARES:

$$\sum_{ijk}\left(x_{ijk}-\bar{x}\right)^2=0$$

i:thickness

j: metal type

k: repetition

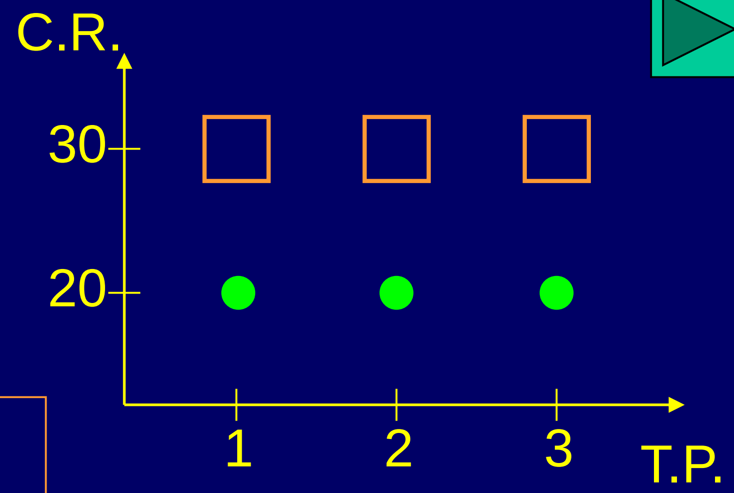
IF THERE IS NO VARIANCE,

NOTHING HAS INFLUENCE !

CASE B:

THICKNESS OF PAINTING

METAL TYPE	1		2		3	
1	20	20	20	20	20	20
2	30	30	30	30	30	30



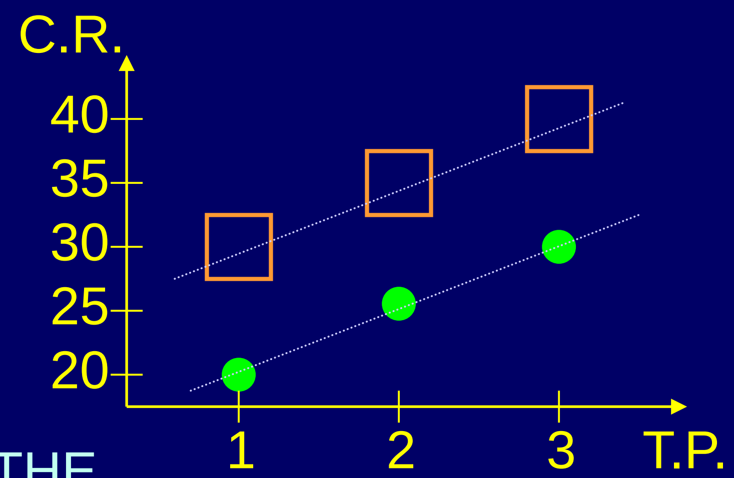
$$SS_{TOTAL} = SS_{METAL}$$

The factor metal type has an effect on the mean.

CASE C:

THICKNESS OF PAINTING

METAL TYPE	1		2		3	
1	20	20	25	25	30	30
2	30	30	35	35	40	40



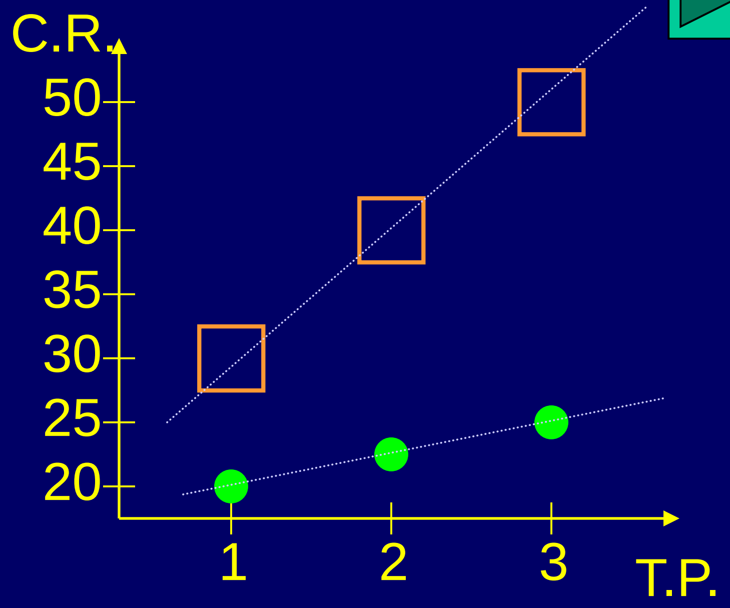
THERE IS VARIABILITY ($SS_{TOTAL} \neq 0$) DUE TO THE EFFECT OF THE METAL TYPE AND THE THICKNESS

$$SS_{TOTAL} = SS_{METAL} + SS_{THICKNESS}$$

CASE D:

THICKNESS OF PAINTING

		1		2		3	
METAL TYPE	1	20	20	25	25	30	30
	2	30	30	40	40	50	50



THERE IS VARIABILITY DUE TO BOTH FACTORS

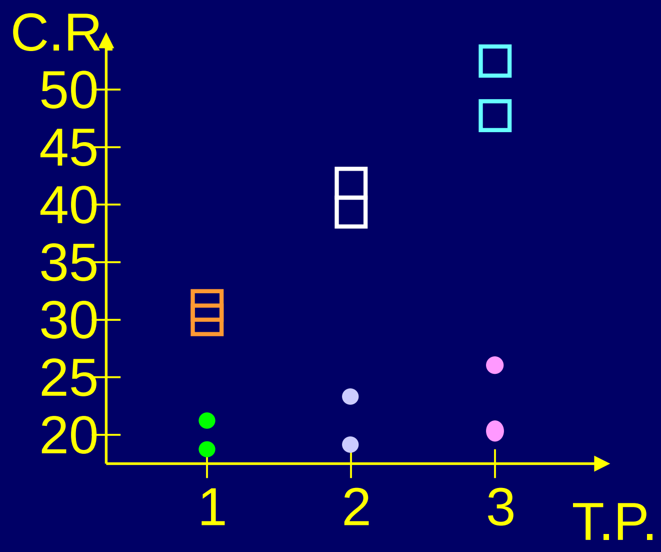
AND THEIR **INTERACTION**

$$SS_{TOTAL} = SS_{METAL} + SS_{THICKNESS} + SS_{INTERACTION}$$

CASE E:

THICKNESS OF PAINTING

		1		2		3	
METAL TYPE	1	19	21	27	24	28	32
	2	30	31	42	39	47	51



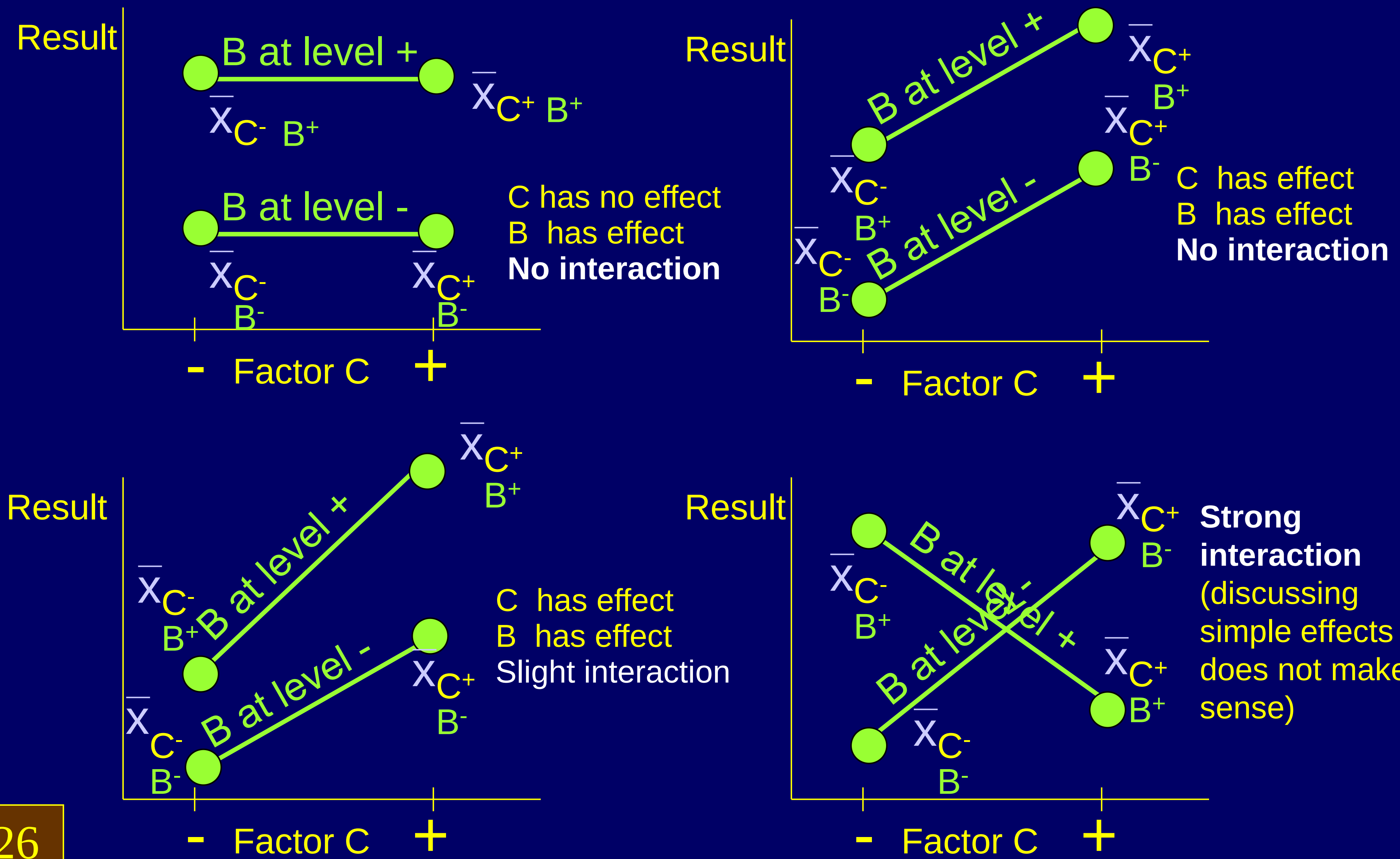
(THE ONLY ONE REALISTIC)

