

DESIGN OF EXPERIMENTS

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Design of experiments

- Usually experimentation (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

- **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

Tests

Test	Dependent variables	Independent variables
T-test	One	One
ANOVA	One	One
Two-way ANOVA	One	Multiple
MANOVA	Multiple	Multiple

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 two different populations?*



Two-factor Experiments

DOE

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 of the grid is labeled "Factor A" and shows levels 1, 2, ..., i, ..., a. The left face is labeled "Factor B" and shows levels 1, 2, ..., i, ..., b. The depth of the grid 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

α_i = effect due to A

e_{ij} = measurement error

Two-factor ANOVA

- Factor A – a input levels
- Factor B – b input levels
- n measurements for each input combination
- abn total measurements

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

α_i = effect due to A

β_j = effect due to B

γ_{ij} = effect due to interaction of A and B

e_{ijk} = measurement error

Sum-of-Squares

- As before, use sum-of-squares identity

$$SST = SSA + SSB + SSAB + SSE$$

- Degrees of freedom
 - ▣ $df(SSA) = a - 1$
 - ▣ $df(SSB) = b - 1$
 - ▣ $df(SSAB) = (a - 1)(b - 1)$
 - ▣ $df(SSE) = ab(n - 1)$
 - ▣ $df(SST) = abn - 1$

Sum-of-Squares

$$\underbrace{\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^r (Y_{ijk} - \bar{Y}_{...})^2}_{SS_{Total}} = \underbrace{r \cdot b \cdot \sum_{i=1}^a (\bar{Y}_{i..} - \bar{Y}_{...})^2}_{SS_A} + \underbrace{r \cdot a \cdot \sum_{j=1}^b (\bar{Y}_{.j.} - \bar{Y}_{...})^2}_{SS_B} \\ + \underbrace{r \times \sum_{i=1}^a \sum_{j=1}^b (\bar{Y}_{ij.} - \bar{Y}_{i..} - \bar{Y}_{.j.} + \bar{Y}_{...})^2}_{SS_{A \times B}} + \underbrace{\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^r (Y_{ijk} - \bar{Y}_{ij.})^2}_{SS_{within}}$$

$$MS_{within} = SS_{within} / df_{within}$$

$n2^k$ Contrasts

- Effects of A, B and interactions.

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

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

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

Two-Factor ANOVA table

Source	Degrees of Freedom	SS	MS	F
A	a-1	SS_A	MS_A	MS_A / MS_{within}
B	b-1	SS_B	MS_B	MS_B / MS_{within}
$A \times B$	(a-1)(b-1)	$SS_{A \times B}$	$MS_{A \times B}$	$MS_{A \times B} / MS_{within}$
Within	ab(r-1)	SS_{within}	MS_{within}	
Total	abr-1	SS_{Total}		

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

Replications are needed

- If $n=1$ (only one measurement of each configuration)
 - ▣ $SSE = 0$
- Since
 - ▣ $SSE = SST - SSA - SSB - SSAB$
- and
 - ▣ $SSAB = SST - SSA - SSB$

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

Two-Factor ANOVA table

	A	B	AB	Error
Sum of squares	SSA	SSB	$SSAB$	SSE
Deg freedom	1	1	1	$2^m(n-1)$
Mean square	$s_a^2 = SSA/1$	$s_b^2 = SSB/1$	$s_{ab}^2 = SSAB/1$	$s_e^2 = SSE/[2^m(n-1)]$
Computed F	$F_a = s_a^2/s_e^2$	$F_b = s_b^2/s_e^2$	$F_{ab} = s_{ab}^2/s_e^2$	
Tabulated F	$F_{[1-\alpha;1,2^m(n-1)]}$	$F_{[1-\alpha;1,2^m(n-1)]}$	$F_{[1-\alpha;1,2^m(n-1)]}$	

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				

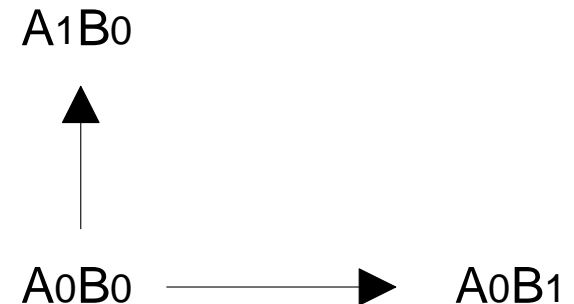
Factorial designs

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: $A_0B_1 - A_0B_0$

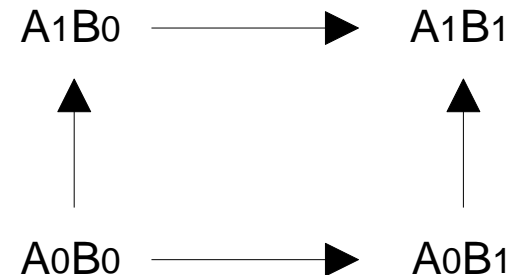


Factorial designs

- 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, $n = 3$
 - ▣ → $3(4^5) = 3,072$ experiments!

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

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

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

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

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

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

Contrasts for $n2^k$ with $k = 3$ factors

Means	Contrast						
	w_a	w_b	w_c	w_{ab}	w_{ac}	w_{bc}	w_{abc}
y_{abc}	-	-	-	+	+	+	-
y_{Abc}	+	-	-	-	-	+	+
y_{aBc}	-	+	-	-	+	-	+
...

$$w_{AC} = y_{abc} - y_{Abc} + y_{aBc} - y_{abC} - y_{ABc} + y_{AbC} - y_{aBC} + y_{ABC}$$

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.

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

Experiment	Factor 1	Factor 2	Factor k	Answer
1	-	-		-	R1
2	+	-		-	R2
3	-	-		-	R3
4	+	-		-	R4
5	-	+		-	R5
6	+	+		-	R6
2^k	+	+		+	$R2^k$

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

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

$$ABC = \frac{y_{21} + y_3 + y_5 + y_8}{4} - \frac{y_1 + y_4 + y_6 + y_7}{4} = 0.5$$

