

# DESIGN OF EXPERIMENTS

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# Design of experiments

- Usually modeling (i.e. simulation) is carry out as a programming exercise.
- Inaccurate statistical methods (no IID).
- Take care of the time required to collect the needed data to apply the statistical techniques, with guaranties of achieve the accomplishment of the objectives.

# Design of experiments

- How to make the **comparisons** between different configurations.
  - ▣ The comparisons must be the more homogeneous as possible.
- Study the **effect** over the answer variable of the values of the different experimental variables.
  - ▣ In a cashier: Answer variable: Queue long; factors: Number of cashiers, service time, time between arrivals.

# Principles

Principles to develop a good design of experiments:

- **Randomization:** Assignment to the random of all the factors that are not controlled by the experimentation.
- **Repetition of the experiment (replication):** Is a good method to reduce the variability between the answers.
- **Statistical homogeneity of the answers:** To compare different alternatives derived from the results, is needed that the executions of the experiments have been done under homogeny conditions. Factorial design helps to obtain this similarity between the experiments.

# Design of Experiments goals

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- **Isolate** effects of each input variable.
- Determine **effects** of interactions.
- Determine **magnitude** of experimental error
- Obtain maximum **information** for given effort

# Terminology

- Response variable
  - ▣ Measured output value
    - E.g. total execution time
- Factors
  - ▣ Input variables that can be changed
    - E.g. cache size, clock rate, bytes transmitted
- Levels
  - ▣ Specific values of factors (inputs)
    - Continuous (~bytes) or discrete (type of system)

# Terminology

- Replication
  - ▣ Completely re-run experiment with same input levels
  - ▣ Used to determine impact of measurement error
- Interaction
  - ▣ Effect of one input factor depends on level of another input factor
- Treatment, scenario, one of the combinations to analyze.

# Tests

Test	Dependent variables	Independent variables
T-test	One	One (two groups)
ANOVA Completely Randomized Design (CRD)	One	One
Two-way ANOVA Randomized Block Design (RBD)	One	Two
MANOVA	Multiple	Multiple



Test	Assumptions					Required sample data							
#	Test name	Check	Statistic		Ind	$\sigma$	$\sigma^1=\sigma^2$	d	$\mu/p$	$\bar{x}/\bar{p};$	n	S	
1	<a href="#">One Sample Z-Test</a>	Mean		✓	✓	✓			✓	✓	✓		
2	<a href="#">One Sample T-Test</a>	Mean		✓	✓	✗			✓	✓	✓	✓	
3	<a href="#">Two Sample Z-Test</a>	Mean		✓	✓	✓		✓		✓	✓		
4	<a href="#">Two Sample T-Test (Pooled variance)</a>	Mean		✓	✓	✗	✓	✓		✓	✓	✓	
5	<a href="#">Two Sample T-Test (Welch's)</a>	Mean		✓	✓	✗	✗	✓		✓	✓	✓	
6	<a href="#">Two Sample Mann-Whitney U Test</a>	Rank			✓			✓					✓
7	<a href="#">Paired T-Test</a>	Mean		✓	Paired								✓
8	<a href="#">Paired Wilcoxon Sign Rank Test</a>	Rank			Paired								✓
9	<a href="#">One Way ANOVA Test</a>	Mean		✓	✓		✓						✓
10	<a href="#">Repeated Measures ANOVA Test</a>	Mean		✓	Dependent groups		<a href="#">Sphericity</a>						✓
11	<a href="#">Kruskal-Wallis Test</a>	Mean			✓								✓
12	<a href="#">Two Way ANOVA Test</a> Fixed model, Mixed model, Random mode, Mixed model with repeats	Mean		✓	✓		✓						✓
<a href="https://www.statskingdom.com/index.html">https://www.statskingdom.com/index.html</a>													
13	<a href="#">One Way MANOVA Test</a>	Mean	F	✓	✓		✓						✓
14	<a href="#">One Sample Proportion Test</a>	Proportion		Binomial	✓				✓	✓	✓		
15	<a href="#">Two Sample Proportion Test</a>	Proportion		Binomial	✓					✓	✓		
16	<a href="#">Chi-Squared Test For Variance</a>	$\sigma$		✓	✓						✓	✓	
17	<a href="#">F Test For Variances</a>	$\sigma$		✓	✓						✓	✓	
18	<a href="#">Levene's Test For Variances</a>	$\sigma$		✗	✓								✓
19	<a href="#">Chi-Squared Test For Goodness Of Fit</a> (McNemar test, Chi-squared test for	Fit			✓								✓

<https://www.statskingdom.com/index.html>

# One-Factor ANOVA

- Separates total variation observed in a set of measurements into:
  - ▣ Variation within one system
    - Due to random measurement errors
  - ▣ Variation between systems
    - Due to real differences + random error
- *One-factor experimental design*
  - ▣ *We have here three or more different populations?*



# Two-factor Experiments

Introduction to Design of Experiments

# Two-factor Experiments

- Two factors (inputs)
  - ▣ A, B
- Separate total variation in output values into:
  - ▣ Effect due to A
  - ▣ Effect due to B
  - ▣ Effect due to interaction of A and B (AB)
  - ▣ Experimental error

# Example – User Response Time

- A = degree of multiprogramming
- B = memory size
- AB = interaction of memory size and degree of multiprogramming

	B (Mbytes)		
A	32	64	128
1	1,125	1,105	1,075
2	1,26	1,225	1,18
3	1,405	1,33	1,25
4	1,75	1,725	1,35

# Two Factors, $n$ Replications

The diagram illustrates a three-way ANOVA design with three factors: Factor A, Factor B, and Factor C. The design is represented as a 3D grid of cells. The top face shows Factor A with levels 1, 2, ..., i, ..., a. The left face shows Factor B with levels 1, 2, ..., i, ..., b. The depth represents Factor C with levels 1, 2, ..., j, ..., n. The cell at the intersection of Factor A level i, Factor B level i, and Factor C level j is labeled  $y_{ijk}$ . The diagram shows multiple replicates of the design, indicated by arrows and the text "n replications".

# One-factor ANOVA

- Each individual measurement is composition of
  - ▣ Overall mean
  - ▣ Effect of alternatives
  - ▣ Measurement errors

$$y_{ij} = \bar{y}_{..} + \alpha_i + e_{ij}$$

$\bar{y}_{..}$  = overall mean

$\alpha_i$  = effect due to A

$e_{ij}$  = measurement error

# Two-factor ANOVA

- Each individual measurement is composition of
  - ▣ Overall mean
  - ▣ Effects
  - ▣ Measurement errors
  - ▣ Interactions

$$y_{ijk} = \bar{y}_{...} + \alpha_i + \beta_j + \gamma_{ij} + e_{ijk}$$

$\bar{y}_{...}$  = overall mean

$\alpha_i$  = effect due to A

$\beta_j$  = effect due to B

$\gamma_{ij}$  = effect due to interaction of A and B

$e_{ijk}$  = measurement error



# $n2^k$ Contrasts

- Effects of A, B and interactions.

$$w_A = y_{AB} + y_{Ab} - y_{aB} - y_{ab}$$

$$w_B = y_{AB} - y_{Ab} + y_{aB} - y_{ab}$$

$$w_{AB} = y_{AB} - y_{Ab} - y_{aB} + y_{ab}$$

# $n2^k$ Sum of Squares

$$SSA = \frac{w_A^2}{n2^k}$$

$$SSB = \frac{w_B^2}{n2^k}$$

$$SSAB = \frac{w_{AB}^2}{n2^k}$$

$$SSE = SST - SSA - SSB - SSAB$$

# Replications are needed

- If no replications,  $n=1$ 
  - ▣  $SSE = 0$ , no information regarding the errors in the measurements.
- Cannot separate effect due to interactions from measurement noise
- Must *replicate* each experiment at least twice

# Example

- Output = user response time (seconds)
- Want to separate effects due to
  - ▣ A = degree of multiprogramming
  - ▣ B = memory size
  - ▣ AB = interaction
  - ▣ Error
- Need **replications** to separate error

	B (Mbytes)		
A	32	64	128
1	1,125	1,105	1,075
2	1,26	1,225	1,18
3	1,405	1,33	1,25
4	1,75	1,725	1,35

# Example

A	B (Mbytes)		
	32	64	128
1	1,125	1,105	1,075
	1,14	1,095	1,055
2	1,26	1,225	1,18
	1,24	1,245	1,15
3	1,405	1,33	1,25
	1,38	1,295	1,305
4	1,75	1,725	1,35
	1,125	1,105	1,075

# Example

ANOVA						
Source of Variation	SS	df	MS	F	P-value	F crit
Sample	0,842854	3	0,280951	460,2617	1,2E-12	3,490295
Columns	0,128802	2	0,064401	105,5034	2,43E-08	3,885294
Interaction	0,107915	6	0,017986	29,46473	1,65E-06	2,99612
Within	0,007325	12	0,00061			
Total	1,086896	23				

# Conclusions From the Example

- 77.6% (SSA/SST) of all variation in response time due to degree of multiprogramming
- 11.8% (SSB/SST) due to memory size
- 9.9% (SSAB/SST) due to interaction
- 0.7% due to measurement error
- 95% confident that all effects and interactions are statistically significant

# Factorial designs

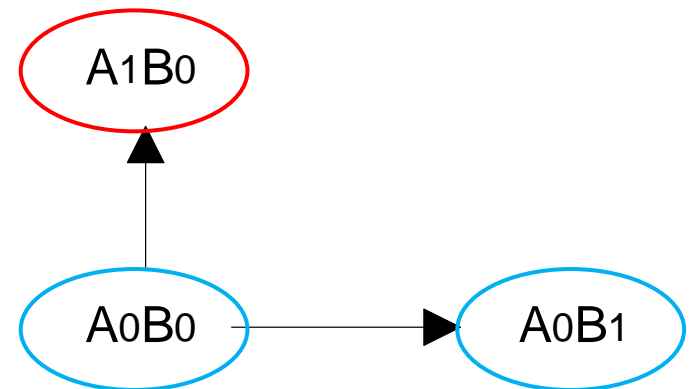
Explore the landscape

Assure that we are analyzing all the combinations  
with economy on the experimentation



# No factorial designs

- To fix two factors and modify all the levels of a third until find a good solution. Fixing this level, start the exploration for the other factors.
- Effect A:  $A_1B_0 - A_0B_0$ .
- Effect B:  $A_0B_1 - A_0B_0$

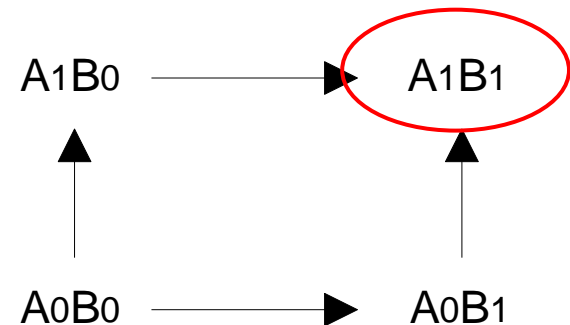


# Factorial designs

□ Take in consideration the interactions.

□ A effect: 
$$\frac{A_1B_0 - A_1B_1}{2} - \frac{A_0B_0 - A_0B_1}{2}$$

□ B effect: 
$$\frac{A_1B_1 - A_0B_1}{2} - \frac{A_0B_0 - A_1B_0}{2}$$



# Factorial designs

- Controlling “k” factors.
- “l” levels for each factor (“li” levels for the i factor).
- $l_1 \cdot l_2 \cdot \dots \cdot l_k$  experiments
- The easiest factorial design is the  $2^k$  with  $l_i = 2 \ \forall i = 1, \dots, k$ .

# A Problem

- *Full factorial design with replication*
  - ▣ Measure system response with all possible input combinations
  - ▣ Replicate each measurement  $n$  times to determine effect of measurement error
- $k$  factors,  $v$  levels,  $n$  replications
  - $n v^k$  experiments
- *Example:*
  - ▣  $k = 5$  input factors,  $v = 4$  levels,  $n = 3$
  - ▣ →  $3(4^5) = 3,072$  executions!

# Fractional Factorial Designs: $n2^k$ Experiments

- Special case of generalized  $m$ -factor experiments
- Restrict each factor to two possible values
  - ▣ High, low
  - ▣ On, off
- Find factors that have largest impact
- Full factorial design with only those factors

# Finding Sum of Squares Terms

Sum of n measurements with (A,B) = (High, Low)	Factor A	Factor B
yAB	High	High
yAb	High	Low
yaB	Low	High
yab	Low	Low

# Yates notation

- Levels: High (+), Low (“-”) for factors A and B

A	B	Yates notation	Meaning
-	-	(1)	Both factors on low level
+	-	a	A in +, B in -
-	+	b	A in - B in +
+	+	ab	A in + B in +

# Contrasts for $n2^k$ with $k = 2$ factors

Measurements	Contrast		
	$W_a$	$W_b$	$W_{ab}$
$y_{AB}$	+	+	+
$y_{Ab}$	+	-	-
$y_{aB}$	-	+	-
$y_{ab}$	-	-	+

$$W_a = y_{AB} + y_{Ab} - y_{aB} - y_{ab}$$

$$W_b = y_{AB} - y_{Ab} + y_{aB} - y_{ab}$$

$$W_{ab} = y_{AB} - y_{Ab} - y_{aB} + y_{ab}$$



# $2^k$ Matrix

Experiment	Factor 1	Factor 2	....	Factor k	Answer
1	-	-		-	R1
2	+	-		-	R2
3	-	-		-	R3
4	+	-		-	R4
5	-	+		-	R5
6	+	+		-	R6
(..)					
$2^k$	+	+		+	$R_{2^k}$

# Important Points

- Experimental design is used to
  - ▣ Isolate the effects of each input variable.
  - ▣ Determine the effects of interactions.
  - ▣ Determine the magnitude of the error
  - ▣ Obtain maximum information for given effort
- Expand 1-factor ANOVA to  $k$  factors
- Use  $n2^k$  design to reduce the number of experiments needed
  - ▣ But loses some information
  - ▣ Useful to underline the tendency with economy of experiments.

# Exercise 1

- We have on a factory three different Machines:
  - A, with speed from 2 to 10
  - B, with speed of 2 and 3
  - C, with speed of 2 but that can be changed for other machine with a speed of 3 for 1000€.
- Define a table for an  $2^k$  experimental design that allows to analyze this.
- What is the time needed to complete the operation?



# Solution

	A	B	C	Answer
1	- (means 2)	-(means 2)	- (means 2)	
2	-	-	+ (means 3, 1000€)	
3	-	+(means 3)	-	
4	-	+	+	
5	+ (means 10)	-	-	
6	+	-	+	
7	+	+	-	
8	+	+	+	

# Yates algorithm

Simplifying the interaction calculus on a  $2^k$  factorial design

# $2^k$ factorial designs

## Advantages

- Determination of the tendency with experiments economy (smoothness).
- Possibility to evolve to composite designs (local exploration).
- Basis for factorial fractional designs (rapid vision of multiple factors).
- Easy analysis and interpretation.