THE EFFECTS OF FACTORS ARE PARTIALLY MASKED (HIDDEN) BY THE RESIDUAL VARIABILITY DUE TO UNCONTROLLED FACTORS

THE CORROSION OF TESTED PROTOTYPES WITH THE SAME METAL AND PAINTING THICKNESS IS NOT EXACTLY THE SAME

$$SS_{TOTAL} = SS_{METAL} + SS_{THICKNESS} + SS_{INTERACTION} + SS_{RESIDUAL}$$

DEFINITION: There is interaction between 2 factors if the effect of one of them is different according to the level of the other factor.



EXERCISE: ANOVA of 2 factors with interaction

One pharmaceutical company wants to improve the yield of a fermentation process (variable Y). For that purpose, an experiment is carried out with 2 factors at 2 levels:

- **Concentration of nitrogen (two levels tested: 40 and 50)**
- **Type of raw material (two types tested: A or B)**

RESULTS

concentr.	raw material	Y	
40	**A**	46	**42**
40	**A**	38	
40	**B**	42	**38**
40	**B**	34	
50	**A**	32	**30**
50	**A**	28	
50	**B**	51	**50**
50	**B**	49	

What concentration and type of raw material should the company choose to maximize the yield?

Highest value -> Solution: conc = 50 raw mat = B

One engineer thinks that, since the highest average value is 50, the optimum conditions would be: conc = 50 and raw material = B

Is this the “best” operative condition?

ONLY IF the effect of both factors or their interaction is statistically significant !

concentr	X_{obs}	$(x_{obs} - \bar{\bar{x}})^2$	X_{pred}	$(x_{pred} - \bar{\bar{x}})^2$
40	46	$(46 - 40)^2$	40	$(40 - 40)^2$
40	38	$(38 - 40)^2$	40	$(40 - 40)^2$
40	42	$(42 - 40)^2$	40	$(40 - 40)^2$
40	34	$(34 - 40)^2$	40	$(40 - 40)^2$
50	32	$(32 - 40)^2$	40	$(40 - 40)^2$
50	28	$(28 - 40)^2$	40	$(40 - 40)^2$
50	51	$(51 - 40)^2$	40	$(40 - 40)^2$
50	49	$(49 - 40)^2$	40	$(40 - 40)^2$
sum:		$490 = SS_{TOTAL}$		$0 = SS_{CONCENTR}$

$$\bar{\bar{x}} = 40$$

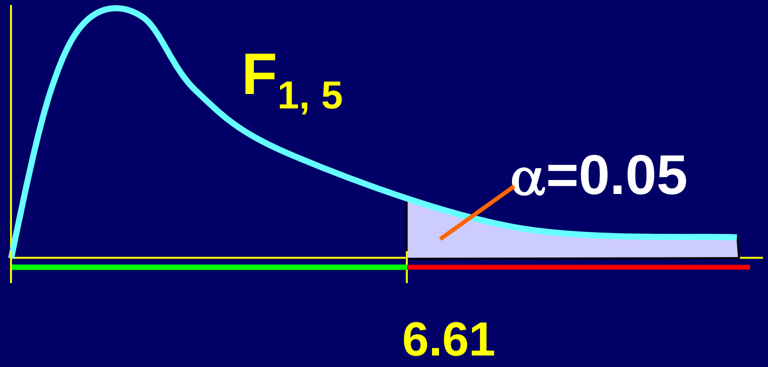
$$\bar{x}_{40} = 40$$

$$\bar{x}_{50} = 40$$

raw_m	X_{obs}	X_{pred}	$(x_{pred} - \bar{\bar{x}})^2$
A	46	36	$(36 - 40)^2$
A	38	36	$(36 - 40)^2$
A	32	36	$(36 - 40)^2$
A	28	36	$(36 - 40)^2$
B	42	44	$(44 - 40)^2$
B	34	44	$(44 - 40)^2$
B	51	44	$(44 - 40)^2$
B	49	44	$(44 - 40)^2$

$SS_{RAW\_M} = 128$

$\bar{x}_A = 36$ $\bar{x}_B = 44$



FACTOR	S.S.	D.F.	M.S.	F_{ratio}
concentration	0	1	0	0
raw material	128	1	128	1.77
RESIDUAL	362	**5**	72.4	
TOTAL	490	7		

<<6.61

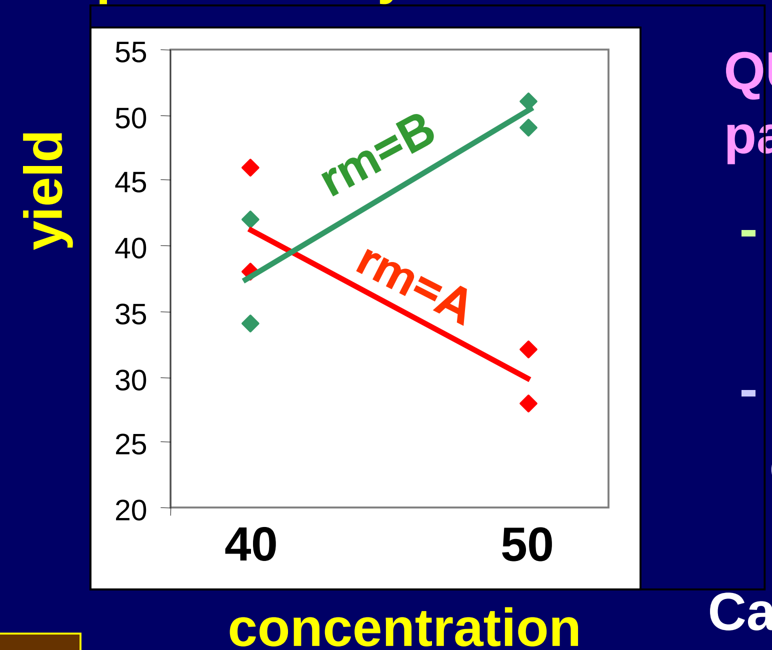
Next step: discard concentration and repeat the ANOVA, but raw material is not statistically significant.

QUESTION: what are the optimum operative conditions in this case?

The analysis is not finished until we check:

- If residuals follow a Normal distributions (no outliers)
- If the interaction between both factors is statistically significant

Graphical study of the interaction:



QUESTION: Do you think that the observed pattern was obtained by random?