Frank Yates



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

Yates algorithm

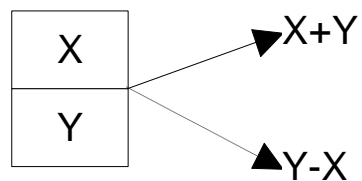
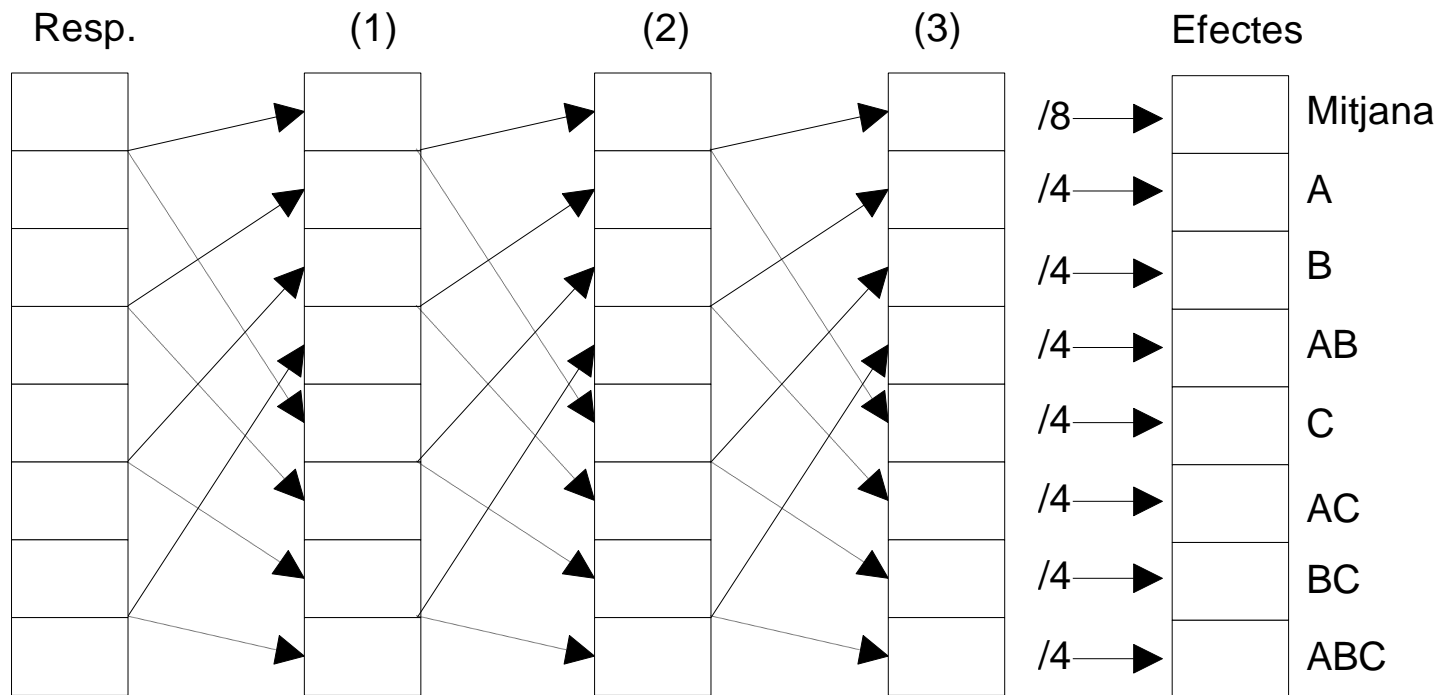
To make systematic the interactions calculus using a table.

- 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 experimental conditions “E”, and the others by the half of “E”.

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 μ that depends on the technology used on the process. This parameter μ 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).
 - ▣ The amount of machines that can be used for glue the different pieces (range from 1 to 5, each machine that increases the number over 2 reduces the time needed by 1 seconds).
 - ▣ The amount 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			μ	1/μ	x1	x2	mean	Yates						
-	-	-	50	0	1	51	0,019607843	20,8852	20,2611	20,57315	55,67501	206,082	246,6539	30,83174	Mean		
-	-	+	50	0	0,5	50,5	0,01980198	33,83603	36,36768	35,10185	150,407	40,57198	-8,42686	-2,10671	Workers		
-	+	-	50	-4	1	47	0,021276596	9,909855	142,0044	75,95712	25,41431	13,02142	84,47532	21,11883	Machines		
-	+	+	50	-4	0,5	46,5	0,021505376	17,76593	131,1337	74,44984	15,15767	-21,4483	-2,71458	-0,67864	Machines*Workers		
+	-	-	10	0	1	11	0,090909091	42,759	0,040152	21,39958	14,5287	94,73195	-165,51	-41,3775	Cleaner		
+	-	+	10	0	0,5	10,5	0,095238095	5,702481	2,326982	4,014731	-1,50728	-10,2566	-34,4697	-8,61743	Cleaner*Workers		
+	+	-	10	-4	1	7	0,142857143	10,48071	8,740406	9,610556	-17,3848	-16,036	-104,989	-26,2471	Cleaner*Machines		
+	+	+	10	-4	0,5	6,5	0,153846154	5,977532	5,116704	5,547118	-4,06344	13,32141	29,35739	7,339348	Cleaner*Machines*Workers		

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

Signification of the effects

The variability is now on the effects

Have the effects significations?

- The effects have been calculated using the answers that owns variability.
 - ▣ The variability goes to the effects.
 - $\hat{A} = \bar{y}(+) - \bar{y}(-)$

Have signification?

- From the variance of the effects.
 - ▣ If we have replications, or if we know an estimation of the answer's variance.
- Using the normal Distribution (and its probabilistic features).
 - ▣ If we do not have replications and we do not have any estimation of the answer's variance.

We have replications

□ Calculation of the variance

□ $S_R^2 = \frac{(n_1-1)s_1^2 + (n_2-1)s_2^2 + \dots + (n_N-1)s_N^2}{n_1 + n_2 + \dots + n_N - N}$, assuming that the amount of replications in each experiment is different.

□ If not $S_R^2 = \frac{s_1^2 + s_2^2 + \dots + s_N^2}{N}$

□ Where $N=2^k$, and $Nt=v*2^k$.

We have replications

- Variance for an effect

- $\widehat{effect} = \overline{y_+} - \overline{y_-}$

- Where $\overline{y_+}$ is the mean of the $N_T/2$ experiments (+ sign), and $\overline{y_-}$ is the mean of the $N_T/2$ experiments (- sign).

- The calculus is:

- $v(\widehat{effect}) = v(\overline{y_+} - \overline{y_-}) = \frac{S^2}{N_T/2} + \frac{S^2}{N_T/2} = \frac{4S^2}{N_T}$

Example

x1	x2	Mean	S2			
60	64	62	8			
72	74	73	2			
54	55	54,5	0,5			
68	70	69	2		v(effect)	12,1942
52	54	53	2			3,492019
83	87	85	8			
45	50	47,5	12,5			
80	85	82,5	12,5			
		S2= 24,38839				

Signification test

- Hypothesis testing

- $H_0: \text{effect}=0$

- $H_1: \text{effect} \neq 0$

- Statistic of the test

- $t = \frac{\widehat{effect}-0}{S_{effect}}$

- t-Student with $n_1+n_2+..+n_n$ -N degrees of freedom
($N=2^k$)

- Calculus of the I.C.