# $2^k$ Matrix example

Experiment	A	B	C	Answer
1	-	-	-	60
2	+	-	-	72
3	-	+	-	54
4	+	+	-	68
5	-	-	+	52
6	+	-	+	83
7	-	+	+	45
8	+	+	+	80

# Effects calculus

$$\text{Effect } A = \frac{A_1B_0 - A_1B_1}{2} - \frac{A_0B_0 - A_0B_1}{2}$$

$$\text{Effect } B = \frac{A_1B_1 - A_0B_1}{2} - \frac{A_0B_0 - A_1B_0}{2}$$

$$\text{Main effect} = \bar{y}_+ - \bar{y}_-$$



# Effects calculus example

$$\text{Main effect} = \bar{y}_+ - \bar{y}_-$$

$$A = \frac{72 + 68 + 83 + 80}{4} - \frac{60 + 54 + 52 + 45}{4} = 23$$

$$B = \frac{54 + 68 + 45 + 80}{4} - \frac{60 + 72 + 52 + 83}{4} = -5$$

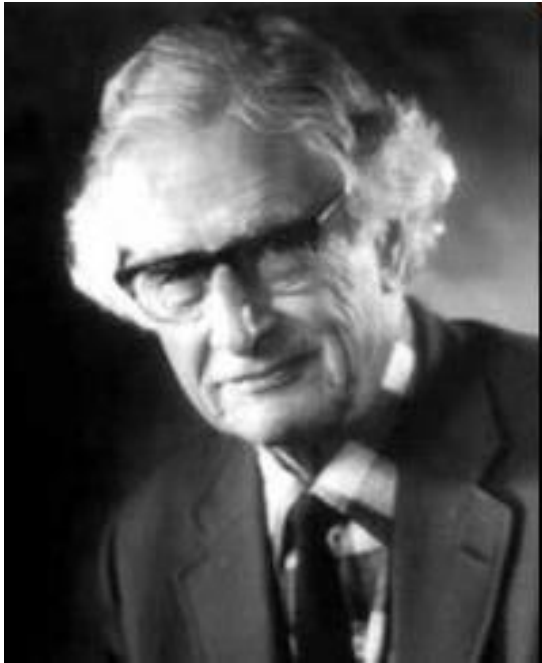
$$C = \frac{52 + 83 + 45 + 80}{4} - \frac{60 + 72 + 54 + 68}{4} = 15$$

# Interactions for 2 and 3 factors

$$AC = \frac{y_1 + y_3 + y_6 + y_8}{4} - \frac{y_2 + y_4 + y_5 + y_7}{4} = 10$$

$$ABC = \frac{y_2 + y_3 + y_5 + y_8}{4} - \frac{y_1 + y_4 + y_6 + y_7}{4} = 0.5$$

# Frank Yates



- A pioneer of the Operation research of the s.XX.

# Yates algorithm

To make systematic the interactions calculus using a table.

- Add the **answer** in the column “i” in the standard form of the matrix of the experimental design.
- Add **auxiliary columns** as factors exists.
- Add a new column dividing the first value of the last auxiliary column by the number of scenarios “E”, and the others by the half of “E”.

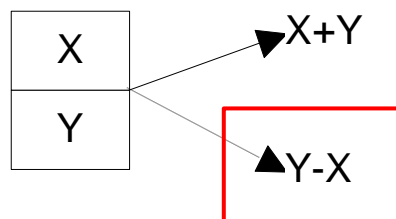
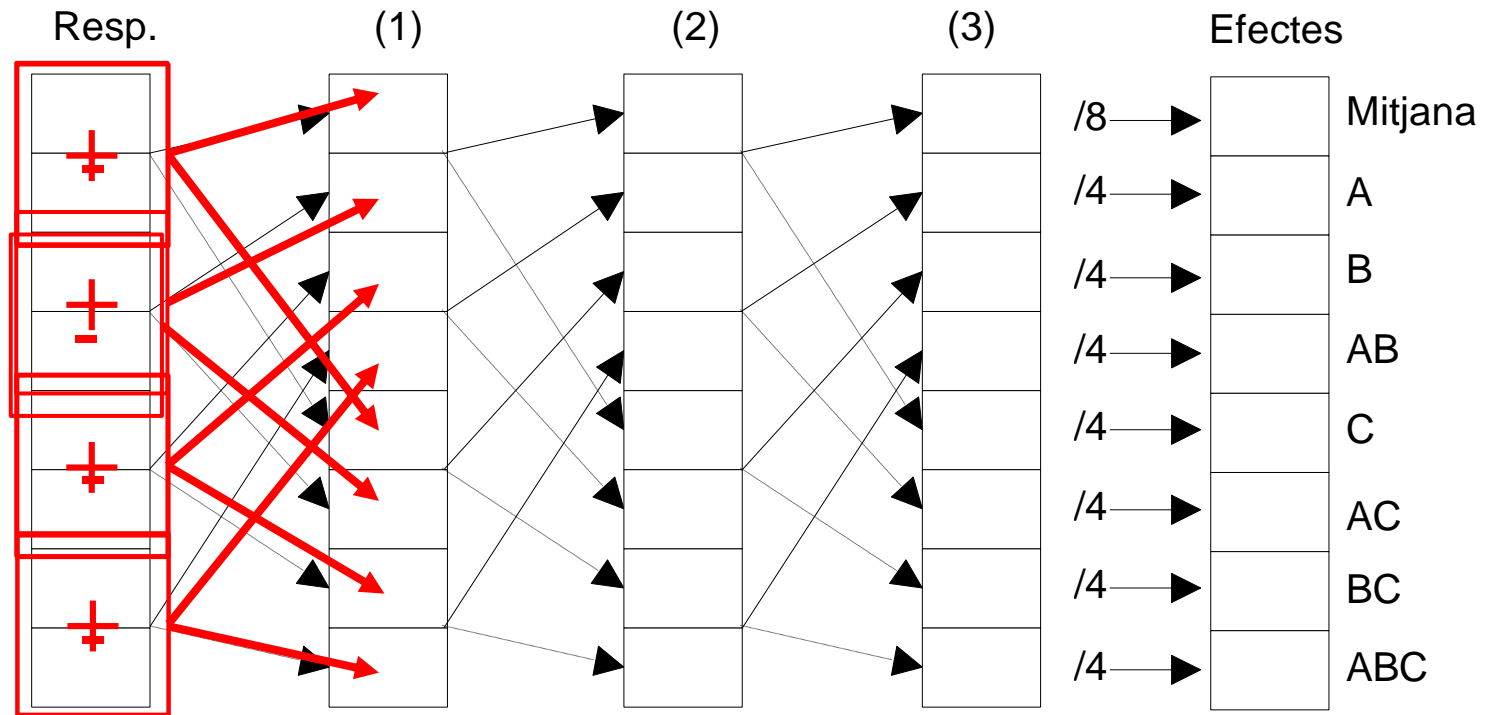
-	-	-
+	-	-
-	+	-
+	+	-
-	-	+
+	-	+
-	+	+
+	+	+

standard form

# Yates algorithm

- In the last column the first value is the mean of the answers, the last values are the effects.
- The correspondence between the values and effects is done through localize the + values in the corresponding rows of the matrix. A value with a single + in the B column is representing the principal effect of B. A row with two + on A and C corresponds to the interaction of AC, etc.

# Yates algorithm



# Yates algorithm example

Exp.	A	B	C	Answer	(1)	(2)	(3)	div.	effect	Id
1	-	-	-	60	132	254	514	8	64.25	Mean
2	+	-	-	72	122	260	92	4	23.0	A
3	-	+	-	54	135	26	-20	4	-5.0	B
4	+	+	-	68	125	66	6	4	1.5	AB
5	-	-	+	52	12	-10	6	4	1.5	C
6	+	-	+	83	14	-10	40	4	10.0	AC
7	-	+	+	45	31	2	0	4	0.0	BC
8	+	+	+	80	35	4	2	4	0.5	ABC

# Wooden industry example

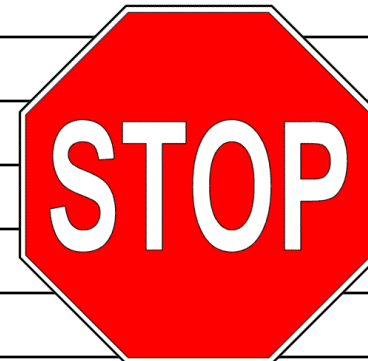


- Wooden industry that allows to reduce the cost.
- 4 variables to consider
  - ▣ Change the light to natural light (open the ceiling).
  - ▣ Increase the speed of the machines.
  - ▣ Increase the lubricant use.
  - ▣ Increase the working space.



# Wooden industry example

Comb.	1	2	3	4	Description	obs.
(1)	-	-	-	-		71
a	+	-	-	-	Natural light	61
b	-	+	-	-	Increase the speed of the machines	90
ab	+	+	-	-		82
c	-	-	+	-	Increase the use of lubricant	68
ac	+	-	+	-		61
bc	-	+	+	-		87
abc	+	+	+	-		80
d	-	-	-	+	Increase the working space.	61
ad	+	-	-	+		50
bd	-	+	-	+		89
abd	+	+	-	+		83
cd	-	-	+	+		59
acd	+	-	+	+		51
bcd	-	+	+	+		85
abcd	+	+	+	+		78



# Wooden industry example

Comb.	obs.	1	2	3	4	Effect	Description
(1)	71						
a	61						
b	90						
ab	82						
c	68						
ac	61						
bc	87						
abc	80						
d	61						
ad	50						
bd	89						
abd	83						
cd	59						
acd	51						
bcd	85						
abcd	78						

# Wooden industry example

Comb.	obs.	1	2	3	4	Effect	Description
(1)	71	132	304	600	1156	72,25	Mean
a	61	172	296	556	-64	-8	A
b	90	129	283	-32	192	24	B
ab	82	167	273	-32	8	1	AB
c	68	111	-18	78	-18	-2,25	C
ac	61	172	-14	114	6	0,75	AC
bc	87	110	-17	2	-10	-1,25	BC
abc	80	163	-15	6	-6	-0,75	ABC
d	61	-10	40	-8	-44	-5,5	D
ad	50	-8	38	-10	0	0	AD
bd	89	-7	61	4	36	4,5	BD
abd	83	-7	53	2	4	0,5	ABD
cd	59	-11	2	-2	-2	-0,25	CD
acd	51	-6	0	-8	-2	-0,25	ACD
bcd	85	-8	5	-2	-6	-0,75	BCD
abcd	78	-7	1	-4	-2	-0,25	ABCD

# Exercise 2: Clean industry

- We have a system that processes some kind of pieces. The time needed to process this pieces can be represented by an **exponential distribution** with a parameter  $1/\mu$  that depends on the technology used on the process. This parameter  $\mu$  can be calculated depending on several factors that affect it. Each factor adds time to the process:
  - ▣ The time needed to clean the pieces by a cleaner machine (range from 10 to 50 seconds).
  - ▣ For glue machines, 1 to 5 machines. If we have 5 machines the time needed is reduced by 4, if one, the time remains the same.
  - ▣ The number of workers that take the finished pieces (1 or 2), with one worker the time is 1 second, with two workers is 0,5 seconds.

# Perform a DOE for the proposed system

- Set the objectives.
- Select the process variables.
- Define an experimental design.
- Execute the design.
- Check that the data are consistent with the experimental assumptions.
- Analyze and interpret the results, detect effects of main factors and interactions.
- Remember:

$$r = 1 - e^{-\alpha \cdot x} \Rightarrow x = \frac{\ln(1-r)}{-\alpha} = \frac{\ln(r)}{-\alpha}$$

# Perform a DOE for the proposed system

- Set the objectives.
  - ▣ Detect the effects and the interactions of the three main factors
- Select the process variables.
  - ▣ Cleaner, Machines, workers.
- Define an experimental design.
  - ▣ We define a 2k experimental design.
- Execute the design.
  - ▣ Using Excel we “simulate” the behavior for each proposed model.
- Check that the data are consistent with the experimental assumptions.
  - ▣ Independence, homoscedasticity, normality, etc?.
- Analyze and interpret the results, detect effects of main factors and interactions.
  - ▣ Done on the Excel

# Answer

Cleaner	Machines	Workers	VALUES		$\mu$	$1/\mu$	x1	x2	mean							
-	-	-	50	0	1	51	0,01960784	150,255	42,6638	96,4594	99,7468	142,996	230,537	<b>28,8171</b>	Mean	
+	-	-	10	0	1	11	0,09090909	3,16628	3,4085	3,28739	43,2496	87,5401	-170,327	<b>-42,5818</b>	Workers	
-	+	-	50	-4	1	47	0,0212766	56,9673	11,246	34,1066	64,7865	-118,136	-98,5301	<b>-24,6325</b>	Machines	
+	+	-	10	-4	1	7	0,14285714	5,95007	12,3359	9,14298	22,7536	-52,1916	129,52	<b>32,3801</b>	Machines*Workers	
-	-	+	50	0	0,5	50,5	0,01980198	28,4253	93,1129	60,7691	-93,172	-56,4972	-55,4563	<b>-13,8641</b>	Cleaner	
+	-	+	10	0	0,5	10,5	0,0952381	3,00539	5,02942	4,0174	-24,9637	-42,0329	65,9441	<b>16,486</b>	Cleaner*Workers	
-	+	+	50	-4	0,5	46,5	0,02150538	8,18413	10,0094	9,09675	-56,7517	68,2084	14,4643	<b>3,61608</b>	Cleaner*Machines	
+	+	+	10	-4	0,5	6,5	0,15384615	11,0781	16,2357	13,6569	4,56014	61,3118	-6,89653	<b>-1,72413</b>	Cleaner*Machines*Workers	

$$r = 1 - e^{-\alpha \cdot x} \Rightarrow x = \frac{\ln(1-r)}{-\alpha} = \frac{\ln(r)}{-\alpha}$$



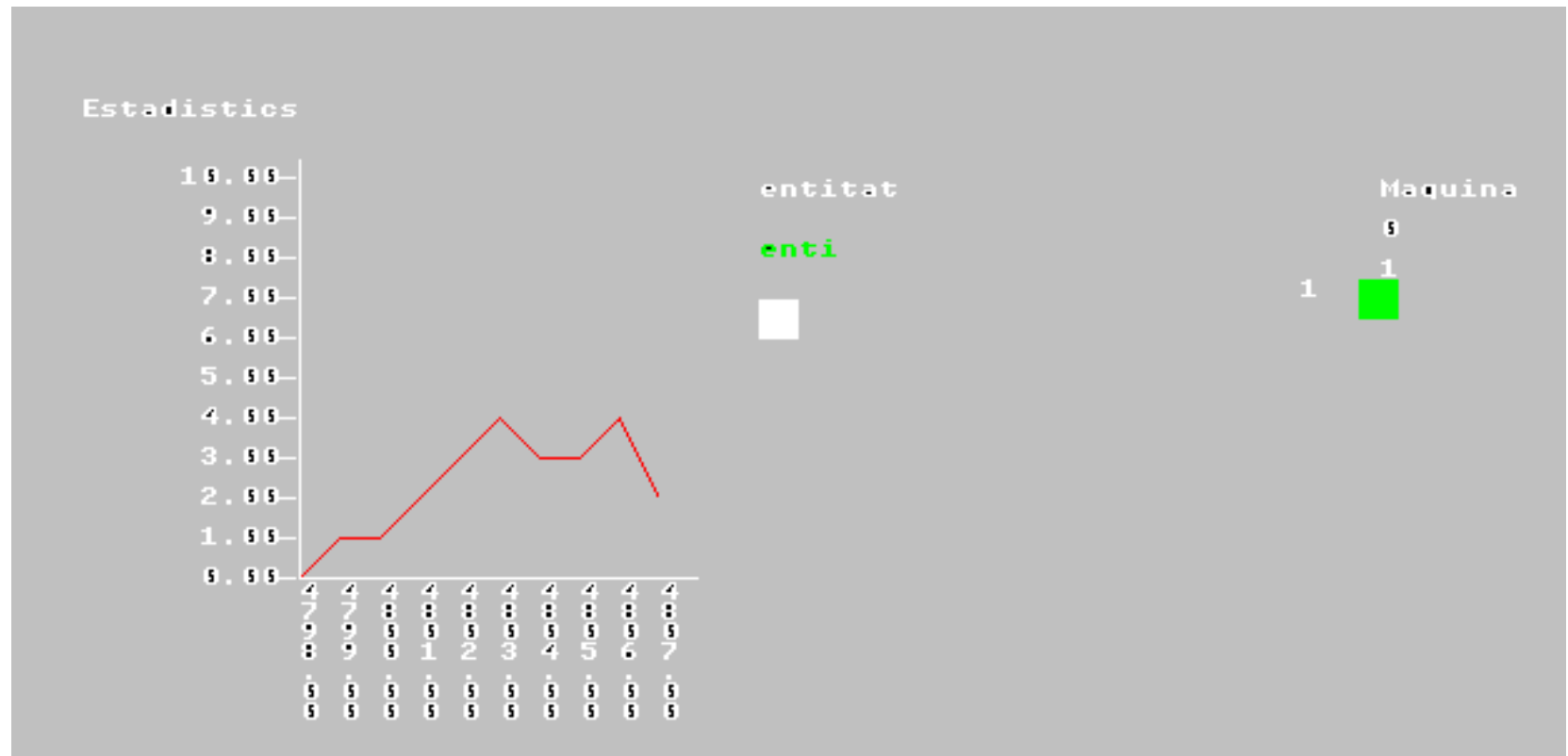
# Replications

Number of replications calculus.