- YES (interaction not significant):
  optimum conditions = either of them
- NO (interaction significant):
  optimum conditions = 50 ; B

Calculate the sum of squares of the interaction and include it in the ANOVA table

Conc	Raw_m	X_{obs}	X_{pred}	$(x_{pred} - \bar{\bar{x}})^2$
40	A	46	42	$(42 - 40)^2$
40	A	38	42	$(42 - 40)^2$
40	B	42	38	$(38 - 40)^2$
40	B	34	38	$(38 - 40)^2$
50	A	32	30	$(30 - 40)^2$
50	A	28	30	$(30 - 40)^2$
50	B	51	50	$(50 - 40)^2$
50	B	49	50	$(50 - 40)^2$

$\Sigma = 416 =$

$= SS_C + SS_{RM} + SS_{C \cdot RM}$

$SS_{CONC \cdot RAWM} = 416 - 128 - 0 = 288$

FACTOR	S.S.	D.F.	M.S.	F_{ratio}	
concentr.	0	1	0	0	<<7.71
raw material	128	1	128	6.92	<7.71
conc x raw m	288	1·1	288	15.6	>7.71
RESIDUAL	74	4	18.5		
TOTAL	490	7			

$F_{1;4}^{0.05} = 7.71$

The interaction between concentration and raw material is statistically significant (at α=0.05) although the simple effect of both factors is not.

In order to maximize the yield, the company should use:

concentration of nitrogen = 50; raw material of type B

Average yield expected at those conditions = (51+49)/2 = 50

RULE: if a double interaction is significant, both factors should always be included in the ANOVA table.

RULE: degrees of freedom of CONCxRAW_M = $(d.f._{CONC})\cdot(d.f._{RAW\_M})$

With >2 factors, triple interactions should also be studied, though in most cases they are not significant.

DESIGN OF EXPERIMENTS

EXPERIMENT: SET OF **TRIALS** CARRIED OUT TO OBTAIN INFORMATION IN ORDER TO IMPROVE A PRODUCT OR PROCESS.

Common approach used optimize industrial processes:

A	B	C	Response
-	-	-	.
-	-	-	.
-	-	-	.
-	-	-	.
+	-	-	.
+	-	-	.
+	-	-	.
+	-	-	.

A^+ better than A^-

A	B	C	Response
+	-	-	.
+	-	-	.
+	-	-	.
+	-	-	.
+	+	-	.
+	+	-	.
+	+	-	.
+	+	-	.

B^+ better than B^-

A	B	C	Response
+	+	-	.
+	+	-	.
+	+	-	.
+	+	-	.
+	+	+	.
+	+	+	.
+	+	+	.
+	+	+	.

C^+ better than C^-

Total number of experimental trials = 24

Optimum Operative Condition (OOC) : $A^+ B^+ C^+$?

Have we tested all possible combinations?

THIS APPROACH (modify one factor each time) IS NOT EFFICIENT:

- **Very expensive (requires many trials).**
- **It does not guarantee obtaining the Optimum Operative Cond.**
- **It is not possible to study the effect of interactions.**

ALTERNATIVE approach, much more effective:

¡ USE A FACTORIAL **EXPERIMENTAL DESIGN** TO STUDY THE SIMULTANEOUS EFFECT OF ALL FACTORS!

A	B	C
-	-	-
+	-	-
-	+	-
+	+	-
-	-	+
+	-	+
-	+	+
+	+	+

- ALL POSSIBLE OPERATIVE CONDITIONS HAVE BEEN TESTED

- ONLY 8 TRIALS ARE NECESSARY (versus 24 trials in the traditional approach)

- ALL EFFECTS ARE ORTHOGONAL AND IT IS POSSIBLE TO STUDY THE EFFECT OF INTERACTIONS

CONTROLED FACTORS: Parameters of the process under study that are tested at two or more levels or variants, in order to investigate the effect over the response variable.

DESIGN OF EXPERIMENTS (DOE)

Quantitative factors => variants ; Qualitative factors => levels

Experimental design with 3 factors: F1 with 2 variants (A, B), F2 with 2 levels (2, 3), F3 with 2 variants (X, Y)

Response variable (measured experimentally):

F1	F2	F3	RV
A	2	X	3.5
B	2	X	4.9
A	3	X	3.2
B	3	X	6.2
A	2	Y	5.3
B	2	Y	4.7
A	3	Y	2.9
B	3	Y	4.8

- **Treatments: different combinations of variants/levels: 2 · 2 · 2 = 8**

- **Repetitions / replicates: number of times that each treatment is tested**

- **Trials: number of experiments carried out**

Trials = treatments x repetitions

Factorial design <u>not replicated</u> (8 treatments, 8 trials)

BALANCED FACTORIAL DESIGN: all treatments are tested the same number $\mathbf{N_R}$ of times. IF $N_R=1$: non-replicated factorial design.

PROPERTY: effect of ALL factors and interactions are orthogonal among them

STEPS TO DESIGN AN EXPERIMENT

0.- TO DEFINE THE PROBLEM AND ESTABLISH THE OBJECTIVE
1.- TO IDENTIFY THE RESPONSE VARIABLE
2.- TO SELECT THE FACTORS AND DECIDE THE LEVELS / VARIANTS
4.- TO DEFINE WHAT WILL CONSTITUTE EACH INDIVIDUAL TRIAL
5.- TO DECIDE THE NUMBER OF TRIALS TO CARRY OUT
5'.- TO DECIDE THE TREATMENT TO USE IN EACH TRIAL
6.- TO ORGANIZE ALL THE WORK; TO CARRY OUT THE EXPERIMENT
7.- TO ANALYZE STATISTICALLY THE RESULTS

IMPORTANT: TRIALS SHOULD ALWAYS BE CARRIED OUT IN A RANDOM ORDER

(to avoid confusion of effects with uncontrolled factors)

ANALYSIS OF RESULTS IN A DOE:

1) Identify with ANOVA which effects are statistic. significant

2) Interpretation of the nature of significant effects:

- if factors are QUALITATIVE : use of LSD INTERVALS

- if factors are QUANTITATIVE and tested at >2 levels: the best method is multiple linear regression

3) Analysis of residuals:

- DETECTION OF OUTLIERS

- EFFECTS OF FACTORS OVER THE VARIANCE OF THE RESPONSE VARIABLE

FACTORS AT 3 LEVELS:

Experiments require a higher number of trials BUT provide more information about linear / quadratic effects that allows a better estimation of the optimum operative conditions.

The data analysis with ANOVA implies 3 assumptions:

1) The populations corresponding to all tested treatments have the SAME variance.

(ANOVA is quite robust though variances are not all equal)

2) NORMALITY:

The response variable has a Normal distribution in all treatments

- If the distribution is highly skewed => use transformations (e.g. work with log(X) or $X^{0.5}$ instead of X)

3) INDEPENDENCE:

The most important !!

Observations from each treatment correspond to individuals extracted randomly from the population considered.

Data resulting from the different treatments are independent among them.

To accomplish this hypothesis it is necessary to randomize the order of all trials in the experiment.

ORTHOGONALITY

F1	F2	F3	RV
A	2	X	3.5
B	3	X	4.9
A	2	X	3.2
B	3	X	6.2
A	2	Y	5.3
B	3	Y	4.7
A	2	Y	2.9
B	3	Y	4.8

3 factors, 8 treatments, 8 trials...

but is there anything "wrong"?

The effect of factor F1 is totally <u>confounded</u> with the effect of factor F2 --> BAD DESIGN!

If this effect is statistically significant, it is NOT possible to know if it was caused by F1, F2 or both.

F1	F2	F3	RV
A	2	X	3.5
B	3	X	4.9
A	2	X	3.2
B	2	X	6.2
A	3	Y	5.3
B	3	Y	4.7
A	2	Y	2.9
B	3	Y	4.8

Is there anything "wrong"?

- **Variant A of F1 was tested 3 times at F2=2 and 1 time at F2=3**
- **Variant B of F1 was tested 1 time at F2=2 and 3 times at F2=3**

F1=A ⟷ F2=2 F1=B ⟷ F2=3

The effect of factor F1 is partly confounded with the effect of factor F2

QUESTION: is this a good or bad DOE ?

F1	F2	RV
2	A	3.5
2	B	4.9
2	A	3.2
2	B	6.2
2	A	5.3
2	B	4.7
3	A	2.9
3	B	4.8
3	A	5.4
3	B	2.7

Is there anything "wrong"?

NO (the design is correct), but F1 was tested 6 times at level 2 and 4 times at level 3.

UNBALANCED DESIGN

If each treatment is tested the same number of times => balanced factorial design

A balanced DOE is better, unless $\sigma^2_{F1=2} > \sigma^2_{F1=3}$

F1=2
- 3 times at F2=A (50%=A)
- 3 times at F2=B (50%=B)

F1=3
- 2 times at F2=A (50%=A)
- 2 times at F2=B (50%=B)

Same proportion:

"F1 and F2 are orthogonal"

(F1 and F2 are not confounded)

Given 2 factors (F_I with I variants and F_J with J variants): the simple effect of both factors will be orthogonal if in each variant of I, the proportions of J variants are the same.

Consequently: it is possible to separate the effect of each factor on the variable under study

QUESTION: is this a good or bad DOE ?