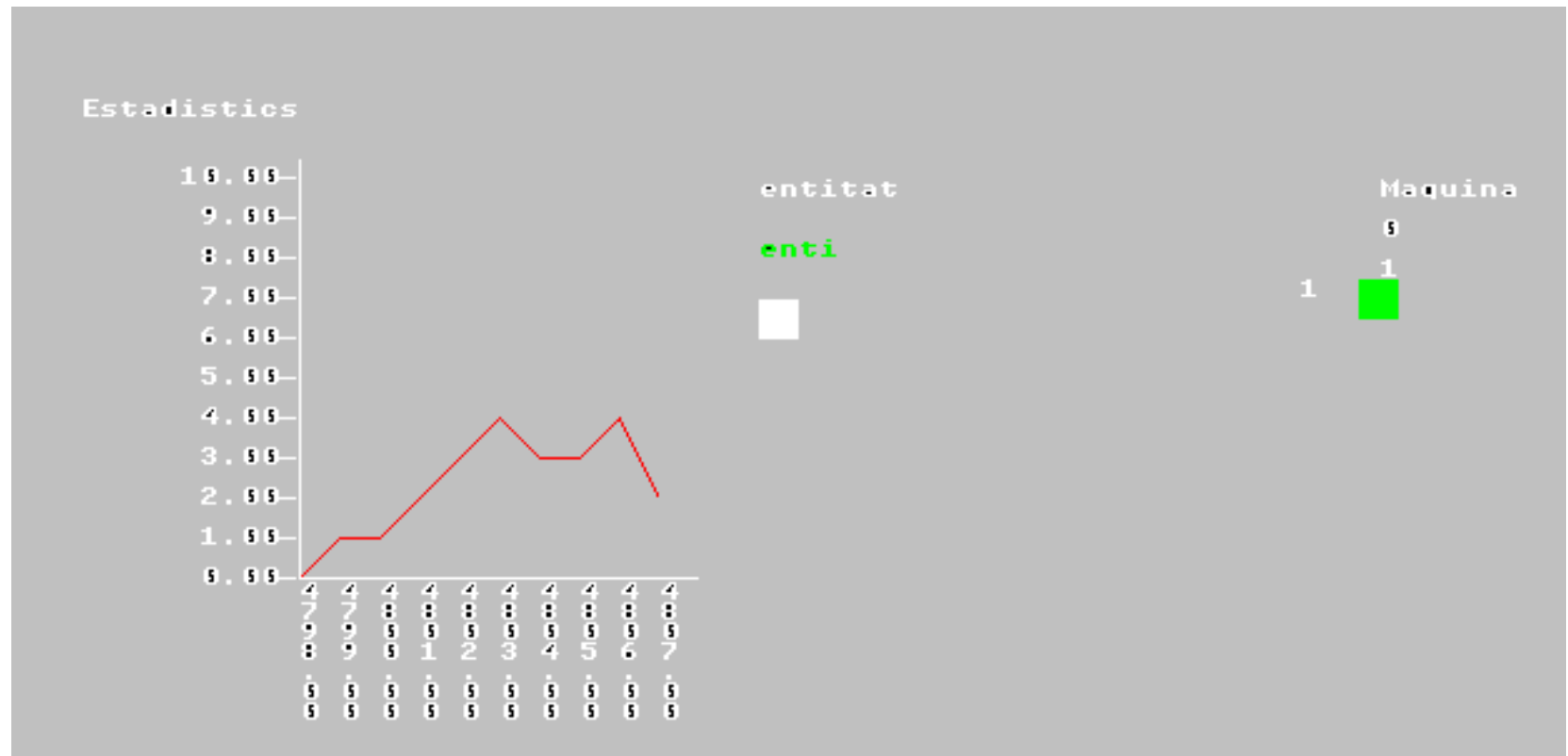
- $\widehat{effect} \pm x * S_{effect}$

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

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

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

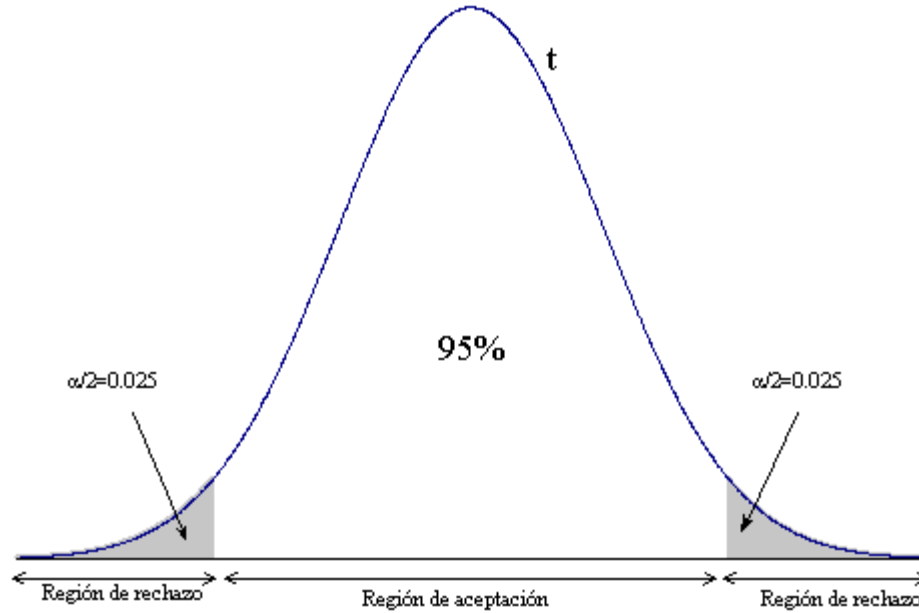
$$s^2 = \frac{n}{n-1} \sigma_y^2 = \frac{n}{n-1} \left(\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2 \right) = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2$$

Confidence interval

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

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

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



$$\bar{y} = 32.4818$$

$$s^2 = 3.5149$$

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 - α							
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

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.

$$n^* = 10 \left(\frac{2.512}{1.62} \right)^2 = 24.04$$

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.