Methods to perform the replications.



# Interest variable calculus



# Experimentation

- Be  $x$  an interest variable

$x_{11}, \dots, x_{1i}, \dots, x_{1m}$

$x_{21}, \dots, x_{2i}, \dots, x_{2m}$

.....

$x_{n1}, \dots, x_{ni}, \dots, x_{nm}$

- $n$  is the number of replications.
- $x_i$  is the value of each one of the replications.

# Sample mean and variance

The use of the term  $n - 1$  is called Bessel's correction, for the *unbiased sample variance*

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$$

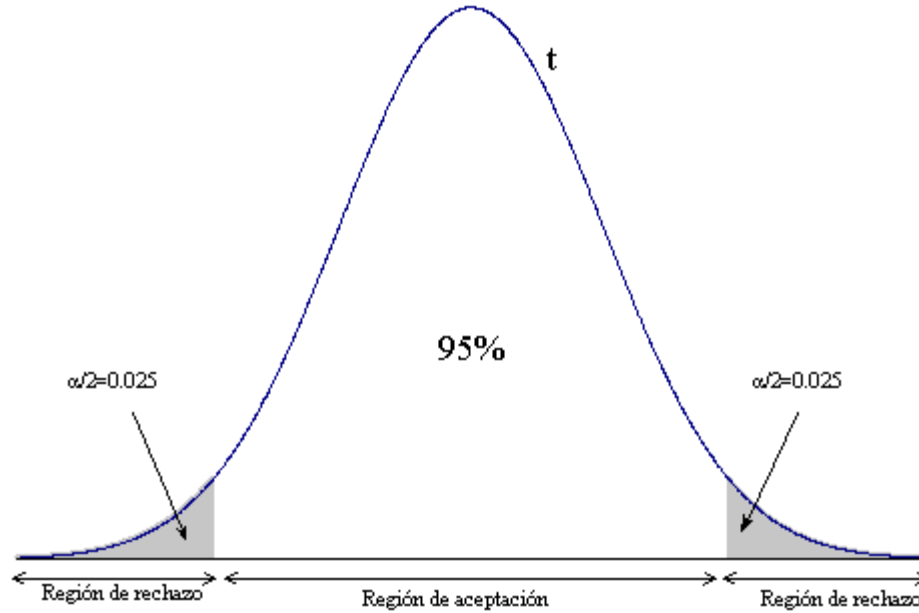
$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2$$

# Confidence interval

- Need to know how far is  $\mu$  and  $\bar{x}$ .
- Student's t-distribution of  $n-1$  degrees of freedom.

$$\bar{x} \pm t_{1-\alpha/2, n-1} \sqrt{\frac{S^2}{n}}$$

# Student's t-distribution



# What is the correct n?

Replication	Value from the model
1	28.841
2	35.965
3	31.219
4	37.090
5	38.734
6	30.923
7	30.443
8	32.175
9	30.683
10	28.745

# Calculus of S and X

- $\bar{x} = 32.4818$

- $S^2 = 12.35$

# Calculus of the self-confidence interval

$$h = t_{1-\alpha/2, n-1} \frac{S}{\sqrt{n}}$$

$$t_{9, 0.975} = 2,26$$

$$h = 2,512$$

	1 - $\alpha$							
r	0.75	0.80	0.85	0.90	0.95	0.975	0.99	0.995
1	1.000	1.376	1.963	3.078	6.314	12.706	31.821	63.657
2	0.816	1.061	1.386	1.886	2.920	4.303	6.965	9.925
3	0.765	0.978	1.250	1.638	2.353	3.182	4.541	5.841
4	0.741	0.941	1.190	1.533	2.132	2.776	3.747	4.604
5	0.727	0.920	1.156	1.476	2.015	2.571	3.365	4.032
6	0.718	0.906	1.134	1.440	1.943	2.447	3.143	3.707
7	0.711	0.896	1.119	1.415	1.895	2.365	2.998	3.499
8	0.706	0.889	1.108	1.397	1.860	2.306	2.896	3.355
9	0.703	0.883	1.100	1.383	1.833	<b>2.262</b>	2.821	3.250
10	0.700	0.879	1.093	1.372	1.812	2.228	2.764	3.169



# Confidence interval:

- (  $32.4818 - 2.512 = 29.9698$ ,  $32.4818 + 2.512 = 34.9938$  )
- The interpretation is that with a probability of 0.95, the random interval  $(29.9698, 34.9938)$  includes the real value of the mean.

# More replications needed.

- If we specify that we want an interval between a 5% of the sample mean with a confidence level of a 95%, we need more replications.
- $0.05 \cdot (32.4818) = 1.62$  but we have 2.512

# Number of needed replications

- where:
- $n$  = initial number of replications.
- $n^*$  = total replications needed.
- $h$  = half-range of the confidence interval for the initial number of replications.
- $h^*$  = half-range of the confidence interval for all the replications (the desired half-range).

$$n^* = n \left( \frac{h}{h^*} \right)^2$$

# Number of replications calculus.

---

$$n^* = \left( \frac{2.512}{1.62} \right)^2 = 24.04$$

# More replications...

Replication	Value from the model
11	33.020
12	29.472
13	27.693
14	31.803
15	30.604
16	33.227
17	28.085
18	35.910
19	30.729
20	30.844
21	32.420
22	39.040
23	32.341
24	34.310
25	28.418

## New mean and variance



$$\bar{y} = 32.1094$$

$$s^2 = 3.1903$$

# New self-confidence interval

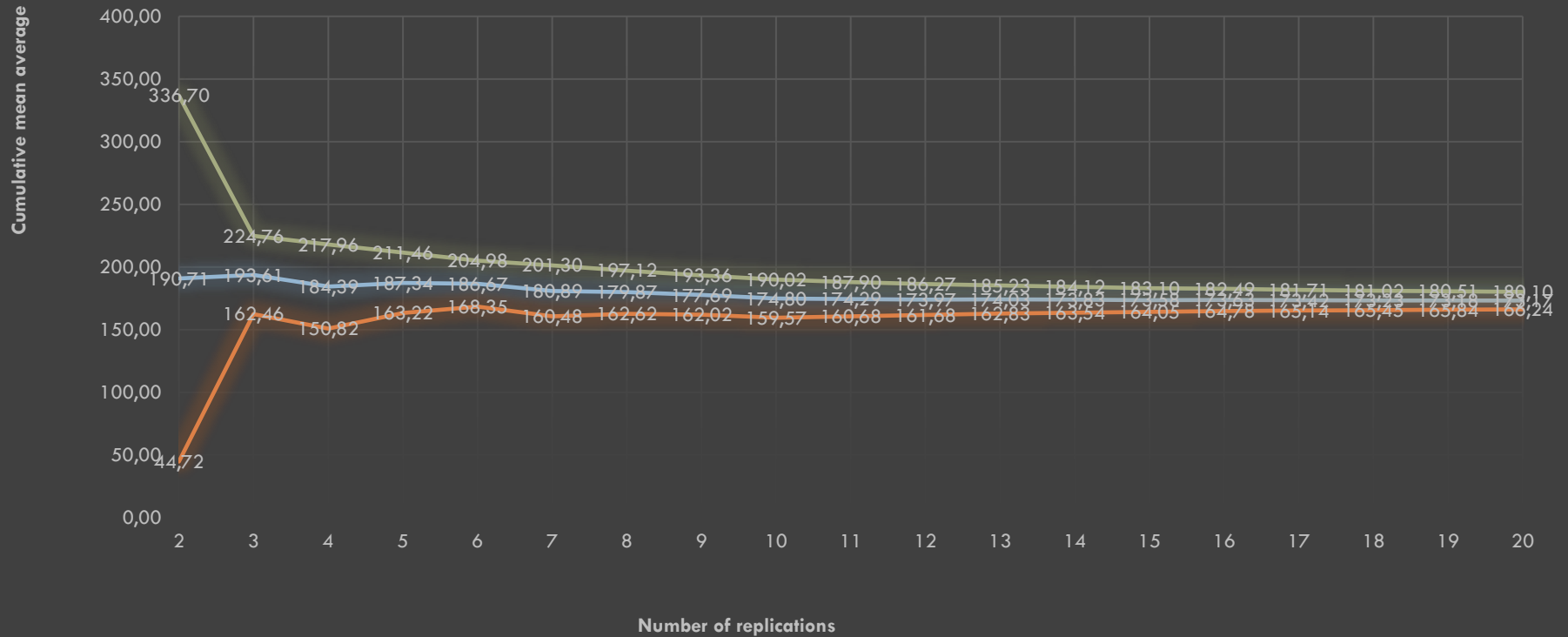
- In that case is enough, but the process can be iterative.

$$h = t_{1-\alpha/2, n-1} \frac{S}{\sqrt{n}}$$

$$h = 1.3144 < 1.62$$

$$n^* = n \left( \frac{h}{h^*} \right)^2$$

# With more replications





# Exercise 3

- Calculate the amount of replications needed for the Exercise 2

Cleaner	Machines	Workers	x1	x2
-	-	-	20,885	20,261
-	-	+	33,836	36,368
-	+	-	9,9099	142
-	+	+	17,766	131,13
+	-	-	42,759	0,0402
+	-	+	5,7025	2,327
+	+	-	10,481	8,7404
+	+	+	5,9775	5,1167

	1 - $\alpha$							
r	0.75	0.80	0.85	0.90	0.95	0.975	0.99	0.995
1	1.000	1.376	1.963	3.078	6.314	12.706	31.821	63.657
2	0.816	1.061	1.386	1.886	2.920	4.303	6.965	9.925
3	0.765	0.978	1.250	1.638	2.353	3.182	4.541	5.841
4	0.741	0.941	1.190	1.533	2.132	2.776	3.747	4.604
5	0.727	0.920	1.156	1.476	2.015	2.571	3.365	4.032
6	0.718	0.906	1.134	1.440	1.943	2.447	3.143	3.707
7	0.711	0.896	1.119	1.415	1.895	2.365	2.998	3.499
8	0.706	0.889	1.108	1.397	1.860	2.306	2.896	3.355
9	0.703	0.883	1.100	1.383	1.833	2.262	2.821	3.250
10	0.700	0.879	1.093	1.372	1.812	2.228	2.764	3.169
11	0.697	0.876	1.088	1.363	1.796	2.201	2.718	3.106
12	0.695	0.873	1.083	1.356	1.782	2.179	2.681	3.055
13	0.694	0.870	1.079	1.350	1.771	2.160	2.650	3.012
14	0.692	0.868	1.076	1.345	1.761	2.145	2.624	2.977
15	0.691	0.866	1.074	1.341	1.753	2.131	2.602	2.947
16	0.690	0.865	1.071	1.337	1.746	2.120	2.583	2.921
17	0.689	0.863	1.069	1.333	1.740	2.110	2.567	2.898
18	0.688	0.862	1.067	1.330	1.734	2.101	2.552	2.878
19	0.688	0.861	1.066	1.328	1.729	2.093	2.539	2.861
20	0.687	0.860	1.064	1.325	1.725	2.086	2.528	2.845
21	0.686	0.859	1.063	1.323	1.721	2.080	2.518	2.831
22	0.686	0.858	1.061	1.321	1.717	2.074	2.508	2.819
23	0.685	0.858	1.060	1.319	1.714	2.069	2.500	2.807
24	0.685	0.857	1.059	1.318	1.711	2.064	2.492	2.797
25	0.684	0.856	1.058	1.316	1.708	2.060	2.485	2.787
26	0.684	0.856	1.058	1.315	1.706	2.056	2.479	2.779
27	0.684	0.855	1.057	1.314	1.703	2.052	2.473	2.771
28	0.683	0.855	1.056	1.313	1.701	2.048	2.467	2.763
29	0.683	0.854	1.055	1.311	1.699	2.045	2.462	2.756
30	0.683	0.854	1.055	1.310	1.697	2.042	2.457	2.750
40	0.681	0.851	1.050	1.303	1.684	2.021	2.423	2.704
60	0.679	0.848	1.046	1.296	1.671	2.000	2.390	2.660
120	0.677	0.845	1.041	1.289	1.658	1.980	2.358	2.617
¥	0.674	0.842	1.036	1.282	1.645	1.960	2.326	2.576

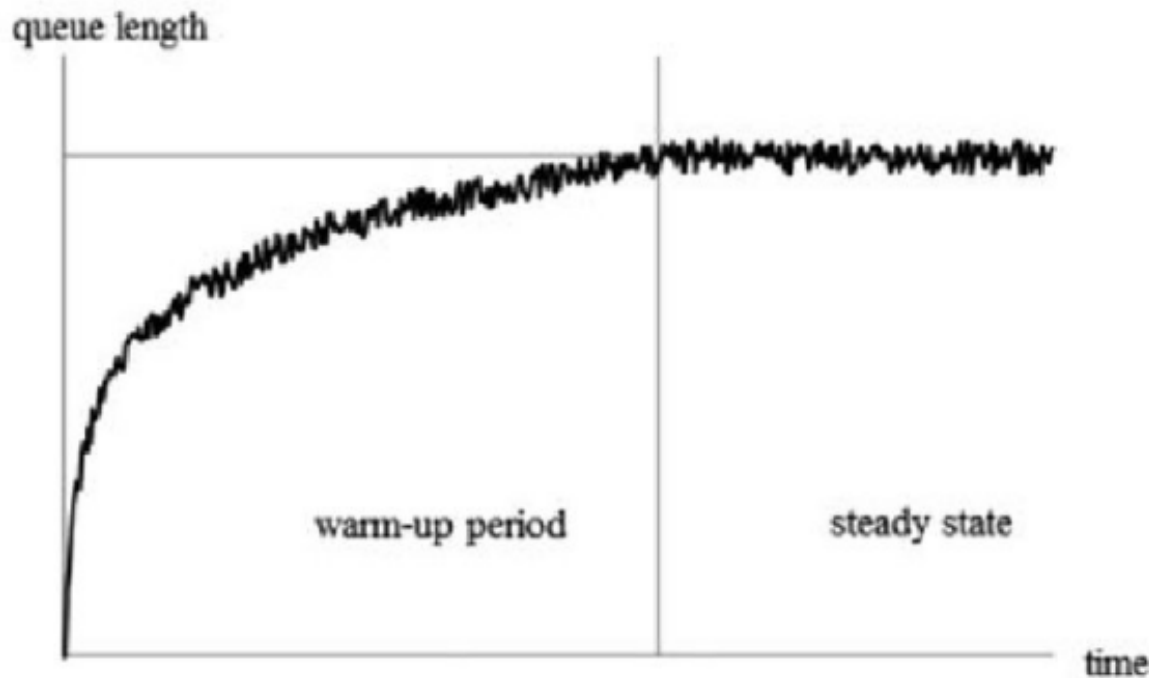
# Replications

Methods to execute the replications.