DOE with 3 factors: A (2 levels), B (3 levels), C (2 levels):

A	B	C
1	1	1
1	2	2
1	3	2
2	1	1
2	2	2
2	3	2

Are A and B orthogonal?

Are A and C orthogonal?

Are B and C orthogonal?

QUESTION:

Is the simple effect of F3 orthogonal to the interaction F1 x F2?

F1	F2	F3	RV
A	2	X	3.5
B	2	X	4.9
A	3	X	3.2
B	3	X	6.2
A	2	Y	5.3
B	2	Y	4.7
A	3	Y	2.9
B	3	Y	4.8

F3=X
- 1 time at F1=A; F2=2 (25%=A·2)
- 1 time at F1=B; F2=2 (25%=B·2)
- 1 time at F2=A; F2=3 (25%=A·3)
- 1 time at F2=B; F2=3 (25%=B·3)

F3=Y
- 1 time at F1=A; F2=2 (25%=A·2)
- 1 time at F1=B; F2=2 (25%=B·2)
- 1 time at F2=A; F2=3 (25%=A·3)
- 1 time at F2=B; F2=3 (25%=B·3)

Same proportion: "F3 is orthogonal to the interaction F1 x F2"

(F3 and the interaction F1 x F2 are not confounded)

Exercise: in a factorial plan 2^4, check that AxB is orthogonal to CxD. Check also that AxBxC is orthogonal to D.

QUESTION:

DOE 1		
F1	F2	F3
1	1	1
2	1	1
1	2	1
2	2	1
1	1	2
2	1	2
1	2	2
2	2	2

In DOE1, check that:
F1 is orthogonal to F2
F1 is orthogonal to F3
F2 is orthogonal to F3
F1 is orthogonal to F2xF3
F2 is orthogonal to F1xF3
F3 is orthogonal to F1xF2

DOE 2			
F1	F2	F3	F4
1	1	1	1
1	2	2	2
1	3	3	3
2	1	2	3
2	2	3	1
2	3	2	2
3	1	3	2
3	2	1	3
3	3	2	1

In DOE2, check that F1 vs F2, F1 vs F3, F1 vs F4, F2 vs F3, F2 vs F4, F3 vs F4 are orthogonal.
Are the simple effects orthogonal to the double interactions?
How many trials would have the “complete” DOE?

What happens if 2 effects are confounded? (for example the simple effect of A and the interaction B·C)

- It is not possible to separate the effect of A vs BC

- We may assume that the effect of A is more important than BC, but this may not be true in practice.

Question: is this DOE good or bad?

F_1	F_2	F_3	RV
A	2	X	3.5
B	3	X	4.9
B	2	Y	3.2
A	3	Y	6.2

Check the orthogonality between F1 vs F2; F1 vs F3 ; F2 vs F3

The effect of F3 is confounded with effect of F1xF2, but this design is the best possible with just 4 trials

Factorial designs 2^k

all factors are tested at 2 levels/variants

- **Experiments are easier as they have a lower number of trials.**
- **The effects of factors and interactions are easy to interpret.**
- **Possible quadratic effects cannot be detected.**

Design 2^K: it is possible to calculate from the data 2^K-1 effects

Relevants in practice

K SIMPLE EFFECTS (each one with 1 degr. freedom)

$\binom{K}{2}$ DOUBLE INTERACTIONS (each one with 1x1 = 1 d.f.)

$\binom{K}{3}$ TRIPLE INTERACTIONS (each one with 1x1x1 = 1 d.f.)

....

$\binom{K}{K}=1$ INTERACTIONS OF ORDER K (with 1 d.f.)

EXAMPLE: **In a 2^4 plan it is possible to calculate 4 simple effects of factors, 6 double interactions, 4 triple int. and 1 quadruple int. = 15 effects**

It is recommended that d.f. residual ≥ 10 (at least d.f. res. ≥ 4)

FRACTIONAL FACTORIAL DESIGN 2^{k-1}

K factors are tested at 2 levels with only HALF of the trials (i.e., 2^{K-1} trials) that would be necessary for the complete design.

In order to build a 2^{K-1} design:

1) Start with a complete 2^K design
2) Multiply the sign of all factors (interaction of highest order)
3) Select those trials with the " + " sign (or -)

In a 2^k design:

- It is not possible to study the effect of the highest-order interaction, but this effect is likely to be the least important.

- The simple effect of a factor is confounded with the (k-1) order interaction of the remaining factors.

- The double interaction of 2 factors is confounded with the (k-2) order interaction of the remaining factors.

- Two effects (simple or interactions) will be completely confounded if their signs are coincident in all trials (for interactions, multiply sings of the factors).

DOE with 4 factors at 2 levels. Which treatments should we select from the complete design to carry out only 8 trials?

	A	B	C	D	ABCD
1	-	-	-	-	+
2					
3					
4	+	+	-	-	+
5					
6	+	-	+	-	+
7	-	+	+	-	+
8					
9					
10	+	-	-	+	+
11	-	+	-	+	+
12					
13	-	-	+	+	+
14					
15					
16	+	+	+	+	+

This is the best possible DOE with 8 trials because:

a) Each factor is tested 4 times at level (-) and 4 times at level (+)

b) The effect of each factor is orthogonal to the remaining factors and to the double interactions!

EXERCISE: check that the simple effect of A is orthogonal to the interaction B·C

Check that the simple effect of A is not orthogonal to the interaction B·C·D

Trials selected so that ABCD = (+)

Example: in a DOE 2^6 (6 factors, 64 trials), it is possible to estimate 63 effects: 6 simple effects, 15 double interactions, 20 triple int., 15 quadruple int., 6 5th-order int., 1 6th-order int.

BUT most of them (interactions of order >2) will be irrelevant !

It is of interest to reduce the number of trials "sacrificing" certain precision and the possibility to study high-order interactions.

A GOOD FRACTIONAL FACTORIAL DESIGN:

A) Should NEVER confound simple effects between them

B) Should TRY (if possible) to avoid confusion between simple effects and double interactions.

(because they exist sometimes, and this confusion would result in a wrong interpretation of results)

C) If possible, should NOT confound double interactions between them (in order to study them).

ORTHOGONAL ARRAYS L_8 , L_{16} , L_{18} , L_{26}

Orthogonal arrays are tables proposed to simplify the design of fractional factorial plans

Developed in Japan by prof. G. Taguchi

Orthogonal array L8:

allows the study of up to 7 factors with 8 trials:

L_8 (2^{7-4})

	1	2	3	4	5	6	7
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	2	2
4	1	2	2	2	2	1	1
5	2	1	2	1	2	1	2
6	2	1	2	2	1	2	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

L_{16}

(2^{15-11})

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2
3	1	1	1	2	2	2	2	1	1	1	1	2	2	2	2
4	1	1	1	2	2	2	2	2	2	2	2	1	1	1	1
5	1	2	2	1	1	2	2	1	1	2	2	1	1	2	2
6	1	2	2	1	1	2	2	2	2	1	1	2	2	1	1
7	1	2	2	2	2	1	1	1	1	2	2	2	2	1	1
8	1	2	2	2	2	1	1	2	2	1	1	1	1	2	2
9	2	1	2	1	2	1	2	1	2	1	2	1	2	1	2
10	2	1	2	1	2	1	2	2	1	2	1	2	1	2	1
11	2	1	2	2	1	2	1	1	2	1	2	2	1	2	1
12	2	1	2	2	1	2	1	2	1	2	1	1	2	1	2
13	2	2	1	1	2	2	1	1	2	2	1	1	2	2	1
14	2	2	1	1	2	2	1	2	1	1	2	2	1	1	2
15	2	2	1	2	1	1	2	1	2	2	1	2	1	1	2
16	2	2	1	2	1	1	2	2	1	1	2	1	2	2	1

ORTOGONAL ARRAY L_{18}

	1	2	3	4	5	6	7	8
1	1	1	1	1	1	1	1	1
2	1	1	2	2	2	2	2	2
3	1	1	3	3	3	3	3	3
4	1	2	1	1	2	2	3	3
5	1	2	2	2	3	3	1	1
6	1	2	3	3	1	1	2	2
7	1	3	1	2	1	3	2	3
8	1	3	2	3	2	1	3	1
9	1	3	3	1	3	2	1	2
10	2	1	1	3	3	2	2	1
11	2	1	2	1	1	3	3	2
12	2	1	3	2	2	1	1	3
13	2	2	1	2	3	1	3	2
14	2	2	2	3	1	2	1	3
15	2	2	3	1	2	3	2	1
16	2	3	1	3	2	3	1	2
17	2	3	2	1	3	1	2	3
18	2	3	3	2	1	2	3	1

L_{18} $(2^1 * 3^7)$

18 trials instead of 4,374

Simple effects account for

1+7x2 = 15 d.f., remaining 2 d.f. that are associated to the interaction F1xF2

EXERCISE: check that the interaction F1xF2 is orthogonal to all simple effects.