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

$$h = 1.3144 < 1.62$$

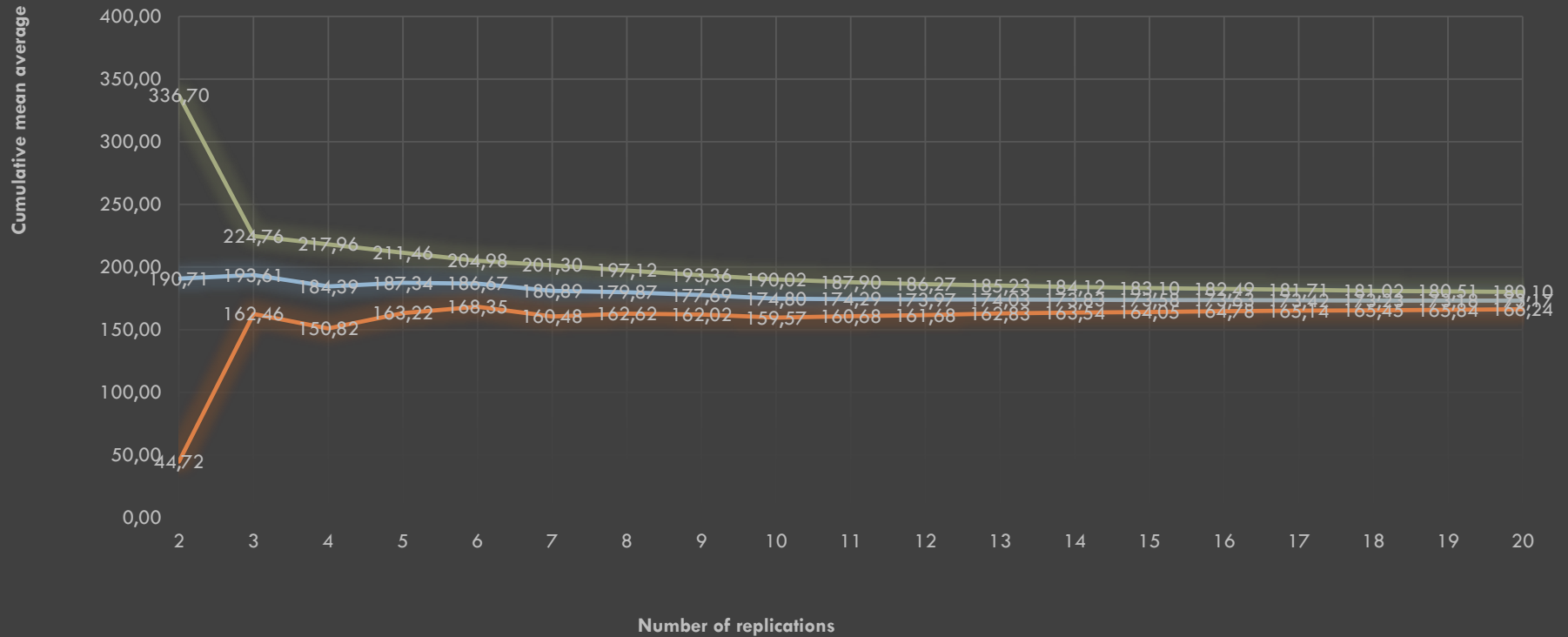
Exercise 3

- 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 - α							
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

With more replications



Replications

Methods to execute the replications.

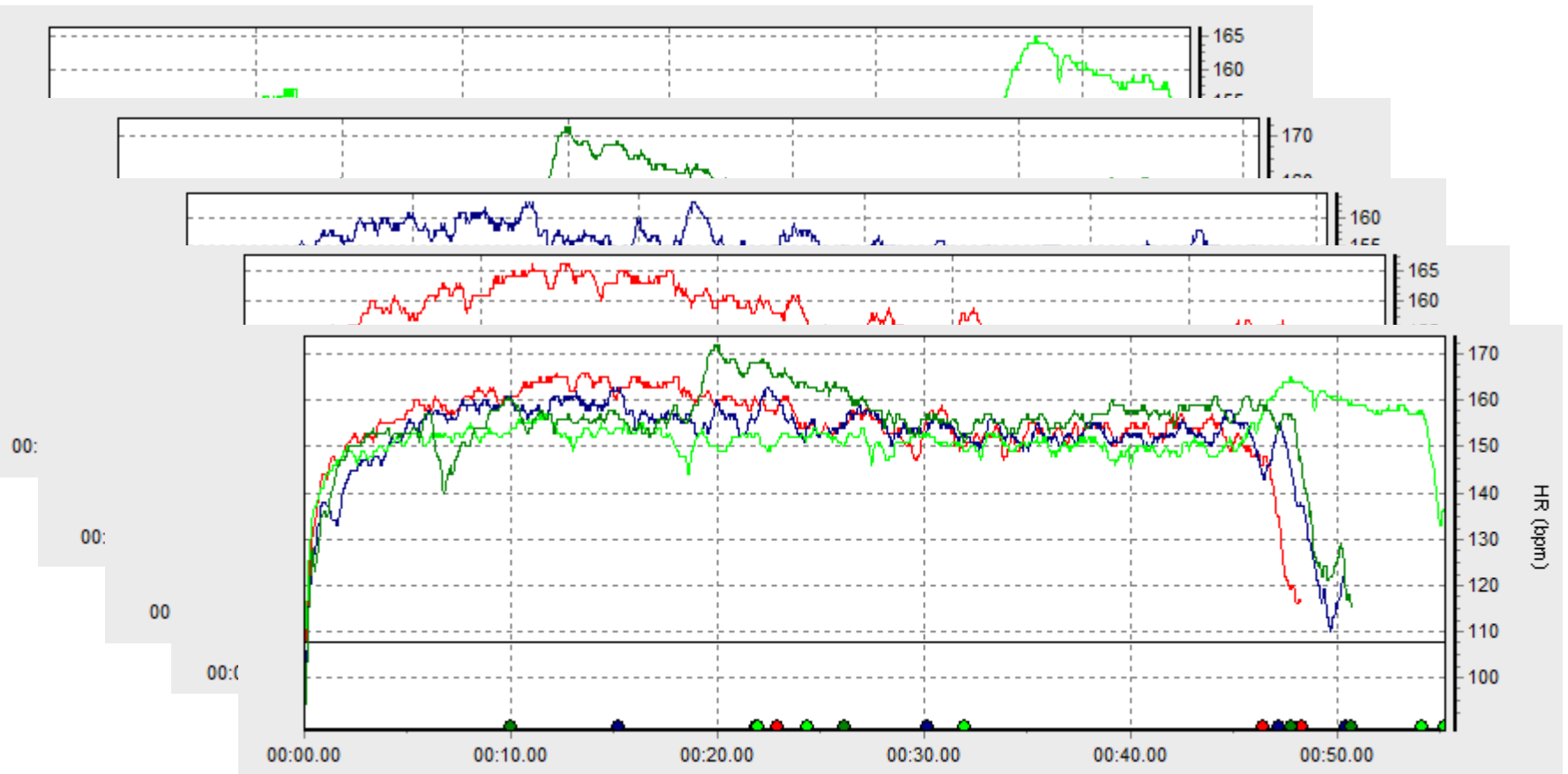
Kind of simulations

- **Finite simulations:** Simulations where a condition defines the end of the execution. Usually time.
- **No finite simulations:** Simulations without this condition.