# Kind of simulations

- **Terminate simulations (for terminate systems):** Simulations where a condition defines the end of the execution. Usually time.
- **Non terminate simulations (for non terminate systems):** Simulations without this condition.

# Transient period

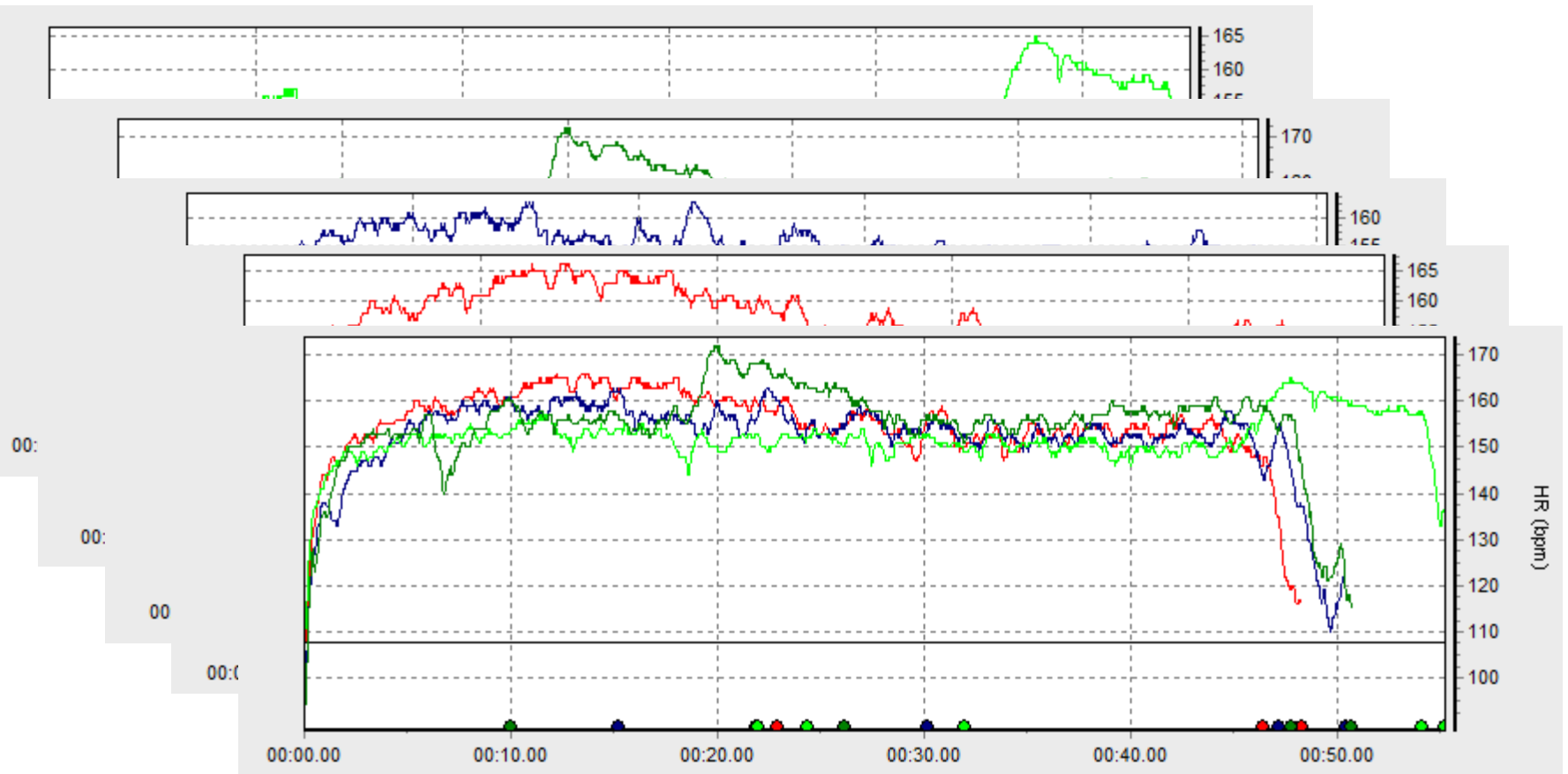


G. Chen and Z. Z. Yang, Methods for estimating vehicle queues at a marine terminal: A computational comparison. *Int. J. Appl. Math. Comput. Sci.* **24**, 611 (2014).

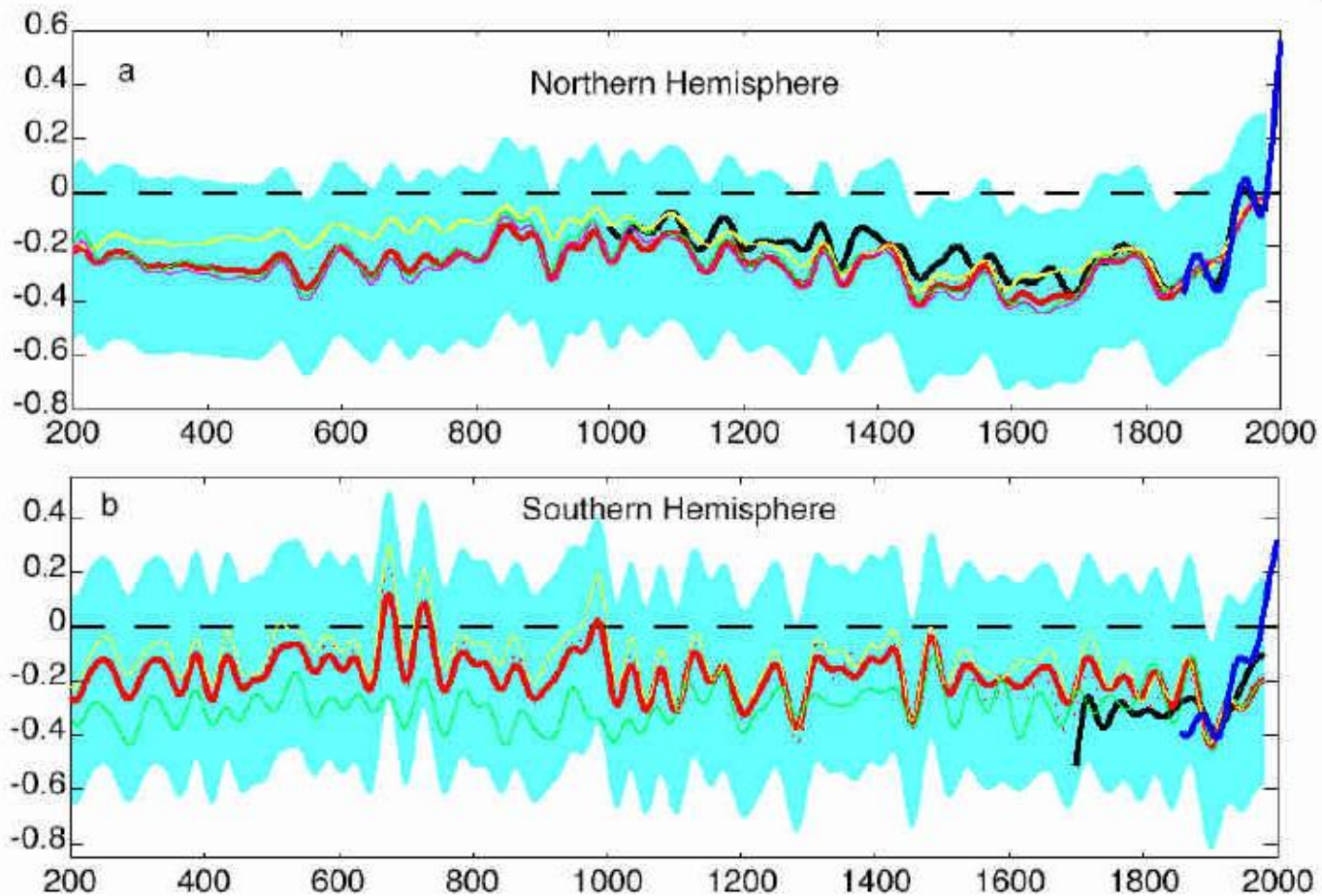
# Independent repetitions

- From the same initial state of the model, that means, with the same parameterizations and behavior, only random numbers to be used in the GAV are changed.
- This different RNG allows test again and again the new system with the different possible values of the variables that are not controlled (random variables).

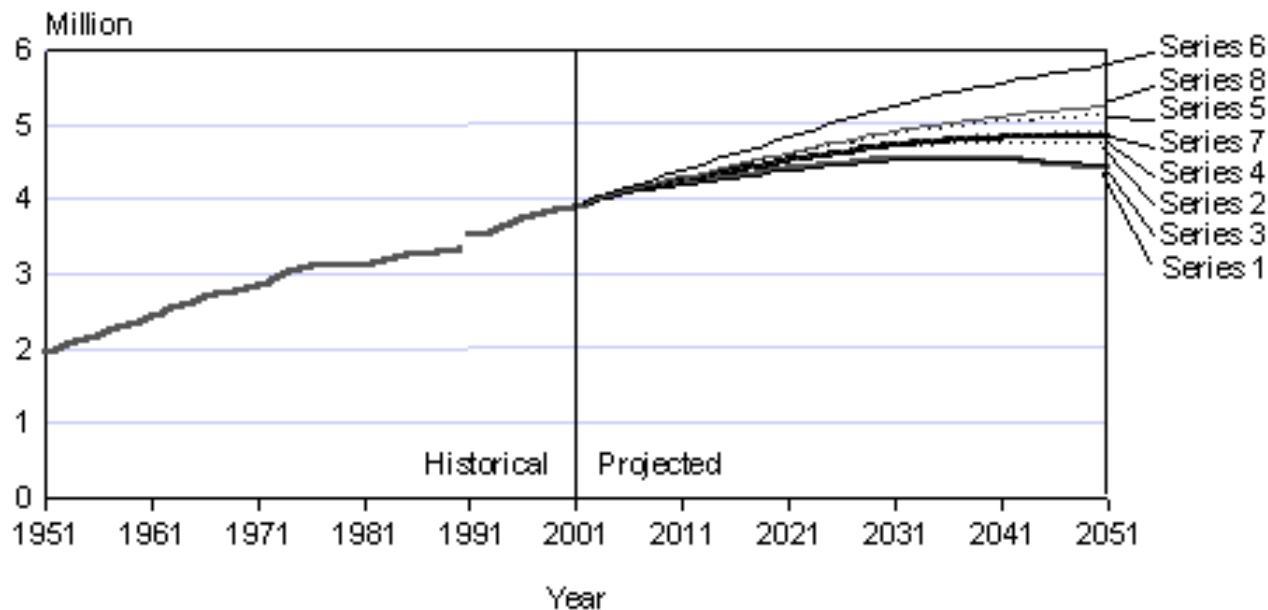
# Independent repetitions



# Independent repetitions



# Independent repetitions



**Note** The break in series between 1990 and 1991 denotes a change from the de facto population concept to the resident population concept.

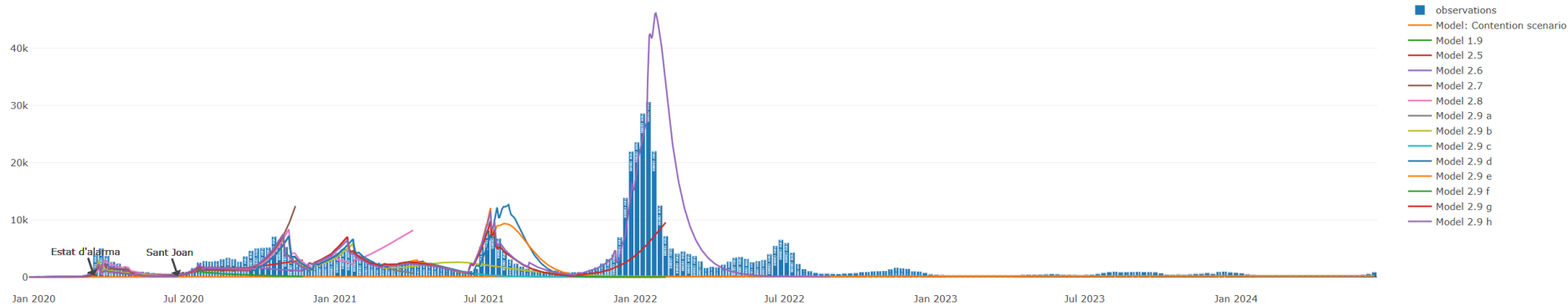


# Independent repetitions

## SDL-PAND KPIs Model actual

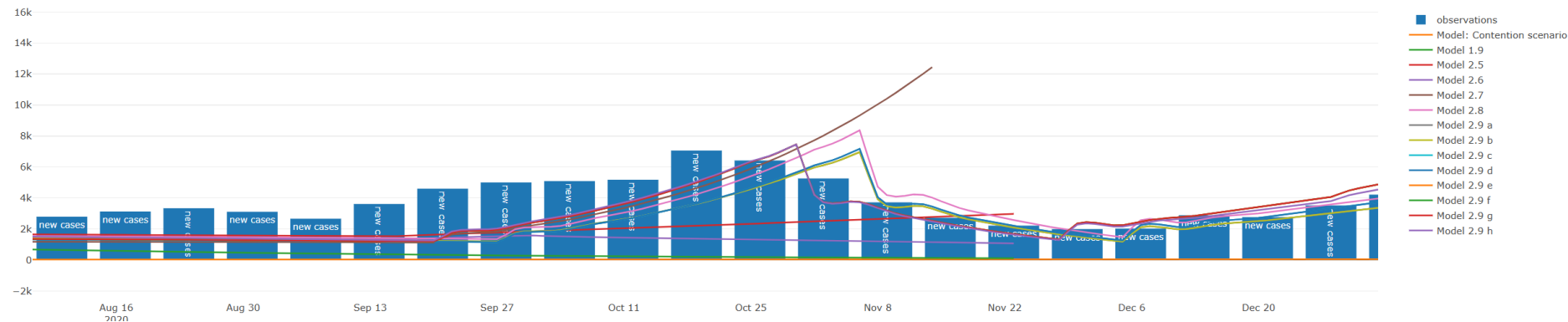
### Previous models

Here we have the models that we have been developing and that have been invalidated by the non-pharmaceutical actions applied to reduce the spread of the virus.