EXERCISE: check that the interaction F1xF3 is NOT orthogonal to the simple effect of F4

ORTOGONAL ARRAY L_{27}

	1	2	3	4	5	6	7	8	9	10	11	12	13
1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	1	1	1	1	2	2	2	2	2	2	2	2	2
3	1	1	1	1	3	3	3	3	3	3	3	3	3
4	1	2	2	2	1	1	1	2	2	2	3	3	3
5	1	2	2	2	2	2	2	3	3	3	1	1	1
6	1	2	2	2	3	3	3	1	1	1	2	2	2
7	1	3	3	3	1	1	1	3	3	3	2	2	2
8	1	3	3	3	2	2	2	1	1	1	3	3	3
9	1	3	3	3	3	3	3	2	2	2	1	1	1
10	2	1	2	3	1	2	3	1	2	3	1	2	3
11	2	1	2	3	2	3	1	2	3	1	2	3	1
12	2	1	2	3	3	1	2	3	1	2	3	1	2
13	2	2	3	1	1	2	3	2	3	1	3	1	2
14	2	2	3	1	2	3	1	3	1	2	1	2	3
15	2	2	3	1	3	1	2	1	2	3	2	3	1
16	2	3	1	2	1	2	3	3	1	2	2	3	1
17	2	3	1	2	2	3	1	1	2	3	3	1	2
18	2	3	1	2	3	1	2	2	3	1	1	2	3
19	3	1	3	2	1	3	2	1	3	2	1	3	2
20	3	1	3	2	2	1	3	2	1	3	2	1	3
21	3	1	3	2	3	2	1	3	2	1	3	2	1
22	3	2	1	3	1	3	2	2	1	3	3	2	1
23	3	2	1	3	2	1	3	3	2	1	1	3	2
24	3	2	1	3	3	2	1	1	3	2	2	1	3
25	3	3	2	1	1	3	2	3	2	1	2	1	3
26	3	3	2	1	2	1	3	1	3	2	3	2	1
27	3	3	2	1	3	2	1	2	1	3	1	3	2

27 trials

instead of 1,584,323

Design completely saturated: simple effects account for 13·2=26 degrees of freedom, which are the total d.f. available (27-1)

EXERCISES

Data in PoliformaT:

recursos \ Transparencias \ English group \ UD 5 DOE-data.xls

EXERCISE-1

In order to study the yield of orange trees, 3 cultivars were tested (A, B, C) as well as different heights of pruning. Results:

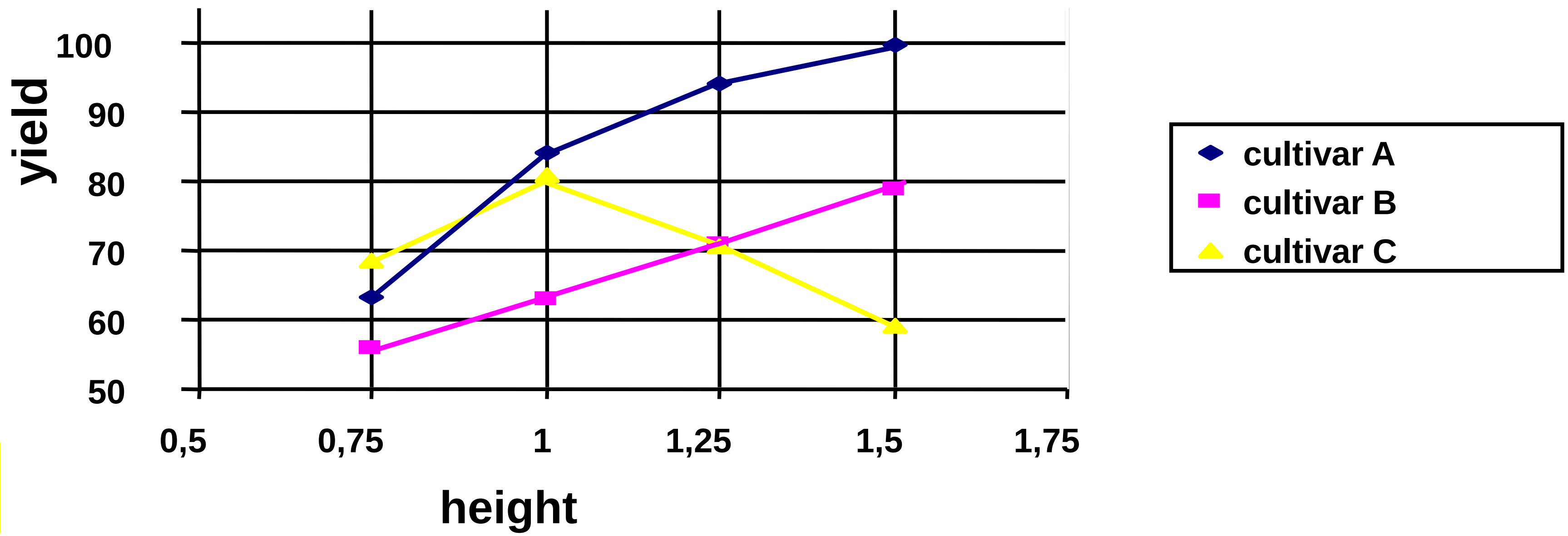
	A	B	C	$\bar{X}_j$
Height 0.75	68 60 $\bar{X}_{11} = 63.33$ 62	52 55 $\bar{X}_{21} = 56$ 61	66 72 $\bar{X}_{31} = 68.67$ 68	$\bar{X}_1 = 62.67$
Height 1	91 75 $\bar{X}_{12} = 84$ 86	62 67 $\bar{X}_{22} = 63$ 60	83 82 $\bar{X}_{32} = 81$ 78	$\bar{X}_2 = 76$
Height 1.25	90 98 $\bar{X}_{13} = 94$ 94	64 75 $\bar{X}_{23} = 71$ 74	72 66 $\bar{X}_{33} = 70.67$ 74	$\bar{X}_3 = 78.56$
Height 1.50	105 95 $\bar{X}_{14} = 99.67$ 99	68 85 $\bar{X}_{24} = 78.67$ 83	61 58 $\bar{X}_{34} = 59$ 58	$\bar{X}_4 = 79.11$

Multifactor ANOVA - yield

Summary table of ANOVA:

Analysis of Variance for yield - Type III Sums of Squares

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
MAIN EFFECTS					
A:cultivar	2287,17	2	1143,58	42,93	0,0000
B:height	1613,64	3	537,88	20,19	0,0000
INTERACTIONS					
AB	2284,61	6	380,769	14,29	0,0000
RESIDUAL	639,333	24	26,6389		
TOTAL (CORRECTED)	6824,75	35			



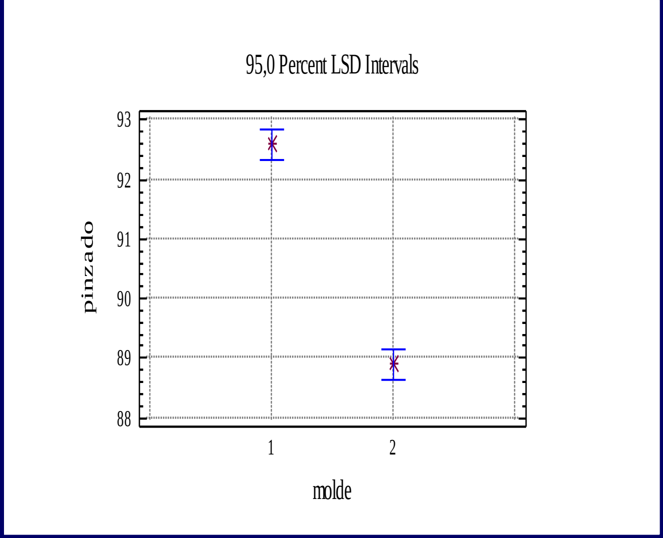
EXERCISE-2:

REPLICATED DESIGN

DESIGN: balanced factorial plan 3x2 with 10 replicates

Experiment to investigate the effect of catalyst and cast type in a quality parameter of PET bottles.

Target: minimize the response variable.