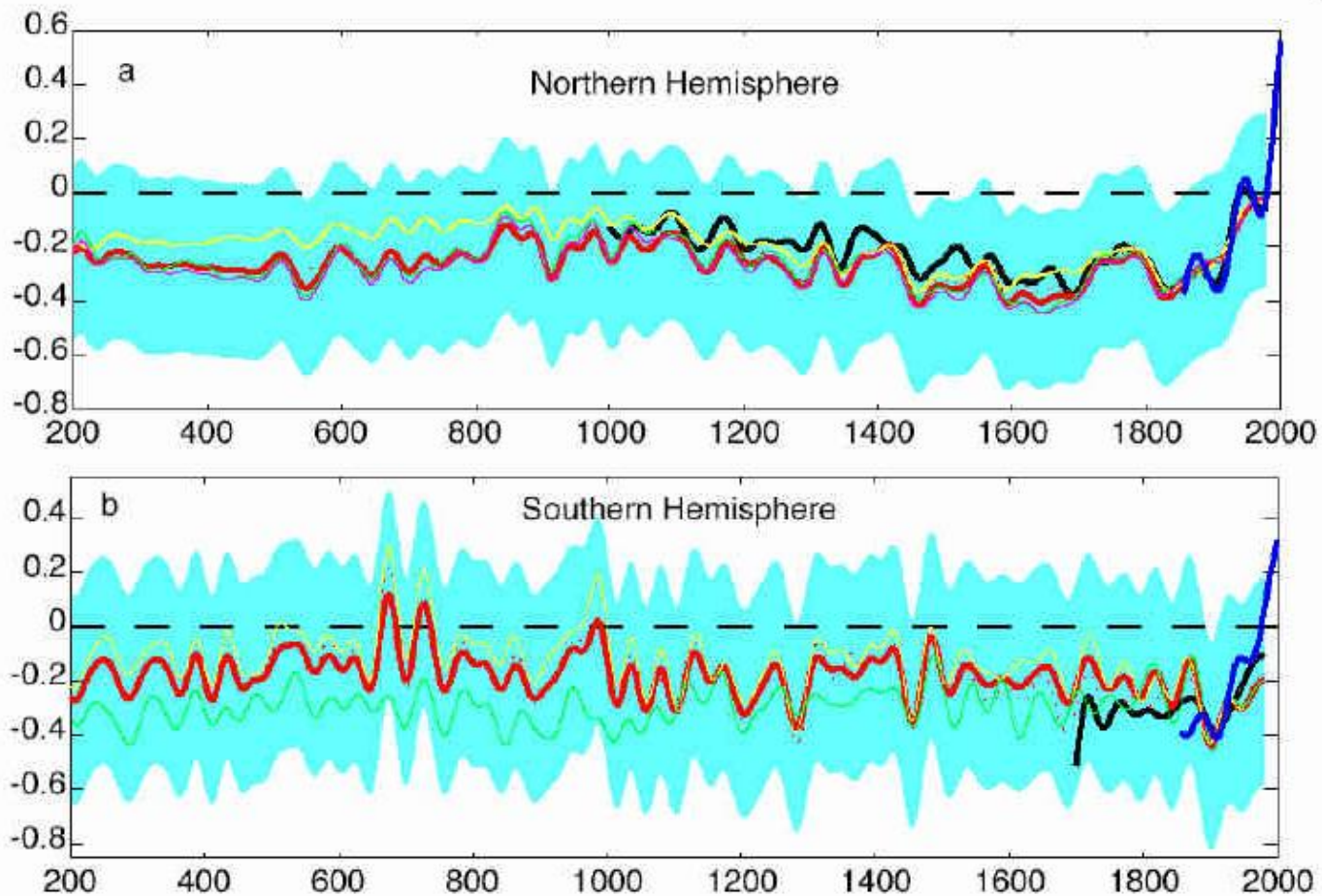
Independent repetitions

- 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).

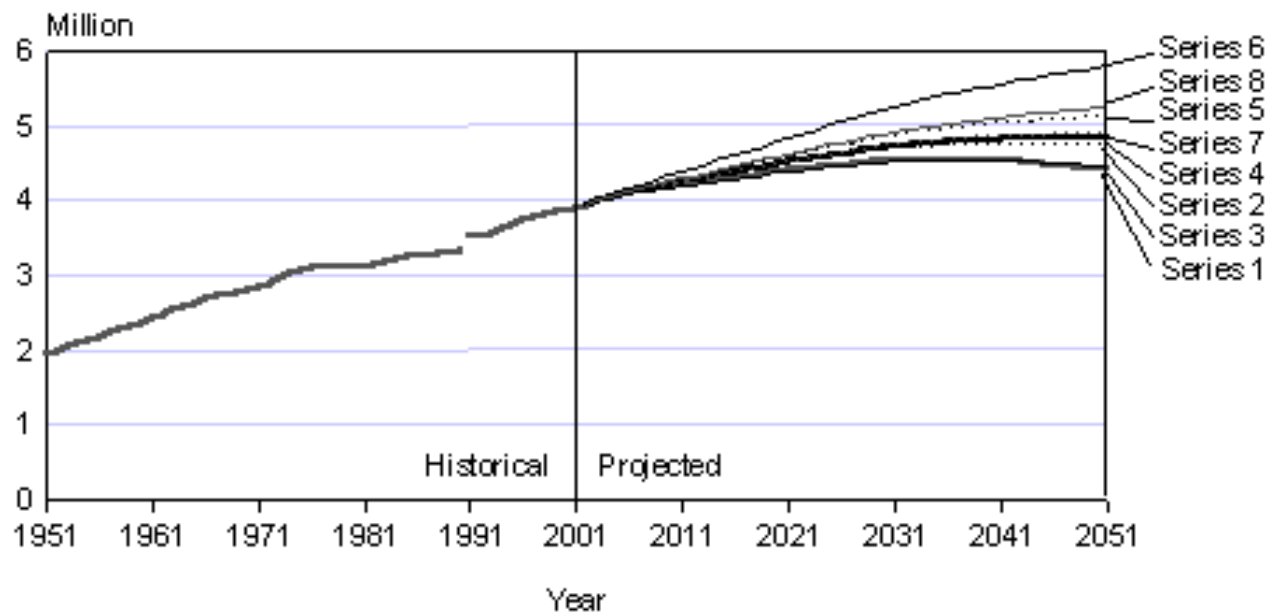
Independent repetitions



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.