### Previous models

Here we have the models that we have been developing and that have been invalidated by the non-pharmaceutical actions applied to reduce the spread of the virus.



# Transient elimination

## □ Definitions:

- $k$ : number of deleted observations.
- $m$ : amount of observations in a single run.
- $n$ : amount of runs (replications).

# Transient elimination

- Step 1: Compute the average of the  $j$  observation's over all runs.
  - ▣  $\bar{x}_j = \frac{1}{m} \sum_{i=1}^m x_{i,j}$
- Step 2: Compute the overall average.
  - ▣  $\bar{\bar{x}} = \frac{1}{n} \sum_{j=1}^n \bar{x}_j$
- Step 3:  $K=1$

# Transient elimination

- Step 4: Compute the overall average of the  $j$  observation's over all runs without the first  $k$  observations.

- $\overline{x_{kj}} = \frac{1}{m-k} \sum_{i=k+1}^m x_{i,j}$   $\overline{\overline{x_k}} = \frac{1}{n} \sum_{j=1}^n \overline{x_{kj}}$

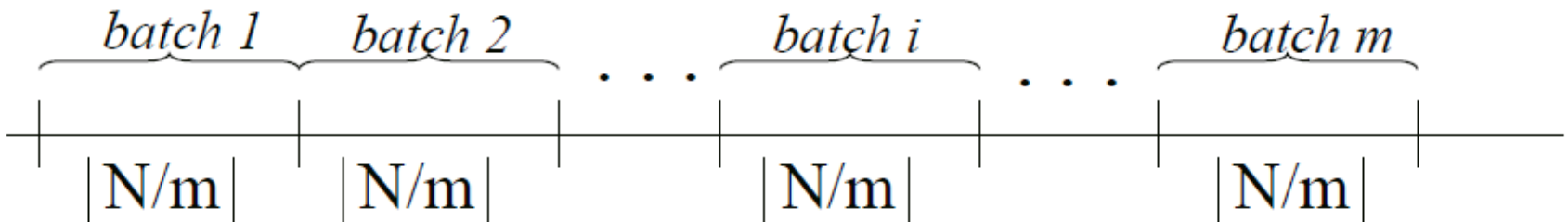
- Step 5: Calculate the relative change

- $\Delta_k = \frac{\overline{\overline{x_k}} - \overline{\overline{x}}}{\overline{\overline{x}}}$

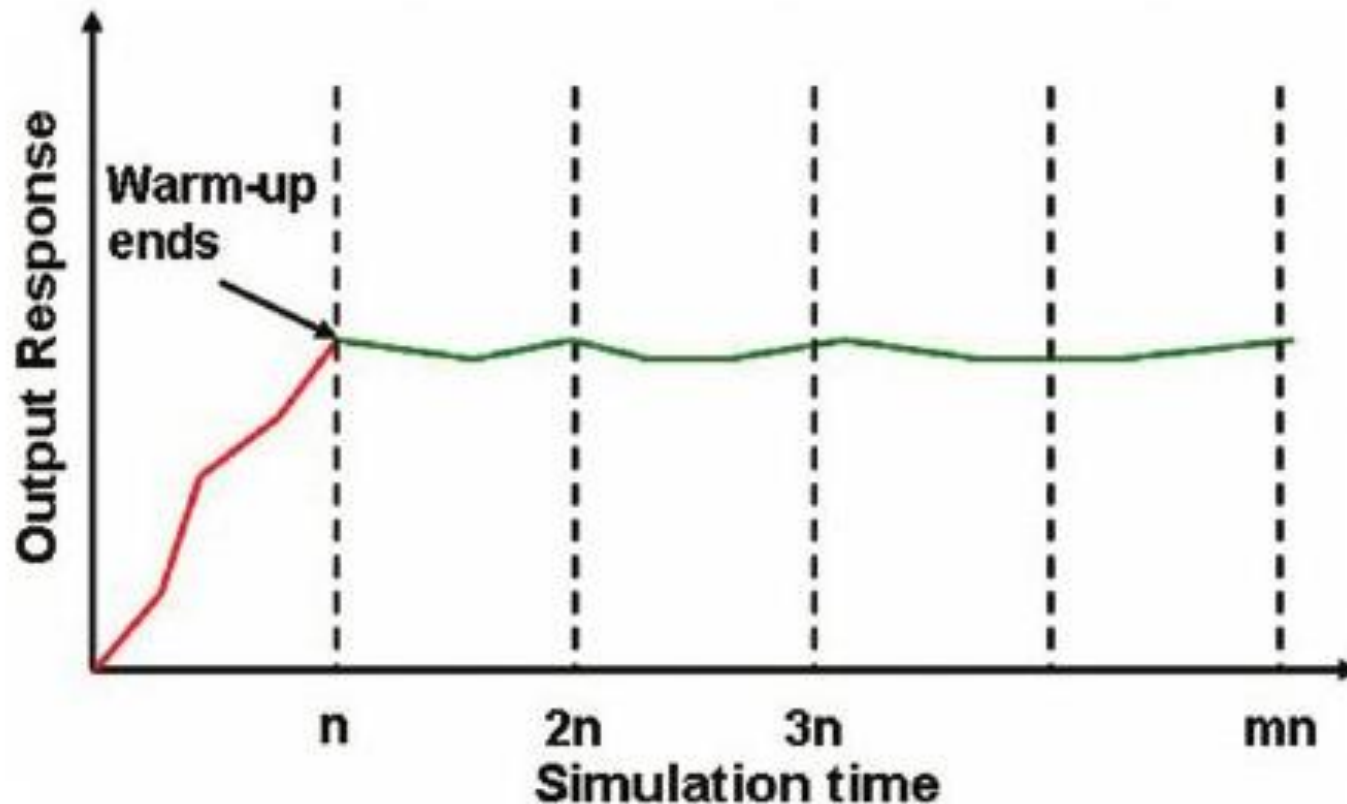
- If  $|\Delta_k - \Delta_{k-1}| > \text{threshold}$  then increment  $k$  and go to step 4, else remove  $k$  observations and use

# Batch means

- Execute a long simulation and then divide it in different blocks, or execution bags “batches”.
  - ▣ We work with the mean values of these observations.
  - ▣ The size of the “batches” is  $n = \lfloor N/m \rfloor$
- Each one of these observations are considered as independent.
- Is desirable to determine what must be the required long of each one of these execution blocks, to assure the correctness of the experiment.



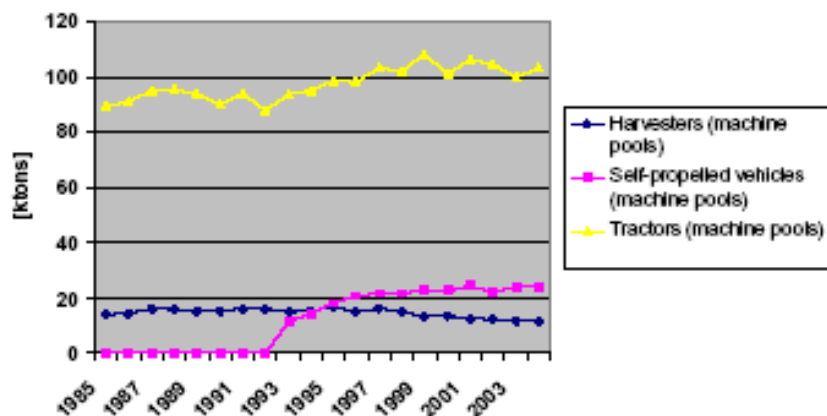
# Batch means



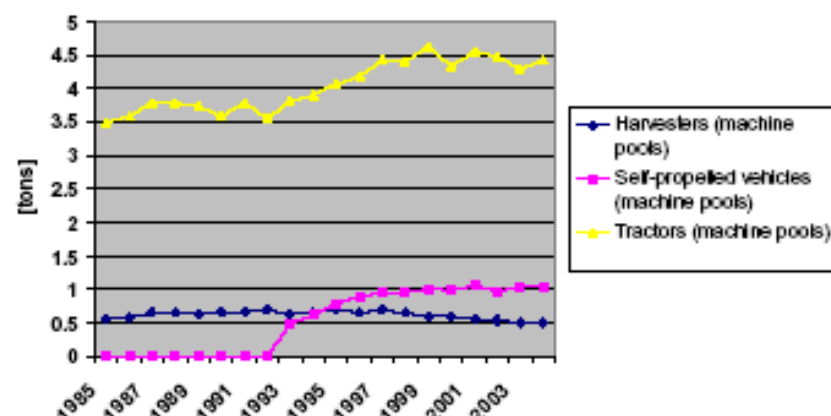
G. Chen and Z. Z. Yang, A review of techniques for the analysis of simulation output, *Int. J. Appl. Math. Comput. Sci.* **24**, 611 (2014).

# Batch means

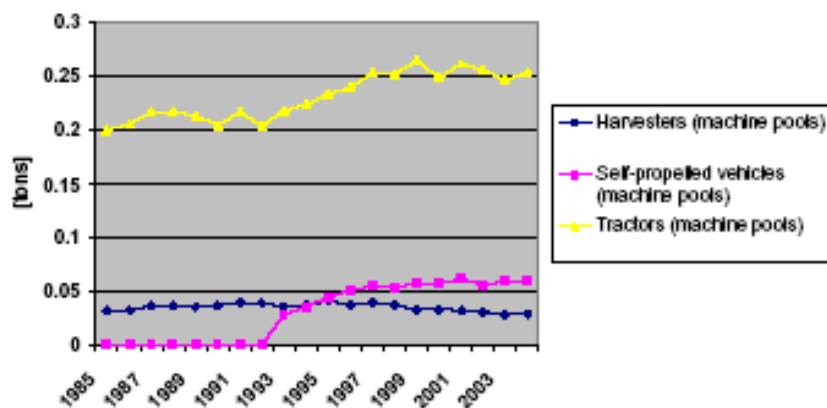
CO<sub>2</sub> emissions



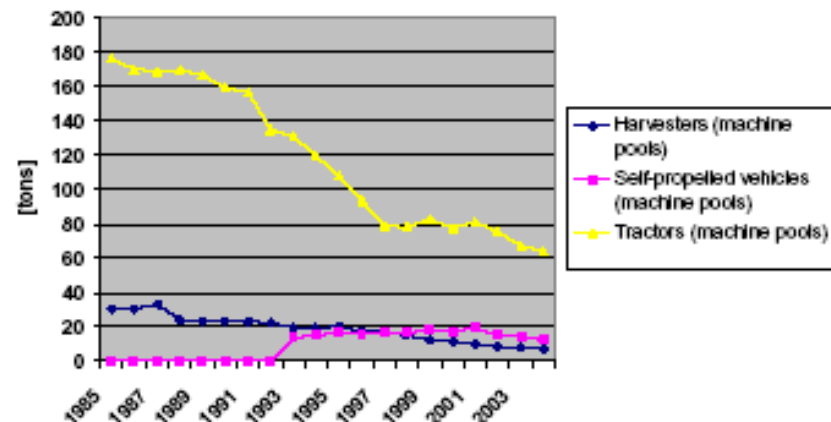
N<sub>2</sub>O emissions



NH<sub>3</sub> emissions



TSP emissions



# Transient elimination

- Step 1: Set  $n=2$
- Step 2: Compute the average of the “i” batch.
  - ▣  $\bar{x}_i = \frac{1}{n} \sum_{j=1}^n x_{i,j}$
- Step 3: Compute the overall average.
  - ▣  $\bar{\bar{x}} = \frac{1}{m} \sum_{i=1}^m \bar{x}_i$
- Step 4: Compute the variance of the batch means.
  - ▣  $Var(\bar{x}) = \frac{1}{m-1} \sum_{i=1}^m (\bar{x}_i - \bar{\bar{x}})^2$

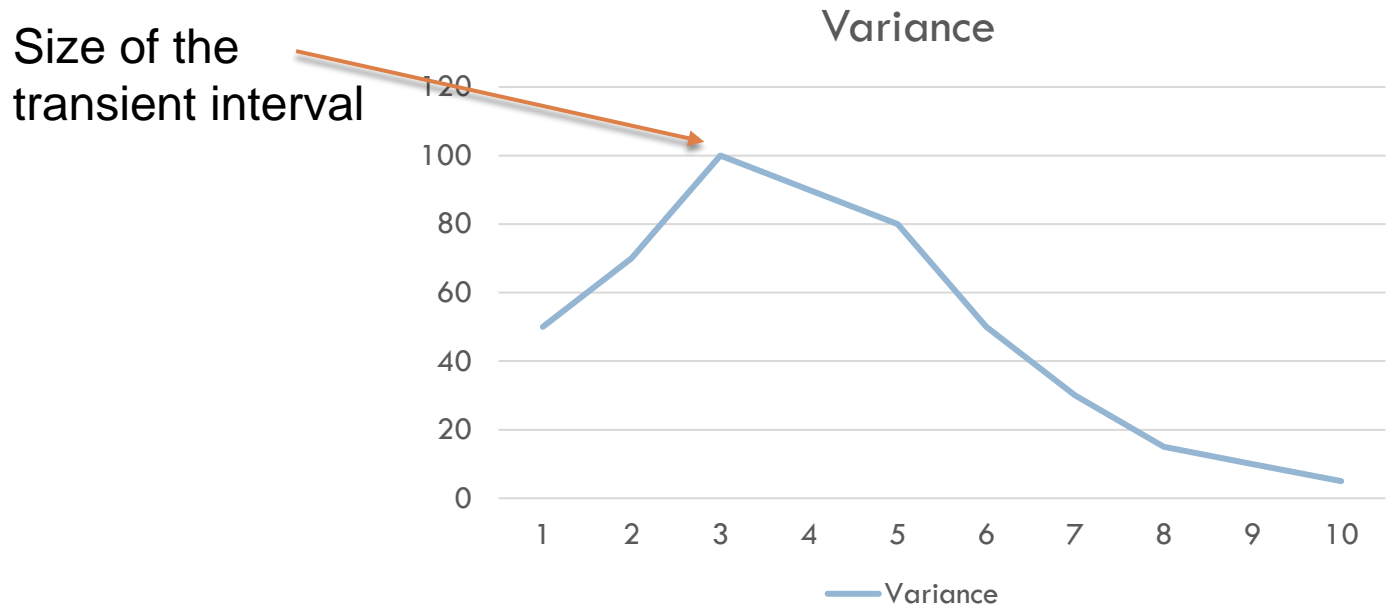
Definitions:

n: amount of observations in a single run.  
m: amount of runs (replications).