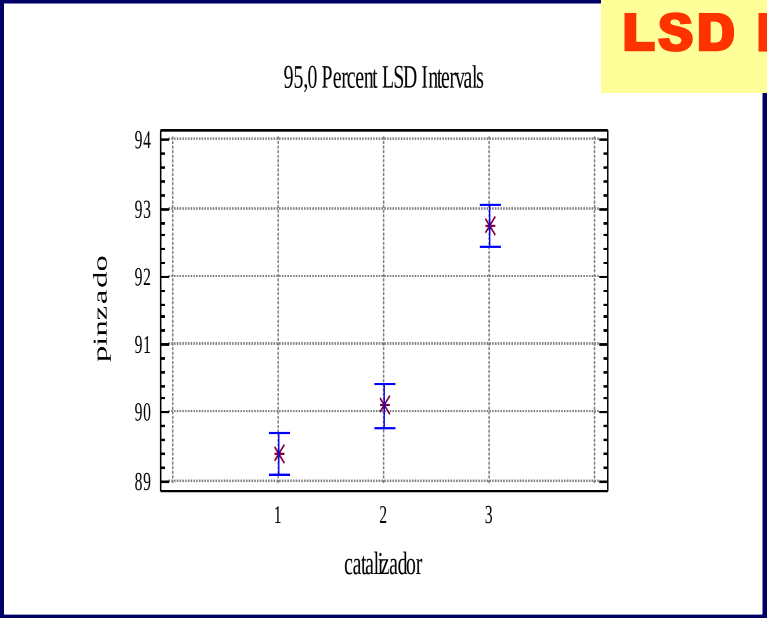


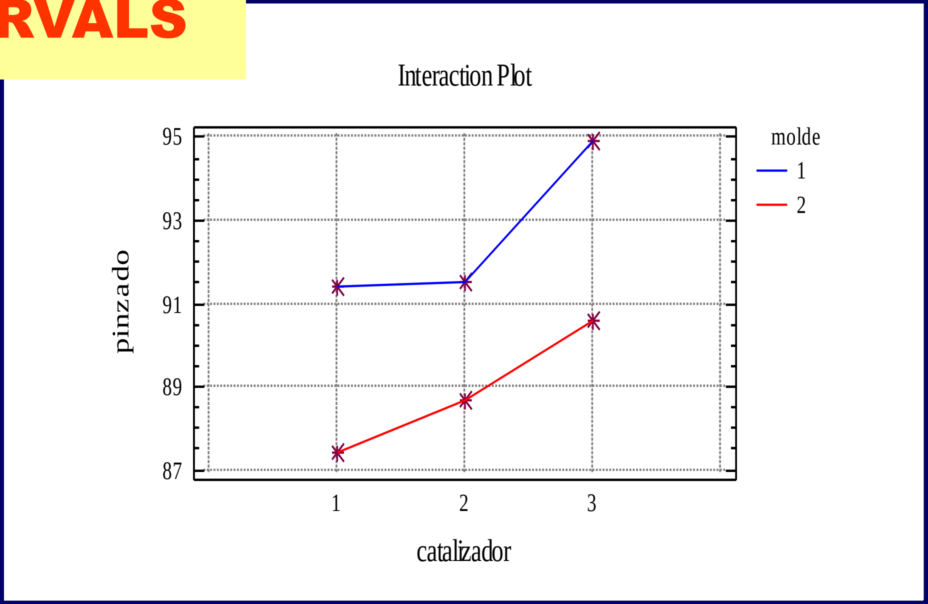
Cast:	Catalyst: A	B	C
1	93	92	95
	93	94	94
	90	90	94
	91	91	94
	92	90	94
	91	91	97
	90	92	95
	91	92	96
	93	92	94
	90	91	96
2	88	90	91
	88	88	90
	87	88	92
	87	88	90
	88	89	91
	87	90	89
	87	89	90
	87	88	91
	87	88	91
	88	89	91

Analysis of Variance for pinzado - Type III Sums of Squares

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
MAIN EFFECTS					
A:catalyst	124,9	2	62,45	63,99	0,0000
B:cast (molde)	205,35	1	205,35	210,42	0,0000
INTERACTIONS					
AB	6,3	2	3,15	3,23	0,0474
RESIDUAL	52,7	54	0,975926		
TOTAL (CORRECTED)	389,25	59			

LSD INTERVALS



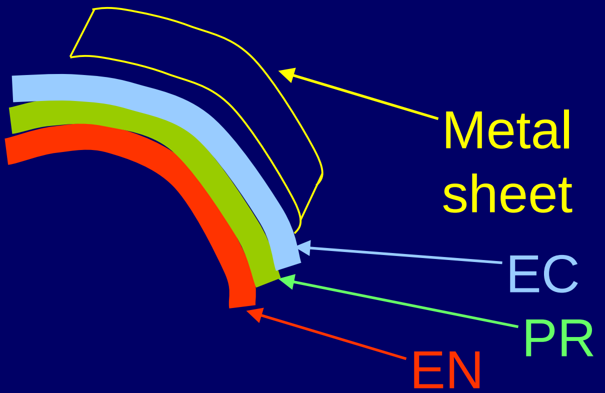


Optimum Operative Condition (to minimize): Catalyst (1), cast (2)

EXERCISE-3: DESIGN 2^3 NON-REPLICATED

RESPONSE VARIABLE: a measurement of the degree of corrosion of vehicle metal sheet (this variable should be kept as low as possible).

FACTORS:
- Electrocoat
- Primer
- Enamel



LEVELS for each factor: 2 different thickness (2 microns vs 5 microns)

EC	PR	EN	corrosion
-	-	-	14
+	-	-	10
-	+	-	8
+	+	-	6
-	-	+	12
+	-	+	4
-	+	+	6
+	+	+	2

NUMBER OF TRIALS = 8 :

2^3 non-replicated

$$SC_{TOTAL} = \sum SC_{EFFECTS} + SC_{RESIDUAL}$$

ANALYSIS OF VARIANCE

What effects are statistically significant?

EFFECT	S.S.	D.f.	M.S.	F-ratio	F-table	P-value
TOTAL	115.5	7	-	-		
EC	40.5	1	40.5	16.2	7.71	0.0158
PR	40.5	1	40.5	16.2	7.71	0.0158
EN	24.5	1	24.5	9.8	7.71	0.0352
RESIDUAL	10	4	2.5			

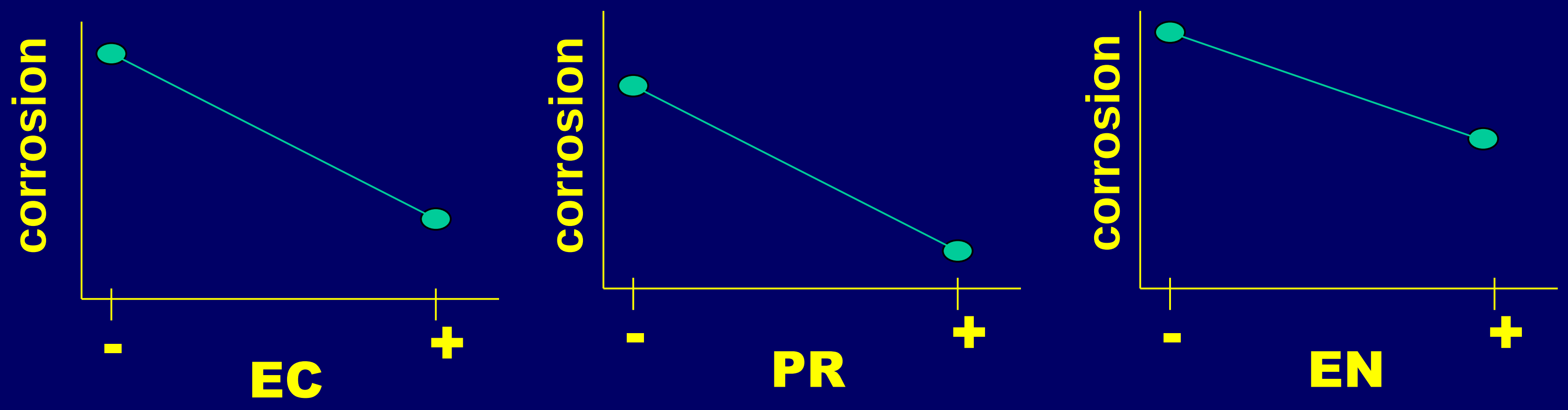
IT IS RECOMMENDED THAT d.f.res $\geq$ 4

How can we get d.f. for the SSresidual? → **Grouping in the $SS_{residual}$ the lowest effects**

OPTIMUM OPERATIVE CONDITION (OOC)

Combination of significant factors that optimize (maximize or minimize) the response variable.

O.O.C. to minimize corrosion: EC^{+} PR^{+} EN^{+} (i.e. thicker layers)



ANALYSIS OF RESIDUALS

Residual for the *i*-th observation:

e_i = (value observed)$_i$ – (mean of the treatment)$_i$

IMPORTANT TO: - Detect outliers

- Check the hypothesis of normality
- Study the effects over the variance of corrosion.