Transient elimination

□ Definitions:

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

Transient elimination

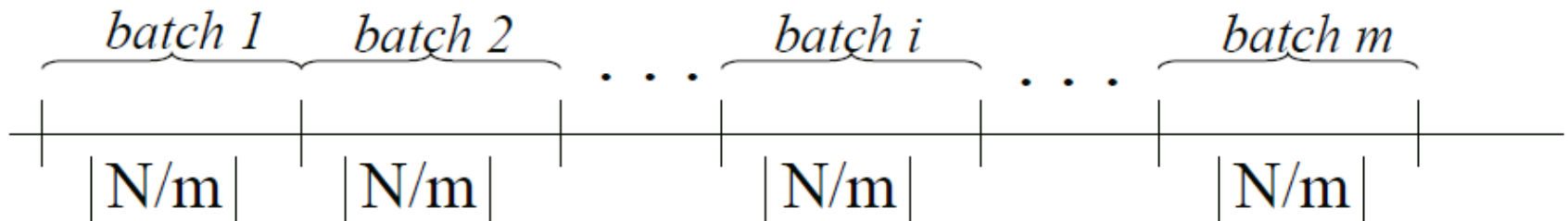
- Step 1: Compute the average of the j observation's over all runs.
 - ▣ $\bar{x}_j = \frac{1}{m} \sum_{i=1}^m x_{i,j}$
- Step 2: Compute the overall average.
 - ▣ $\bar{\bar{x}} = \frac{1}{n} \sum_{j=1}^n \bar{x}_j$
- Step 3: $K=1$

Transient elimination

- Step 4: Compute the overall average of the j observation's over all runs without the first k observations.
 - ▣ $\bar{\bar{x}}_k = \frac{1}{n-k} \sum_{j=k+1}^n \bar{x}_j$
- Step 5: Calculate the relative change
 - ▣ $\Delta = \frac{\bar{\bar{x}}_k - \bar{\bar{x}}}{\bar{\bar{x}}}$
- If $|\Delta_k - \Delta_{k-1}| > \text{threshold}$ then increment k and go to step 4, else remove k observations and use

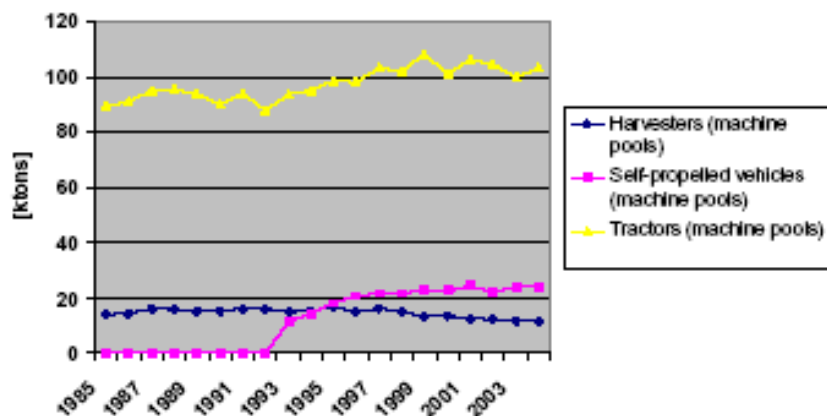
Batch means

- 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.

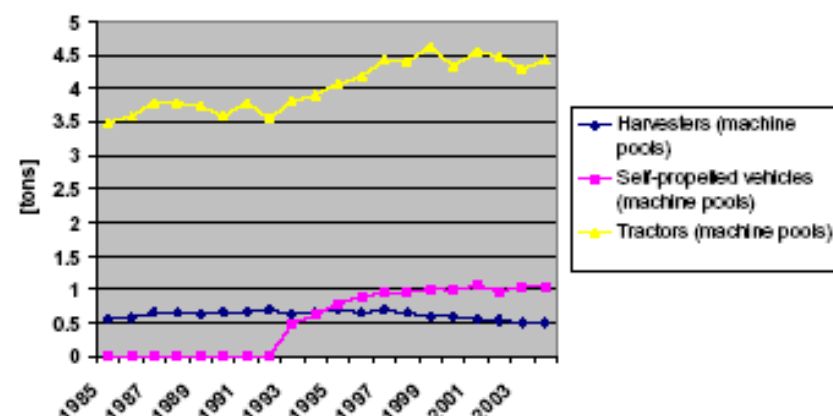


Batch means

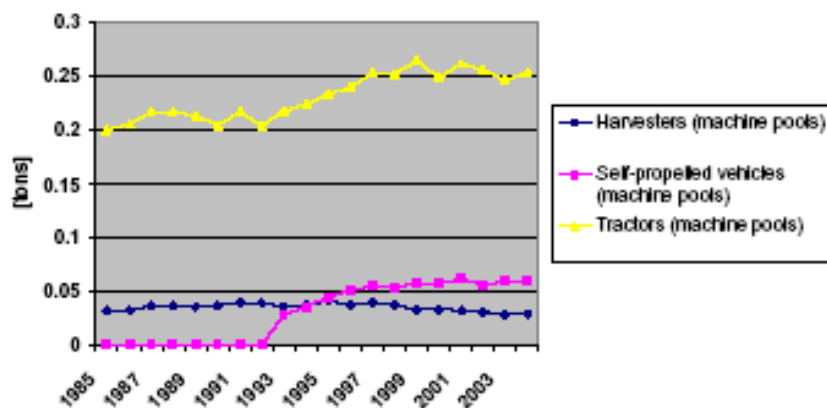
CO₂ emissions



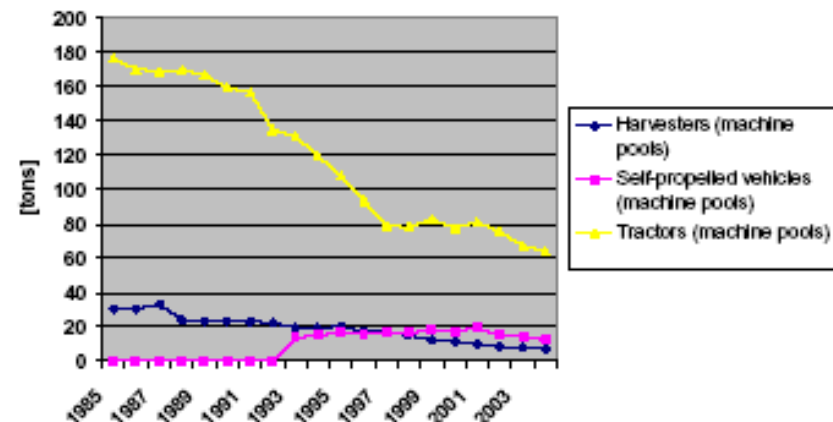
N₂O emissions



NH₃ 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.
 - ▣ $Var(\bar{x}) = \frac{1}{m-1} \sum_{i=1}^m (\bar{x}_i - \bar{\bar{x}})^2$