# Transient elimination

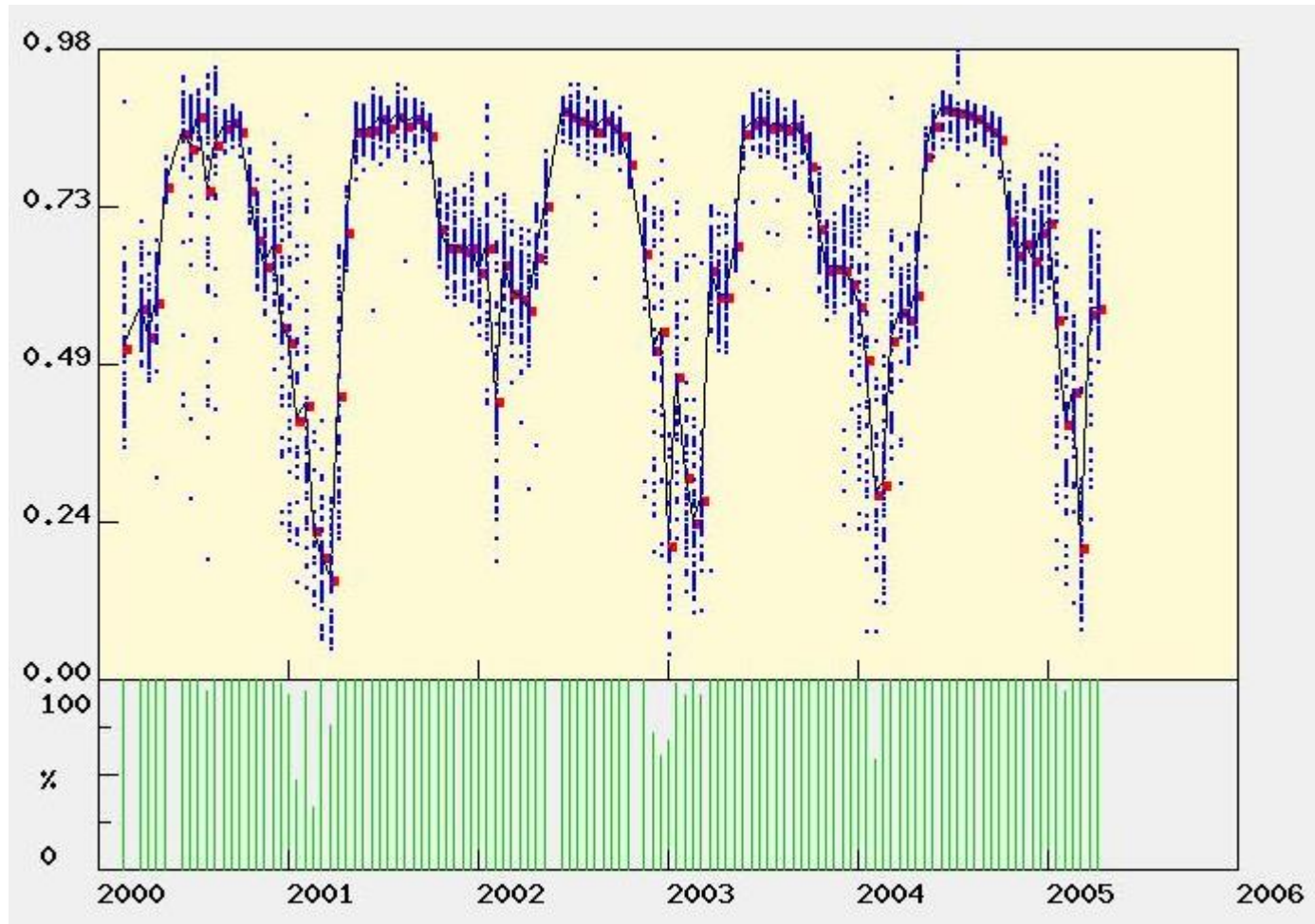
- Step 5: Increase  $n$  by 1 and go to step 2 and plot the variance as a function of  $n$ . The point at which the variance starts to decrease is the length of the transient interval.



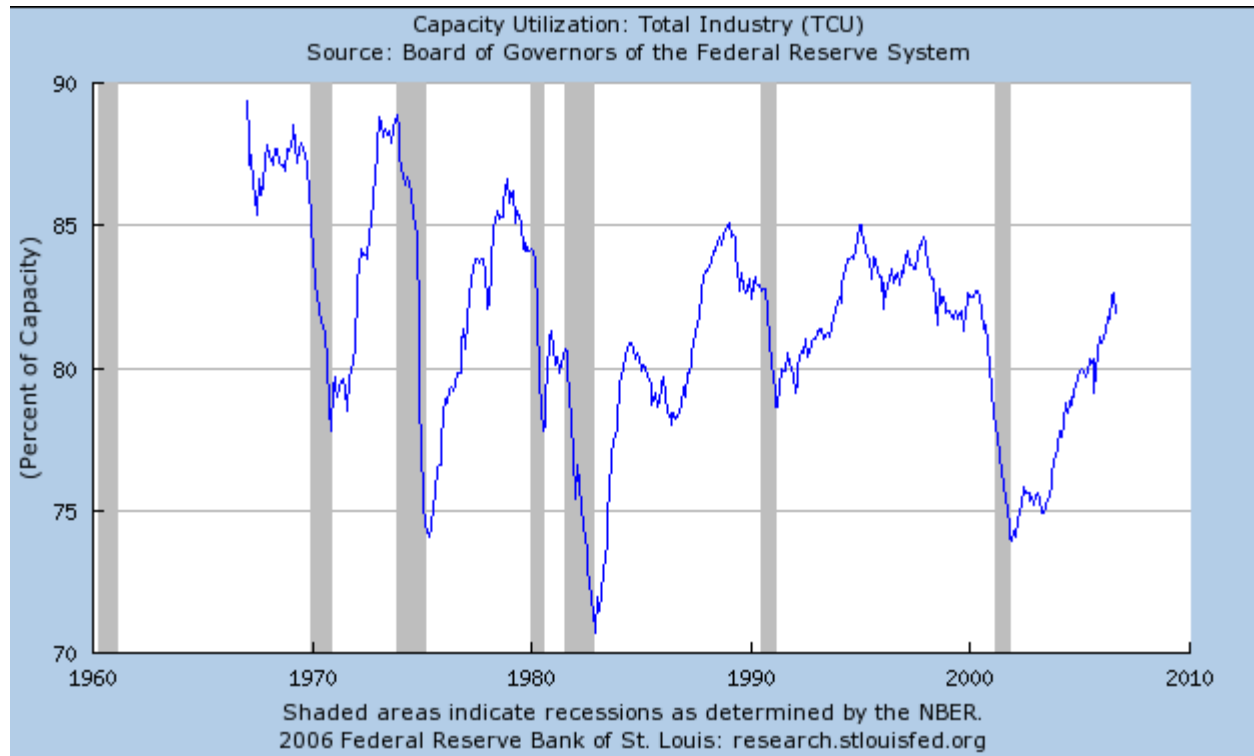
# Regenerative methods

- If the variables observed in the execution of the simulation model, represents, in some way a cyclical restart, that allows suppose the existence of cycles (in the life of the variable). Is likely to consider each one of theses cycles as a replication
- This method is not always applicable. Depends on the existence of cycles in the variables. Also the longitude of this replications must be small; if the longitude of this cycles is big we obtain a small sum of replications.

# Regenerative methods

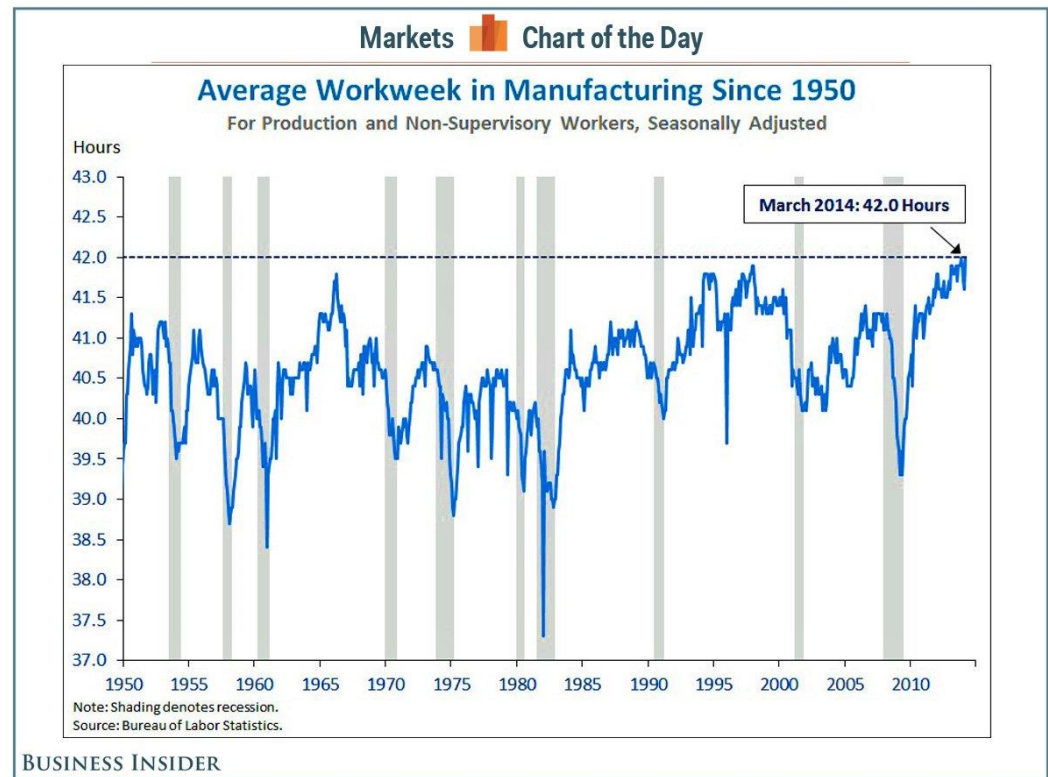


# Regenerative methods



# Regarding the chart

- Nobel laureate and Yale University economist Robert Shiller is in the camp of experts who believe the odds of a recession are very low.
- Read more: <http://www.businessinsider.com/shiller-chart-shows-why-recession-is-years-away-2014-4#ixzz30lcrlnl2>



# Regenerative methods

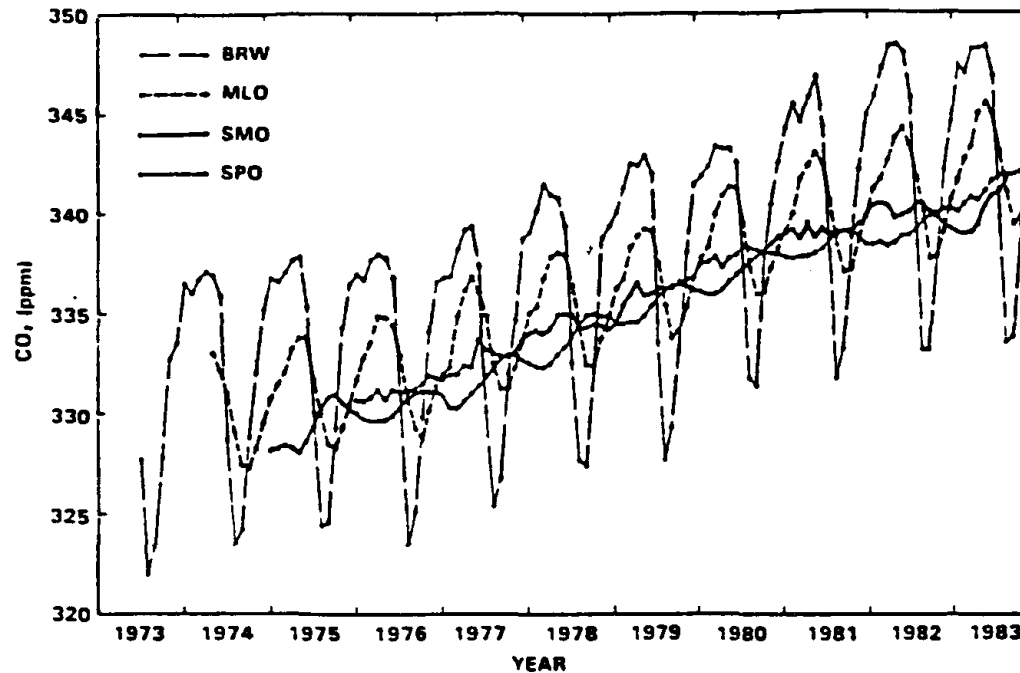


Fig. 1. Selected monthly mean carbon dioxide concentrations from continuous measurements (Barrow, Alaska (BRW); Mauna Loa, Hawaii (MLO); American Samoa (SMO); South Pole (SPO). From: WMO, 1985.

# Applicability

	Terminating simulations	Nonterminating simulations
Loading period needed	Independent repetitions	Independent repetitions
Loading period unneeded	Independent repetitions erasing the loading period/ Batch means	Batch means



# Variance reduction techniques

Reduce the number of replications



# Motivation

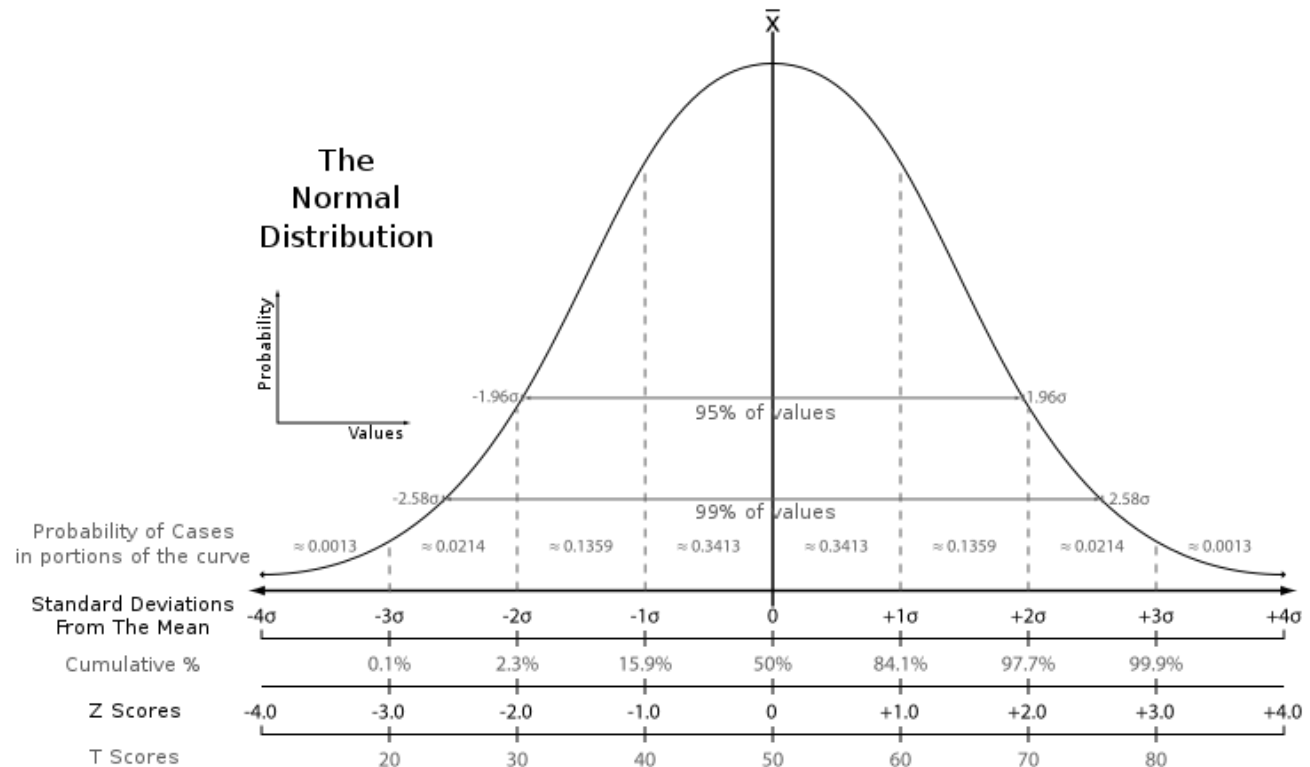
- Interest to reduce the variability introduced in the answer variable due to the use of RNG.
- The value that estimates a specific answer variable, that is represented by its confidence interval, must be adjusted (as possible).

$$\left( \bar{x} - k \frac{s}{\sqrt{n}}, \bar{x} + k \frac{s}{\sqrt{n}} \right)$$

# Motivation

- Obviously, increasing  $n$ , that is the number of observations, the standard error decreases. Variance reduction techniques try to reduce this variability without the need of increase the number of observations.

$$\frac{s}{\sqrt{n}}$$



# Antithetic variables

- Use of antithetic values o the random numbers stream used.
- In the first execution the random numbers used can be  $(a, b, c, ..) \in [0,1)$ .
- In the second execution we use its antithetic values, that means  $(1-a, 1-b, 1-c, ..) \in [0,1)$ .
- Is needed to establish a synchronization method between both streams

# Control variables

- Simulation allows the observation of the system evolution during the execution of the experiment.
- This allows, in certain grade, to compare the values of the answer variables with the observed values.
- We can add modification to the model to reduce the difference.