EXERCISE-4: REPLICATED DESIGN 2^2

In a chemical reaction, the target is to improve the quality of a mixture used to incorporate certain additive to a polymer.

Response variable: % additive **Target: maximize**

2 FACTORS:

- **Stirring speed in the mixing process**
- **Stirring time**

SPEED \ TIME	3 ’	6 ’
600 rpm	17.2 17.0 17.1 $\bar{X} = 17.1$	16.4 16.8 15.6 $\bar{X} = 16.267$
1000 rpm	18.7 19.0 18.6 $\bar{X} = 18.767$	19.4 17.7 17.4 $\bar{X} = 18.167$

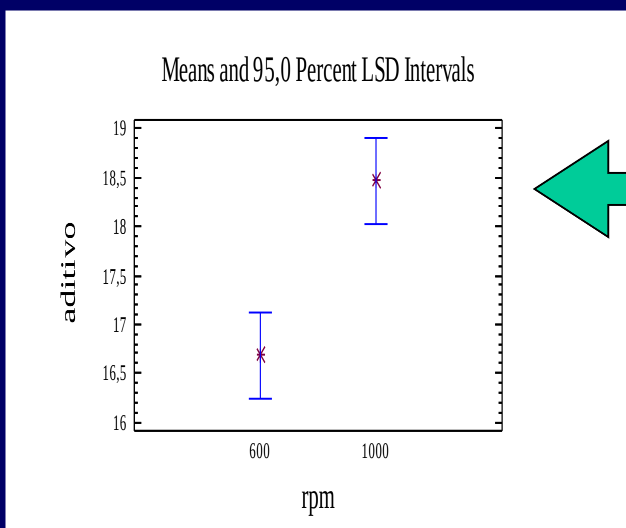
Analysis of Variance for aditivo

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
A:time	1,54083	1	1,54083	3,88	0,0845
B:speed	9,54083	1	9,54083	24,00	0,0012
AB:time*speed	0,04083	1	0,04083	0,10	0,7568
Total error	3,18	8	0,3975		
Total (corr.)	14,3025	11			

Effect “nearly” significant

Clearly significant

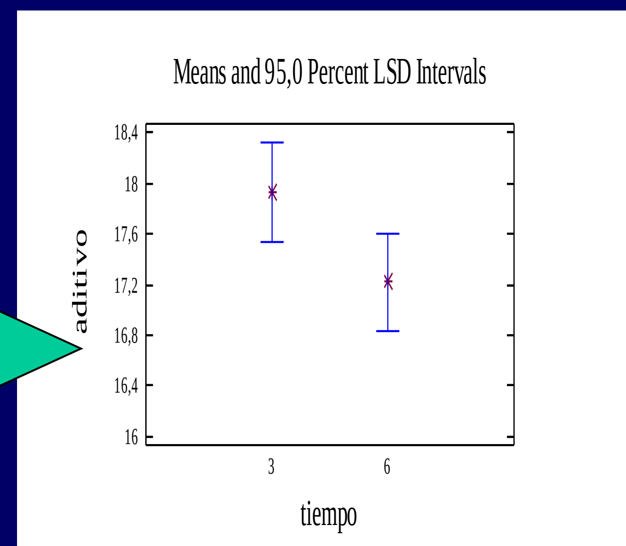
No evidence of interaction between both factors



EFFECT OF:

SPEED

TIME



As the effect of time is nearly significant, it seems convenient to take it into account.

What would be the OOC ?

EXERCISE-5: Factorial design 2^{4-1}

The effect of 4 factors in the stability of a chemical product is tested (target: maximize the stability)

	Variable	-	+
1	Concentration of acid (%)	20	30
2	Concentration of catalyst (%)	1	2
3	Temperature (° C)	100	150
4	Concentration of monomers	25	50

trial	V1	V2	V3	V4	STABILITY
1	-	-	-	-	20
2	+	-	-	+	14
3	-	+	-	+	17
4	+	+	-	-	10
5	-	-	+	+	19
6	+	-	+	-	13
7	-	+	+	-	14
8	+	+	+	+	10

Analysis of Variance for STABILITY - Type III Sums of Squares

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
A:ACID	66,125	1	66,125	144,27	0,0012
B:TEMPERATURE	3,125	1	3,125	6,82	0,0796
C:MONOMER	1,125	1	1,125	2,45	0,2152
D:CATALYST	28,125	1	28,125	61,36	0,0043
RESIDUAL	1,375	3	0,458333		
TOTAL (CORRECTED)	99,875	7			

Analysis of Variance for STABILITY - Type III Sums of Squares

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
MAIN EFFECTS					
A:ACID	66,125	1	66,125	58,78	0,0006
B:CATALYST	28,125	1	28,125	25,00	0,0041
RESIDUAL	5,625	5	1,125		
TOTAL (CORRECTED)	99,875	7			

Exercise: determine the optimum operative conditions

EXERCISE-6

In order to improve the yield of a chemical process (target: maximize the response variable), 5 factors are studied

Trat.	resp.	A	B	C	D	E
1	15.6	-	-	-	-	-
2	13.5	+	-	-	-	-
3	16.3	-	+	-	-	-
4	17.1	+	+	-	-	-
5	26.8	-	-	+	-	-
6	25	+	-	+	-	-
7	30	-	+	+	-	-
8	28.9	+	+	+	-	-
9	15.4	-	-	-	+	-
10	12.7	+	-	-	+	-
11	15.3	-	+	-	+	-
12	15.9	+	+	-	+	-
13	20.3	-	-	+	+	-
14	21.3	+	-	+	+	-
15	27	-	+	+	+	-
16	24.1	+	+	+	+	-
17	28.9	-	-	-	-	+
18	29	+	-	-	-	+
19	33.7	-	+	-	-	+
20	33.6	+	+	-	-	+

Trat.	resp.	A	B	C	D	E
21	47.4	-	-	+	-	+
22	44.2	+	-	+	-	+
23	52.6	-	+	+	-	+
24	46.2	+	+	+	-	+
25	27.8	-	-	-	+	+
26	29.5	+	-	-	+	+
27	30.1	-	+	-	+	+
28	29.6	+	+	-	+	+
29	35.9	-	-	+	+	+
30	36.4	+	-	+	+	+
31	41	-	+	+	+	+
32	38.6	+	+	+	+	+

1) ANOVA results with data from the 32 trials:

Source of variation	Sum of Squares	Df	Mean Square	F-Ratio	Sig. Level
TOTAL	3514.4847	31			
B	79.0653	1	79.0653	21.656	.0001
C	1031.7153	1	1031.7153	282.35	.0000
D	144.0753	1	144.0753	39.462	.0000
E	2101.1403	1	2101.1403	575.499	.0000
C*D	63.562812	1	63.562812	17.410	.0003
RESIDUAL	94.925625	26	3.6509856		

2) ANOVA results if ONLY the 16 trials in red had been conducted:

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
B	47,2656	1			
C	530,151	1			
D	60,4506	1			
E	1028,81	1			
INTERACTIONS					
BC	50,0556	1			
RESIDUAL					
TOTAL (CORRECTED)	1774,76				

(complete the table and obtain conclusions)

- Check that relevant effects are nearly the same with only 16 trials
- Obtain the optimum conditions (solution: $B^+ C^+ D^- E^+$)

EXERCISE-7: FRACTIONAL DOE 2^{6-3}

DOE to study the best conditions for improving the resistance against corrosion of metal sheets

6 factors studied (all at 2 levels)

	A	B	C	D	E	F	RESP.
1	-	-	-	+	+	+	8
2	+	-	-	-	-	+	6
3	-	+	-	-	+	-	7
4	+	+	-	+	-	-	7
5	-	-	+	+	-	-	10
6	+	-	+	-	+	-	8
7	-	+	+	-	-	+	8
8	+	+	+	+	+	+	9

FACTOR	SS	D.F.	MS	$F_{COMPUTED}$
A	1.125	1	1.125	9
B	0.125	1	0.125	1
C	6.125	1	6.125	49
D	3.125	1	3.125	25
E	0.125	1	0.125	1
F	0.125	1	0.125	1
RESIDUAL	0.125	1	0.125	

It is convenient to group in the $SS_{RESIDUAL}$ those factors clearly not significant in order to have at least 4 residual degrees of freedom

FACTOR	SS	D.F.	MS	$F_{COMPUTED}$
A	1.125	1	1.125	9
C	6.125	1	6.125	49
D	3.125	1	3.125	25
RESIDUAL	0.5	4	0.125	

$F_{1,4}$ (α=0.05) = 7.71

Which effects are statistically significant?

What would be the operative conditions to maximize the resistance?