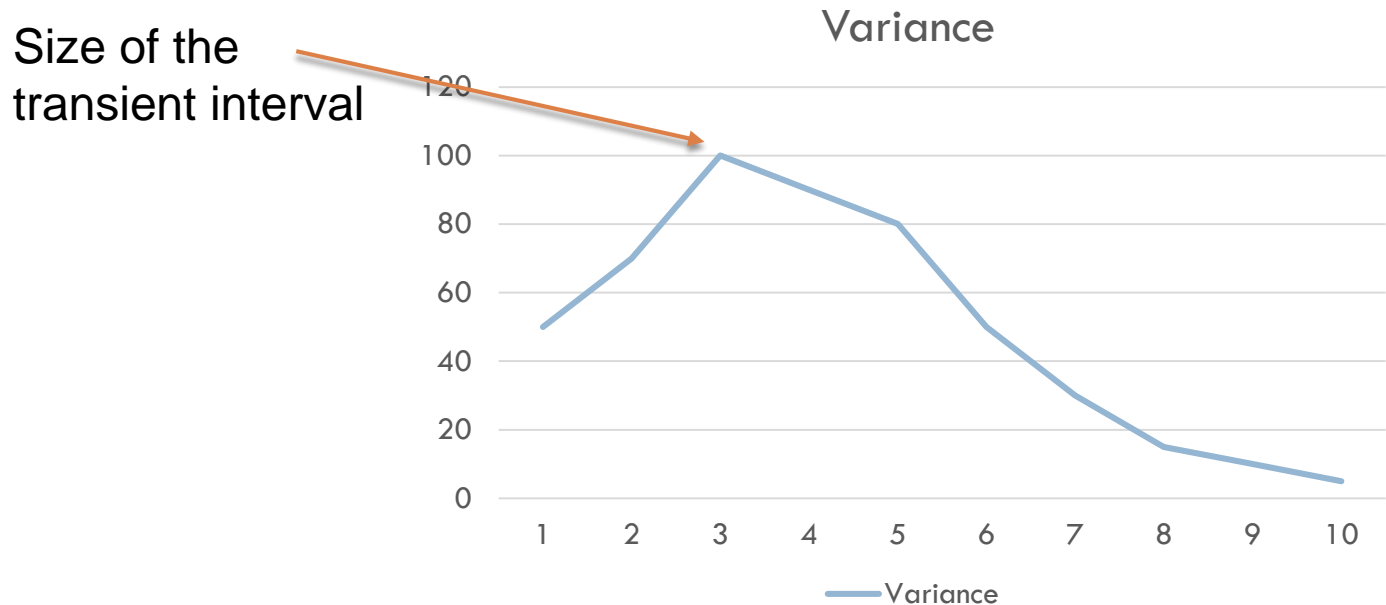
Definitions:

n: amount of observations in a single run.

m: amount of runs (replications).

Transient elimination

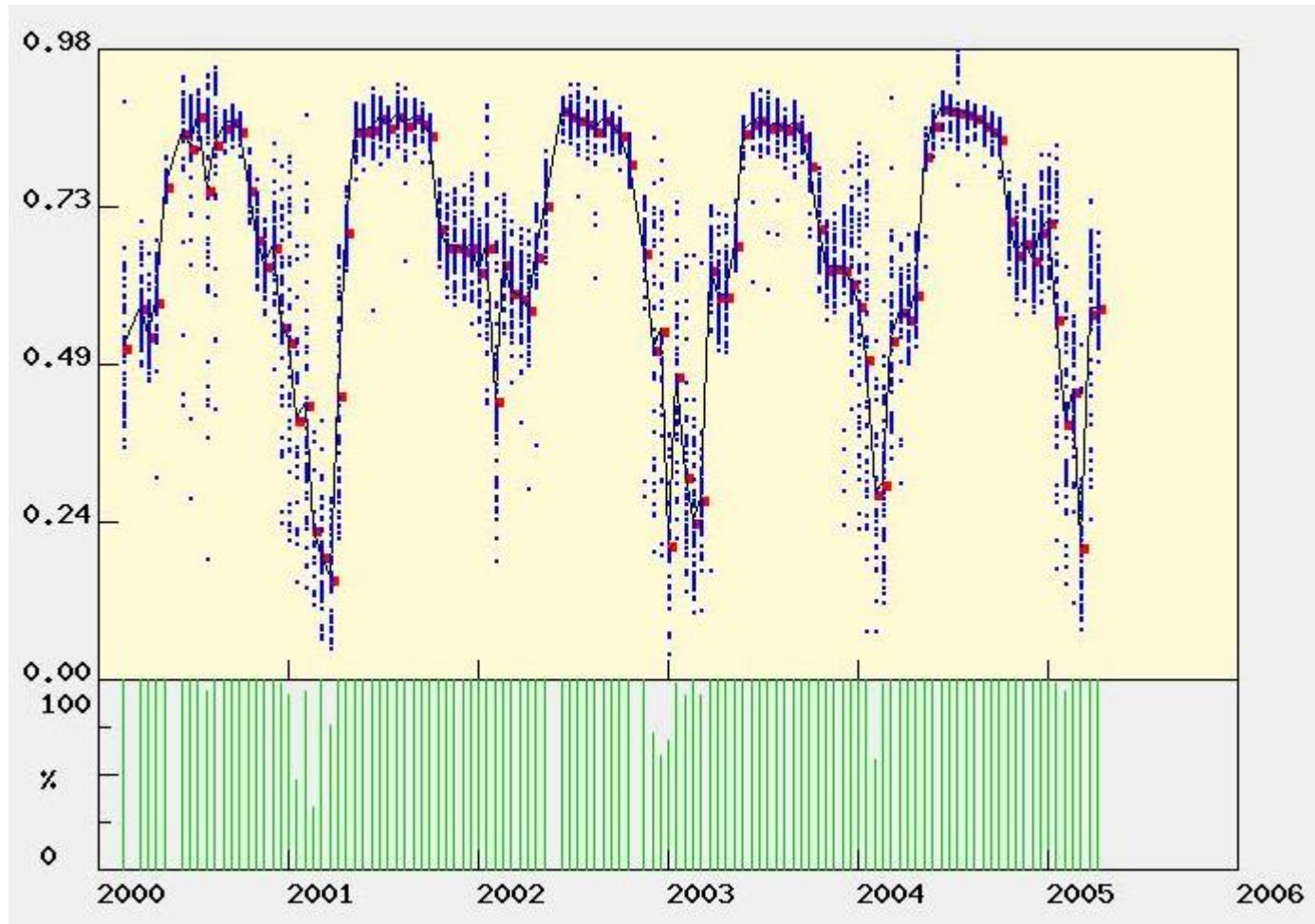
- Step 5: Increase n by 1 and go to step 2 and plot the variance as a function of n . The point at which the variance starts to decrease is the length of the transient interval.