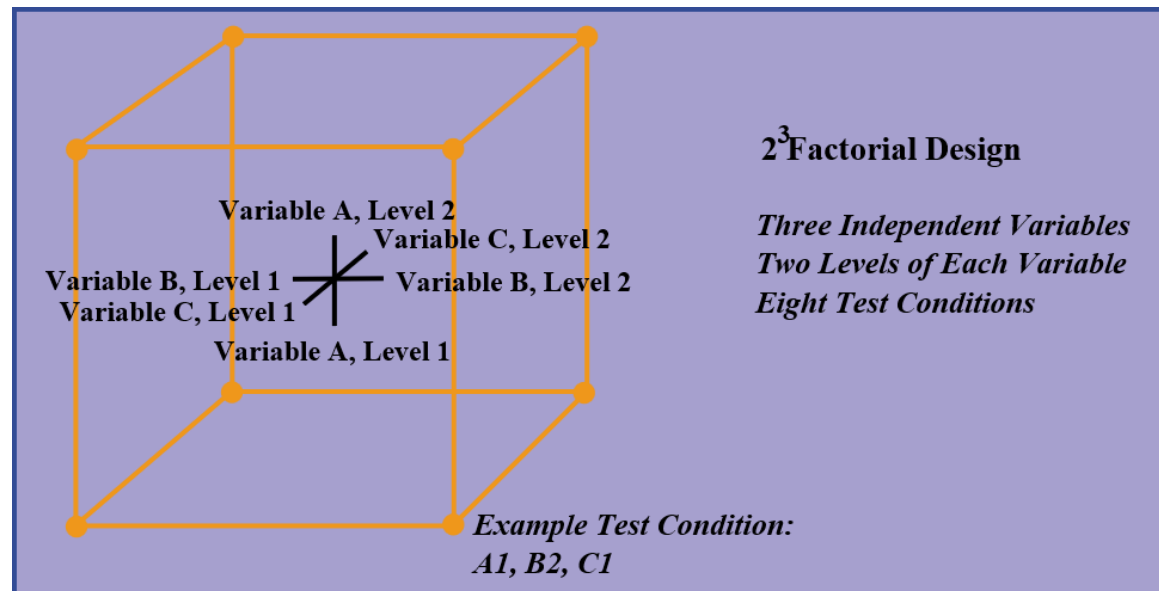
# Fractional factorial design

# Fractional factorial design

- A factorial experiment in which only an **adequately chosen fraction** of the treatment combinations (scenarios) required for the complete factorial experiment **is selected to be run**.

# A $2^{3-1}$ design (half of a $2^3$ )

- Consider the two-level, full factorial design for three factors, namely the  $2^3$  design. This implies eight runs (not counting replications or center points).



# $2^3$ Two-level, Full Factorial Design

	X1	X2	X3	Y
1	-1	-1	-1	$y_1 = 33$
2	+1	-1	-1	$y_2 = 63$
3	-1	+1	-1	$y_3 = 41$
4	+1	+1	-1	$y_4 = 57$
5	-1	-1	+1	$y_5 = 57$
6	+1	-1	+1	$y_6 = 51$
7	-1	+1	+1	$y_7 = 59$
8	+1	+1	+1	$y_8 = 53$

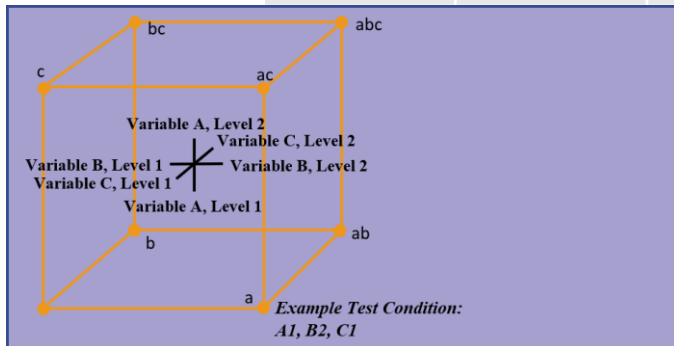


# Computing the effects

- Effect of  $X_1 = (1/4)(y_2 + y_4 + y_6 + y_8) - (1/4)(y_1 + y_3 + y_5 + y_7)$
- $X_1 = (1/4)(63+57+51+53) - (1/4)(33+41+57+59) = 8.5$
- Suppose, however, that we only have enough resources to do four runs. It is still possible to estimate the main effect for  $X_1$ ? Or any other main effect?
  - ▣ The answer is yes, and there are even different choices of the four runs that will accomplish this.

# Only 4 runs

		C1	C2	C3	Y
Y1	1	-1	-1	-1	$y_1 = 33$
Y2	2	+1	-1	-1	$y_2 = 63$
Y3	3	-1	+1	-1	$y_3 = 41$
Y4	4	+1	+1	-1	$y_4 = 57$
Y5	5	-1	-1	+1	$y_5 = 57$
Y6	6	+1	-1	+1	$y_6 = 51$
Y7	7	-1	+1	+1	$y_7 = 59$
Y8	8	+1	+1	+1	$y_8 = 53$



$$C1 = \frac{y_4 + y_6}{2} - \frac{y_1 + y_7}{2}$$

$$C2 = \frac{y_4 + y_7}{2} - \frac{y_1 + y_6}{2}$$

# Main effects

## □ C1 main effect:

- $c1 = (1/2) (y4 + y6) - (1/2) (y1 + y7)$

- $c1 = (1/2) (57+51) - (1/2) (33+59) = 8$

## □ C2 main effect

- $c2 = (1/2) (y4 + y7) - (1/2) (y1 + y6)$

- $c2 = (1/2) (57+59) - (1/2) (33+51) = 16$

## □ C3 main effect

- $c3 = (1/2) (y6 + y7) - (1/2) (y1 + y4)$

- $c3 = (1/2) (51+59) - (1/2) (33+57) = 10$

# Selecting the experiments to execute

- Note that, mathematically,  $2^{3-1} = 2^2$

	X1	X2
1	-	-
2	+	-
3	-	+
4	+	+

# Adding the column of the interactions

- We add a new column that represents the interactions between X1 and X2

	X1	X2	X1*X2
1	-	-	+
2	+	-	-
3	-	+	-
4	+	+	+

# Adding the column for the new factor

- Now we can substitute this new column for X3

	X1	X2	X3
1	-	-	+
2	+	-	-
3	-	+	-
4	+	+	+

# Example

- We have 4 factors P, T, D, E.
- $2^4$ .
- We want to perform at maximum 8 experiments.

# Example

	P	T	D	$E=P*T$
1	-	-	-	+
2	+	-	-	-
3	-	+	-	-
4	+	+	-	+
5	-	-	+	+
6	+	-	+	-
7	-	+	+	-
8	+	+	+	+



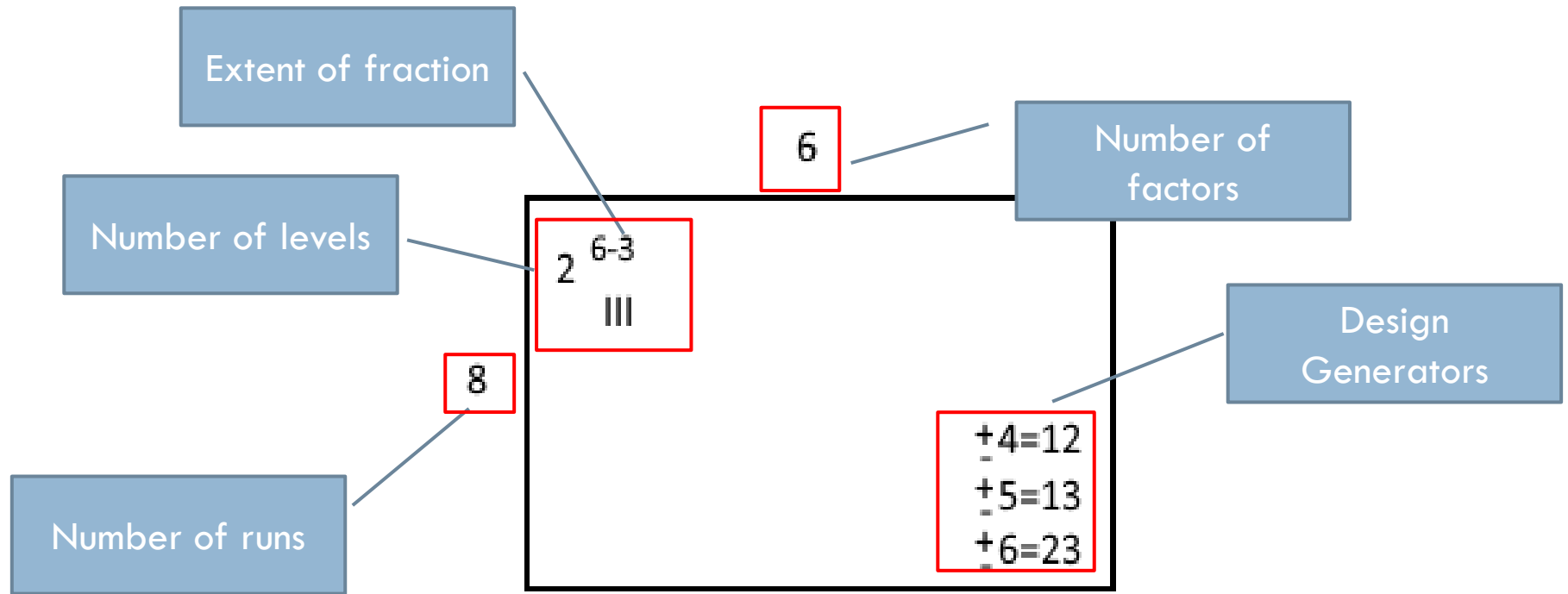
# Confounding

- A confounding design is one where some treatment effects (main or interactions) are estimated by the same linear combination of the experimental observations as some blocking effects.

# The price

- One price we pay for using the design table column  $X1 * X2$  to obtain column  $X3$  is, clearly, our **inability** to obtain an **estimate of the interaction effect** for  $X1 * X2$  (i.e.,  $c12$ ) that is separate from an estimate of the main effect for  $X3$ .
- We have **confounded** the **main effect** estimate for factor  $X3$  (i.e.,  $c3$ ) with the **estimate of the interaction effect** for  $X1$  and  $X2$  (i.e., with  $c12$ )

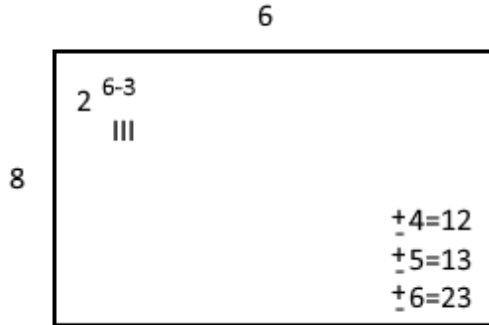
# Definition of the experiment



# Construct a Fractional Factorial Design From the Specification

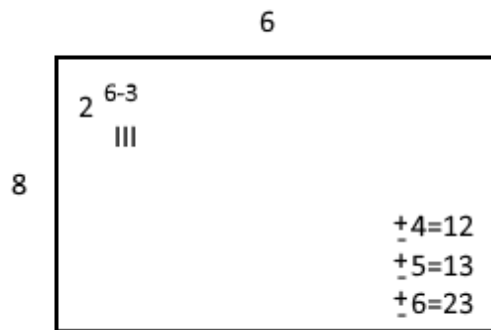
- **Write down a full factorial design** in standard order for  $k-p$  factors ( $6-3 = 3$  factors for the example above). In the specification above we start with a  $2^3$  full factorial design. Such a design has  $2^3 = 8$  rows.
- **Add a fourth column** to the design table for factor 4, using  $4 = 12$  to manufacture it (i.e., create the new column by multiplying the indicated old columns together).
- **Do likewise** for factor 5 and for factor 6, using the appropriate design generators.
- The resultant design matrix gives the **8 trial runs** for an 6-factor fractional factorial design.

# Example: $2^{6-3}$



X1	X2	X3	X4	X5	X6
-1	-1	-1			
1	-1	-1			
-1	1	-1			
1	1	-1			
-1	-1	1			
1	-1	1			
-1	1	1			
1	1	1			

# Example: $2^{6-3}$



X1	X2	X3	X4	X5	X6
-1	-1	-1	1	1	1
1	-1	-1	-1	-1	1
-1	1	-1	-1	1	-1
1	1	-1	1	-1	-1
-1	-1	1	1	-1	-1
1	-1	1	-1	1	-1
-1	1	1	-1	-1	1
1	1	1	1	1	1

# Resolution

- The length of the shortest word in the defining relation is called the resolution of the design.
- Resolution describes the degree to which estimated main effects are confounded (or aliased) with estimated 2-level interactions, 3-level interactions, etc.
- Resolution is added as a Roman numeral to the experiment definition.