EXERCISE-8: FRACTIONAL DOE 2^{6-2}

A DOE is conducted to study the effect of 6 parameters of a chemical process over the resistance obtained in one adhesive (target: MAX.)

VARIABLE (units)	LEVEL	
	-1	1
SACAROSE (GR)	43	71
PARAFORMOL	30	42
NaOH (GR)	6	10
WATER (GR)	16	20
MAX. TEMPER. (ºC)	80	90
TIME	25	35

X_1	X_2	X_3	X_4	X_5	X_6	y
-1	-1	-1	-1	-1	-1	162
1	-1	-1	-1	1	-1	146
-1	1	-1	-1	1	1	182
1	1	-1	-1	-1	1	133
-1	-1	1	-1	1	1	228
1	-1	1	-1	-1	1	143
-1	1	1	-1	-1	-1	223
1	1	1	-1	1	-1	172
-1	-1	-1	1	-1	1	168
1	-1	-1	1	1	1	128
-1	1	-1	1	1	-1	175
1	1	-1	1	-1	-1	186
-1	-1	1	1	1	-1	197
1	-1	1	1	-1	-1	175
-1	1	1	1	-1	1	196
1	1	1	1	1	1	173

Simple effects are NOT confounded with double interactions

It is possible to calculate in total 15 effects (N-1):

- **6 SIMPLE EFFECTS**
  (confounded with interactions of order > 2)
- **7 DOUBLE INTERACTIONS**
  (confounded with interactions of order > 2)
- **2 INTERACTIONS OF ORDER >2**

Analysis of Variance for Y - Type III Sums of Squares

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
A:F1	4726,56	1	4726,56	14,23	0,0023
B:F3	3220,56	1	3220,56	9,69	0,0082
RESIDUAL	4319,31	13	332,255		
TOTAL (CORRECTED)	12266,4	15			

We should also check that none of double interactions are significant

Which would be the optimum operative conditions to maximize the resistance?

(solution: F1 at level - and F3 at level +)

EXERCISE-9

In a certain process, TIME is a quality parameter that should be minimized.

FACTORS STUDIED:

- 3 at 2 LEVELS (A C E)
- 5 at 3 LEVELS (B D F G H)

Design used: L_{18} by adapting 3rd and 5th columns to set factors at 3 levels

TRIAL	A	B	C	D	E	F	G	H	TIME
1	1	1	1	1	1	1	1	1	852
2	1	1	2	2	2	2	2	2	540
3	1	1	2	3	2	3	3	3	417
4	1	2	1	1	2	2	3	3	1282
5	1	2	2	2	2	3	1	1	505
6	1	2	2	3	1	1	2	2	445
7	1	3	1	2	1	3	2	3	852
8	1	3	2	3	2	1	3	1	482
9	1	3	2	1	2	2	1	2	707
10	2	1	1	3	2	2	2	1	492
11	2	1	2	1	1	3	3	2	975
12	2	1	2	2	2	1	1	3	450
13	2	2	1	2	2	1	3	2	722
14	2	2	2	3	1	2	1	3	402
15	2	2	2	1	2	3	2	1	732
16	2	3	1	3	2	3	1	2	482
17	2	3	2	1	2	1	2	3	855
18	2	3	2	2	1	2	3	1	515

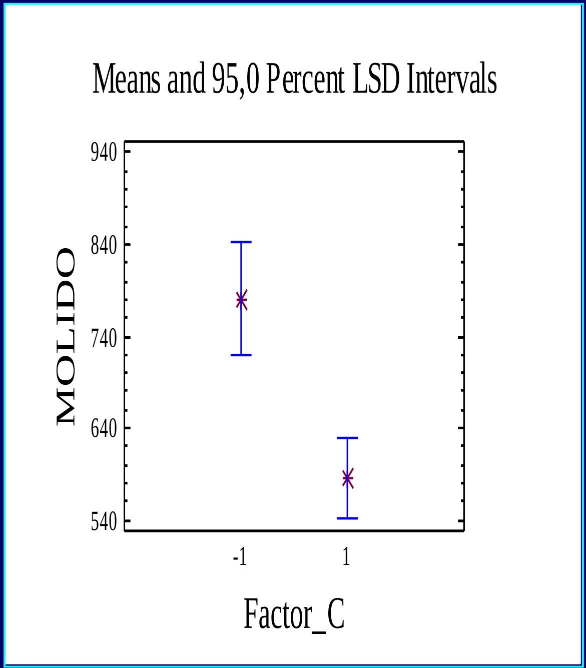
Analysis of Variance for TIME - Type III Sums of Squares

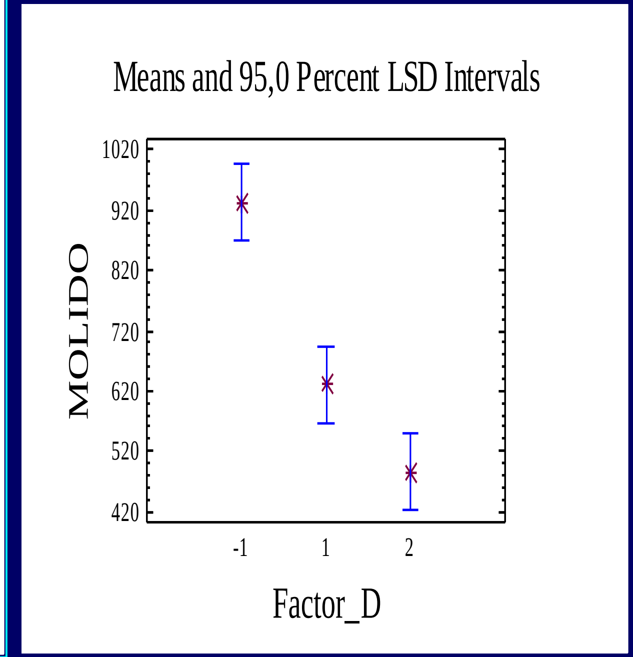
Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
A:Factor_A	11602,7	1	11602,7	1,00	0,3729
B:Factor_B	10942,1	2	5471,06	0,47	0,6536
C:Factor_C	151970,0	1	151970,0	13,16	**0,0222**
D:Factor_D	625208,0	2	312604,0	27,07	**0,0047**
E:Factor_E	4807,11	1	4807,11	0,42	0,5539
F:Factor_F	2372,11	2	1186,06	0,10	0,9047
G:Factor_G	82548,8	2	41274,4	3,57	**0,1287**
H:Factor_H	38778,8	2	19389,4	1,68	0,2955
RESIDUAL	46186,5	4	11546,6		
TOTAL (CORRECTED)	974416,0	17			

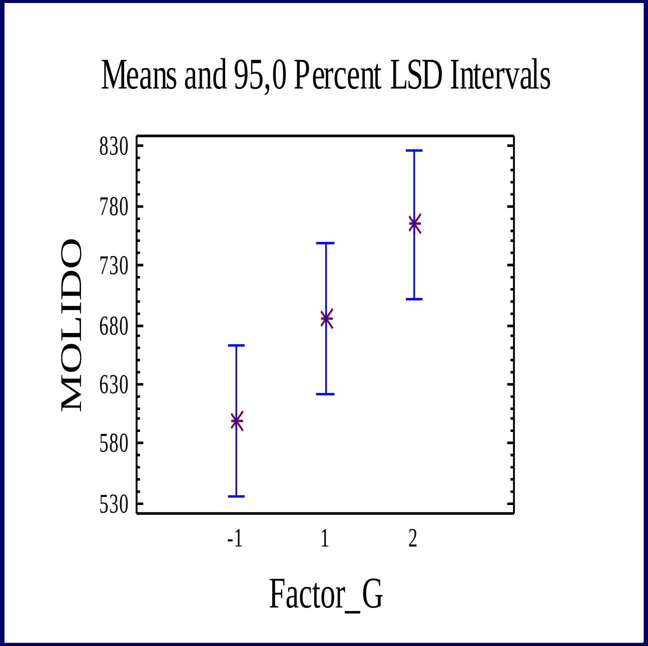
Analysis of Variance for TIME - Type III Sums of Squares

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
A:Factor_D	625208,0	2	312604,0	32,71	0,0000
B:Factor_G	82548,8	2	41274,4	4,32	0,0387
C:Factor_C	151970,0	1	151970,0	15,90	0,0018
RESIDUAL	114689,0	12	9557,45		
TOTAL (CORRECTED)	974416,0	17			

Factors C, D, G are statistically significant







Optimum operative conditions to minimize: C (2) D (3) G (1)

Certain quadratic effect is observed in factor D

(it could be studied with multiple linear regression)

The effect of G is clearly linear (not quadratic) in the interval tested. Thus, if possible, it would be better to decrease even more the level of factor G.