	Ability	Example
I	Not useful: an experiment of exactly one run only tests one level of a factor and hence can't even distinguish between the high and low levels of that factor	$2^1 - 1$ with defining relation $I = A$
II	Not useful: main effects are confounded with other main effects	$2^2 - 1$ with defining relation $I = AB$
III	Estimate main effects, but these may be confounded with two-factor interactions	$2^3 - 1$ with defining relation $I = ABC$
IV	Estimate main effects unconfounded by two-factor interactions Estimate two-factor interaction effects, but these may be confounded with other two-factor interactions	$2^4 - 1$ with defining relation $I = ABCD$
V	Estimate main effects unconfounded by three-factor (or less) interactions Estimate two-factor interaction effects unconfounded by two-factor interactions Estimate three-factor interaction effects, but these may be confounded with other two-factor interactions	$2^5 - 1$ with defining relation $I = ABCDE$
VI	Estimate main effects unconfounded by four-factor (or less) interactions Estimate two-factor interaction effects unconfounded by three-factor (or less) interactions Estimate three-factor interaction effects, but these may be confounded with other three-factor interactions	$2^6 - 1$ with defining relation $I = ABCDEF$



# Selection

Número de factores, k	Fracción	Número de combinaciones	Generadores de diseño
3	$2^{3-1}$	4	C=AB
4	$2^{4-1}$	8	D=ABC
5	$2^{5-1}$	16	E=ABCD
	$2^{5-2}$	8	D=AB      E=AC
6	$2^{6-1}$	32	F=ABCDE
	$2^{6-2}$	16	E=ABC      F=BCD
	$2^{6-3}$	8	D=AB      F=BC
			E=AC
7	$2^{7-1}$	64	G=ABCDEF
	$2^{7-2}$	32	F=ABCD      G=ABDE
	$2^{7-3}$	16	E=ABC      G=ACD
			F=BCD
	$2^{7-4}$	8	D=AB      F=BC E=AC      G=ABC
8	$2^{8-2}$	64	G=ABCD      H=ABEF
	$2^{8-3}$	32	F=ABC      H=BCDE
			G=ABD
	$2^{8-4}$	16	E=BCD      G=ABC F=ACD      H=ABD
9	$2^{9-2}$	128	H=ACDFG      J=BCEFG
	$2^{9-3}$	64	G=ABCD      J=CDEF
			H=ACEF
	$2^{9-4}$	32	F=BCDE      H=ABDE
			G=ACDE      J=ABCE
	$2^{9-5}$	16	E=ABC      H=ABD F=BCD      J=ABCD G=ACD



# Example

- We have a limited budget to analyze the different factors to consider on our model. Each individual experiment costs 100€ and we have a total budget of 20.000€ to be destined to experimentation. Define an experiment design, with this constraint, considering that we need at least 3 replications for each experiment.

GORE	C1: BUSH	C2: BUCHANAN	C3: NADER	C4: BROWNE	C5: HAGELIN	C6: HARRIS	C7: MCREYNOLDS	C8: MOOREHEAD	C9: PHILLIPS
ALACHUA	47300	34062	262	3215	658	42	4	658	21
BAKER	2392	5610	73	53	17	3	0	0	3
BAY	18850	38637	248	828	171	18	5	3	37
BRADFORD	3072	5413	65	84	28	2	0	0	3
BREVARD	97318	115185	570	4470	643	39	11	11	76

More than 100 cases...

# Answer

- We consider that GORE categorical variable are not going to be used on our analysis.
- Assuming that we can spend all the budget in an initial experimentation without considering the possible inconvenient that can appear due to possible high variability of certain variables (that lead us to increase the number of needed replications that is initial considered by 3), the maximum amount of experiment is 64:
  - ▣  $64 \text{ experiment} * 3 \text{ replications} * 100\text{€} = 19200\text{€}$

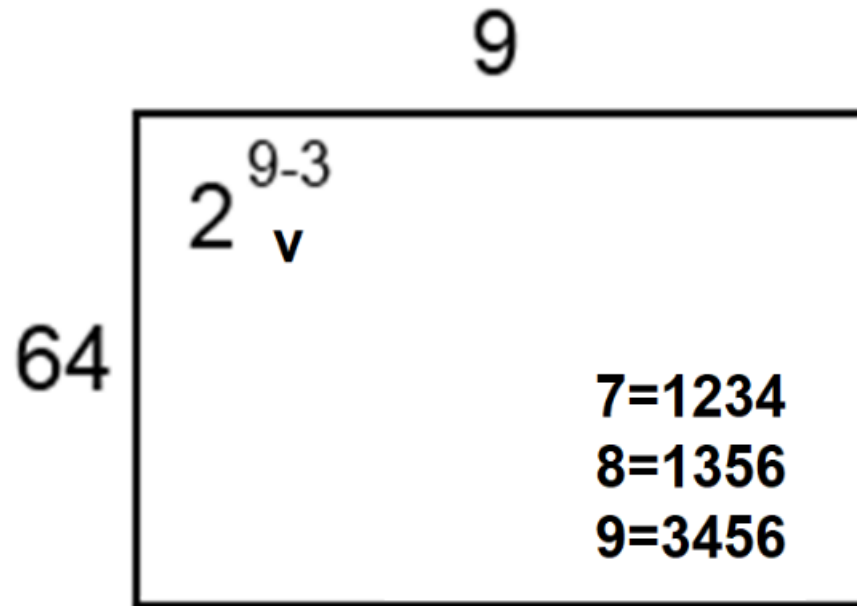
# Answer

- This design don't allow a complete experimentation considering all the factors we have on our model, we have 9 factors that implies a  $2^9$  experiments meaning 512 experiments with 3 replications each one of them.
- This implies that we need to reduce the amount of variables to be considered using a fractional factorial design.

# Answer

- To do this it is needed to define a confounding pattern and select those factors that are going to be confounded.
- The design will be defined as:
  - ▣  $2^{9-3}$
- Hence 3 confounding patterns must be defined.
- We select in our case the last three variables to be confounded using the first 6 variables.

# Answer





# Plackett-Burman designs

# Plackett-Burman designs

- In 1946, R.L. Plackett and J.P. Burman published their now famous paper "The Design of Optimal Multifactorial Experiments" in *Biometrika* (vol. 33). This paper described the construction of very economical designs with the run number a multiple of four (rather than a power of 2).
- Plackett-Burman designs are very efficient screening designs when only main effects are of interest.



# Plackett and Burman designs (1946)

- Effects of main factors only
  - ▣ Logically minimal number of experiments to estimate effects of  $m$  input parameters (factors)
  - ▣ Ignores interactions
- Requires  $O(m)$  experiments
  - ▣ Instead of  $O(2^m)$  or  $O(v^m)$

# Plackett and Burman Designs

- PB designs exist only in sizes that are multiples of 4
- Requires  $X$  experiments for  $m$  parameters
  - ▣  $X = \text{next multiple of } 4 \geq m$
- PB design matrix
  - ▣ Rows = configurations
  - ▣ Columns = factor's values in each configuration
    - High/low = +1 / -1
  - ▣ First row = from P&B paper
  - ▣ Subsequent rows = circular right shift of preceding row
  - ▣ Last row = all (-1)

# Plackett and Burman Designs

- PB designs also exist for 20-run, 24-run, and 28-run (and higher) designs.
- With a 20-run design you can run a screening experiment for up to 19 factors, up to 23 factors in a 24-run design, and up to 27 factors in a 28-run design.

# PB Design Matrix

Config	Input Parameters (factors)							Response
	A	B	C	D	E	F	G	
1	+1	+1	+1	-1	+1	-1	-1	
2	-1	+1	+1	+1	-1	+1	-1	
3	-1	-1	+1	+1	+1	-1	+1	
4	+1	-1	-1	+1	+1	+1	-1	
5	-1	+1	-1	-1	+1	+1	+1	
6	+1	-1	+1	-1	-1	+1	+1	
7	+1	+1	-1	+1	-1	-1	+1	
8	-1	-1	-1	-1	-1	-1	-1	
Effect								

# PB Design Matrix

Config	Input Parameters (factors)							Response
	A	B	C	D	E	F	G	
1	+1	+1	+1	-1	+1	-1	-1	10
2	-1	+1	+1	+1	-1	+1	-1	12
3	-1	-1	+1	+1	+1	-1	+1	3
4	+1	-1	-1	+1	+1	+1	-1	5
5	-1	+1	-1	-1	+1	+1	+1	6
6	+1	-1	+1	-1	-1	+1	+1	5
7	+1	+1	-1	+1	-1	-1	+1	8
8	-1	-1	-1	-1	-1	-1	-1	9
Effect								

# PB Design Matrix

Config	Input Parameters (factors)							Response
	A	B	C	D	E	F	G	
1	+1	+1	+1	-1	+1	-1	-1	10
2	-1	+1	+1	+1	-1	+1	-1	12
3	-1	-1	+1	+1	+1	-1	+1	3
4	+1	-1	-1	+1	+1	+1	-1	5
5	-1	+1	-1	-1	+1	+1	+1	6
6	+1	-1	+1	-1	-1	+1	+1	5
7	+1	+1	-1	+1	-1	-1	+1	8
8	-1	-1	-1	-1	-1	-1	-1	9
Effect	-0,5							

$$-0.5 = (+1(10) + 1(5) + 1(5) + 1(8))/4 - (-1(12) + -1(3) + -1(6) + -1(6))/4$$

# PB Design Matrix

Config	Input Parameters (factors)							Response
	A	B	C	D	E	F	G	
1	+1	+1	+1	-1	+1	-1	-1	10
2	-1	+1	+1	+1	-1	+1	-1	12
3	-1	-1	+1	+1	+1	-1	+1	3
4	+1	-1	-1	+1	+1	+1	-1	5
5	-1	+1	-1	-1	+1	+1	+1	6
6	+1	-1	+1	-1	-1	+1	+1	5
7	+1	+1	-1	+1	-1	-1	+1	8
8	-1	-1	-1	-1	-1	-1	-1	9
Effect	-0,5	3,5	0,5	-0,5	-2,5	-0,5	-3,5	

# PB Design

- Magnitude of effect is important, sign is meaningless.
- In the previous example (from most important to least important effects): B, G, E, A, C, D and F.



[illegible]

Plackett RL and Burman J . P. (1946). THE DESIGN OF OPTIMUM MULTIFACTORIAL EXPERIMENTS Design of optimum multifactorial experiments Suppose also that the extreme value of  $x_i$  under consideration is  $x_i^*$ . Then the main effect of  $x_i$  is  $\frac{1}{2}(y_i^* - y_i)$ . *Biometrika*, 33(4), 305–325.

# Example

- A statistical approach to the experimental design of the sulfuric acid leaching of gold-copper ore.
- [http://www.scielo.br/scielo.php?script=sci\\_arttext&pid=S0104-663220030003000010](http://www.scielo.br/scielo.php?script=sci_arttext&pid=S0104-663220030003000010)

# Our factors



**Table 4: Mineralogical analysis of transition ore sample and sulfuric acid leach residue**

Minerals	Molecular formulae	Assay (%)	
		Transition ore	Leach residue
Native Cu	Cu	0.39	0.30
Chalcopyrite	CuFeS <sub>2</sub>	r	r
Bornite	Cu <sub>5</sub> FeS <sub>4</sub>	r	r
Chalcocite	Cu <sub>2</sub> S	rr	rr
Covelite	CuS	rr	rr
Cuprite	Cu <sub>2</sub> O	t	-
Malachite	Cu <sub>2</sub> (CO <sub>3</sub> )(OH) <sub>2</sub>	t	-
Goethite/Limonite	HFeO <sub>2</sub> /Fe <sub>2</sub> O <sub>3</sub> .H <sub>2</sub> O	26	21
Iron oxide	Fe <sub>2</sub> O <sub>3</sub> , Fe <sub>3</sub> O <sub>4</sub>	8	7
Clorite	(Mg,Al,Fe) <sub>12</sub> [(Si,Al) <sub>8</sub> O <sub>20</sub> ](OH) <sub>16</sub>	33	35
Quartz	SiO <sub>2</sub>	26	33

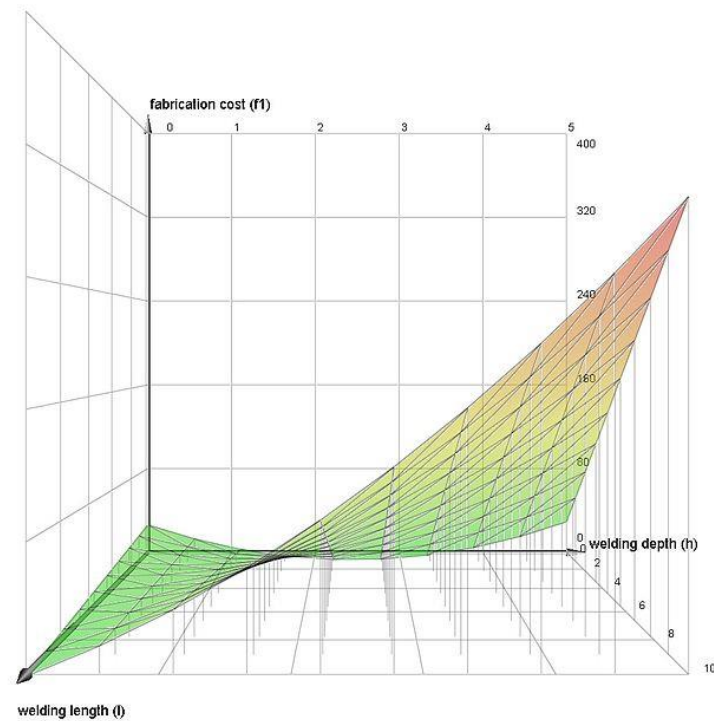
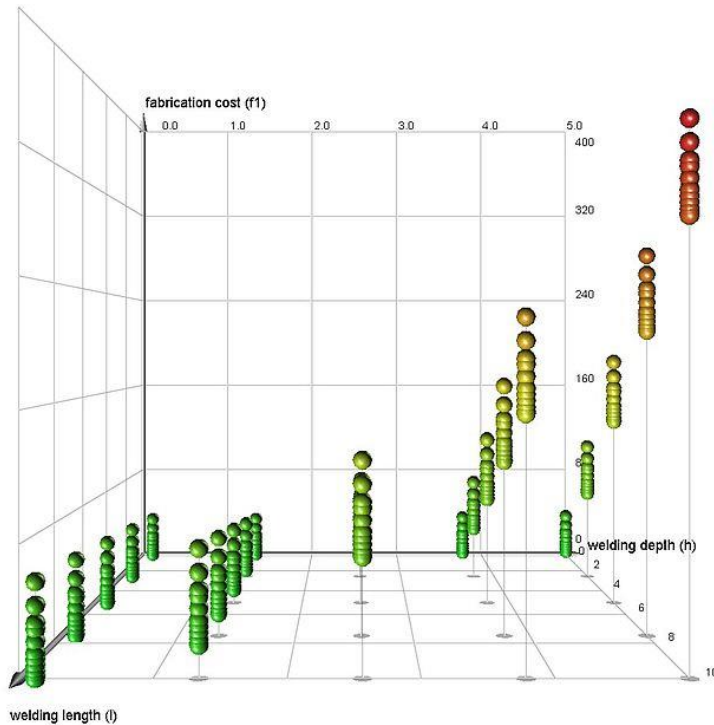
Notations -: not detected rr: very rare (some cristals) r: rare (~0.2%) t: trace (~0.5%) <1: ~0.8%





# Response surface methods

# From full factorial design to the surface



# Planning and running DOE

- Check performance of gauges/measurement devices first.
- Keep the experiment as simple as possible.
- Check that all planned runs are feasible.
- Watch out for process drifts and shifts during the run.
- Avoid unplanned changes (e.g., swap operators at halfway point).
- Allow some time (and back-up material) for unexpected events.
- Obtain buy-in from all parties involved.
- Maintain effective ownership of each step in the experimental plan.
- Preserve all the raw data--do not keep only summary averages!
- Record everything that happens.
- Reset equipment to its original state after the experiment.