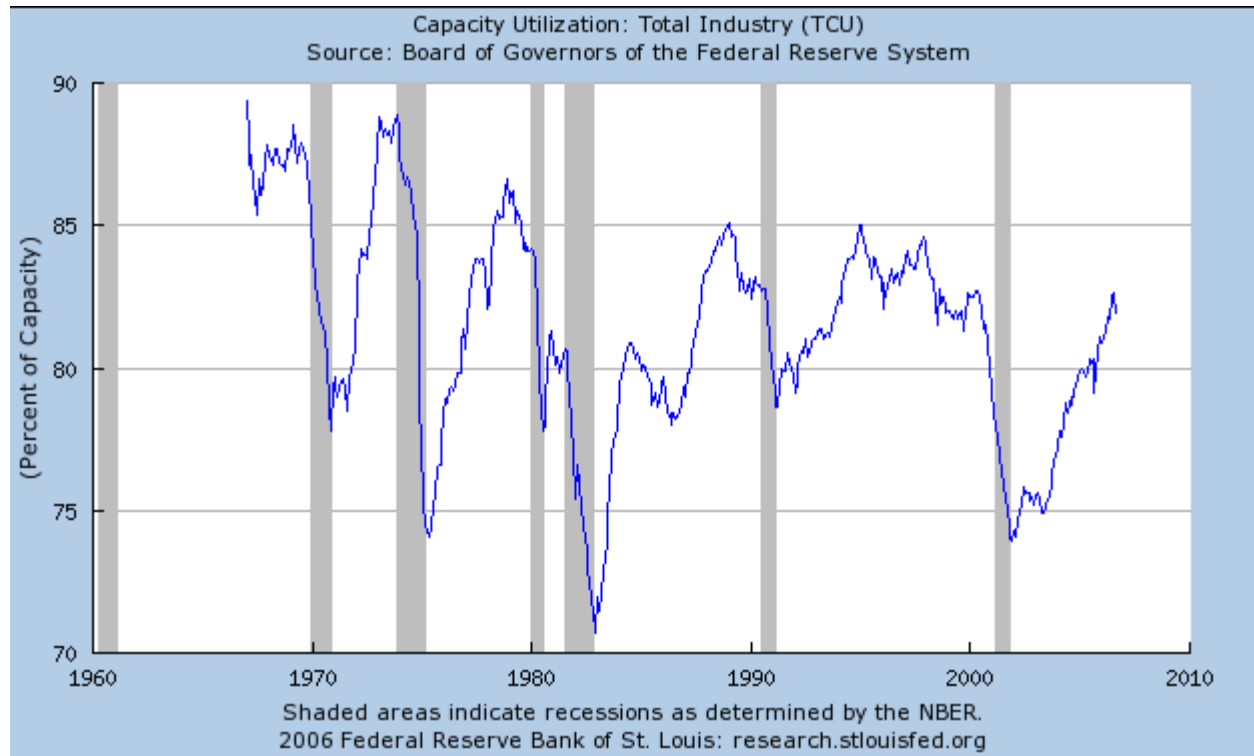
Regenerative methods

- 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

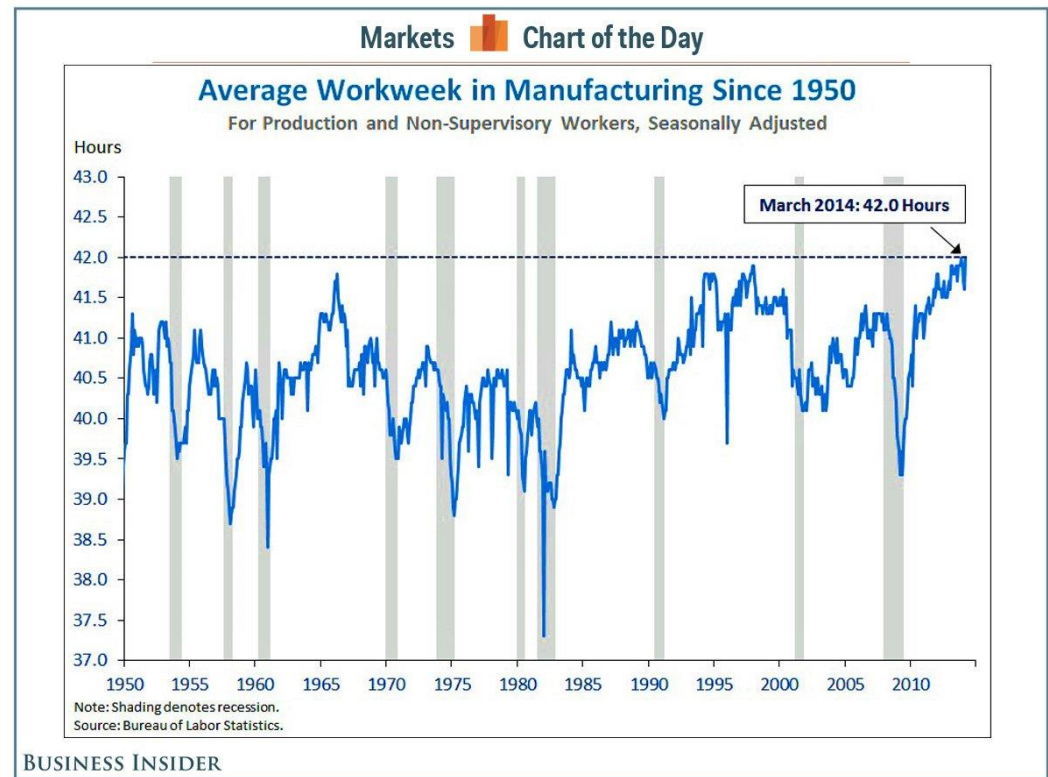


Regenerative methods



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

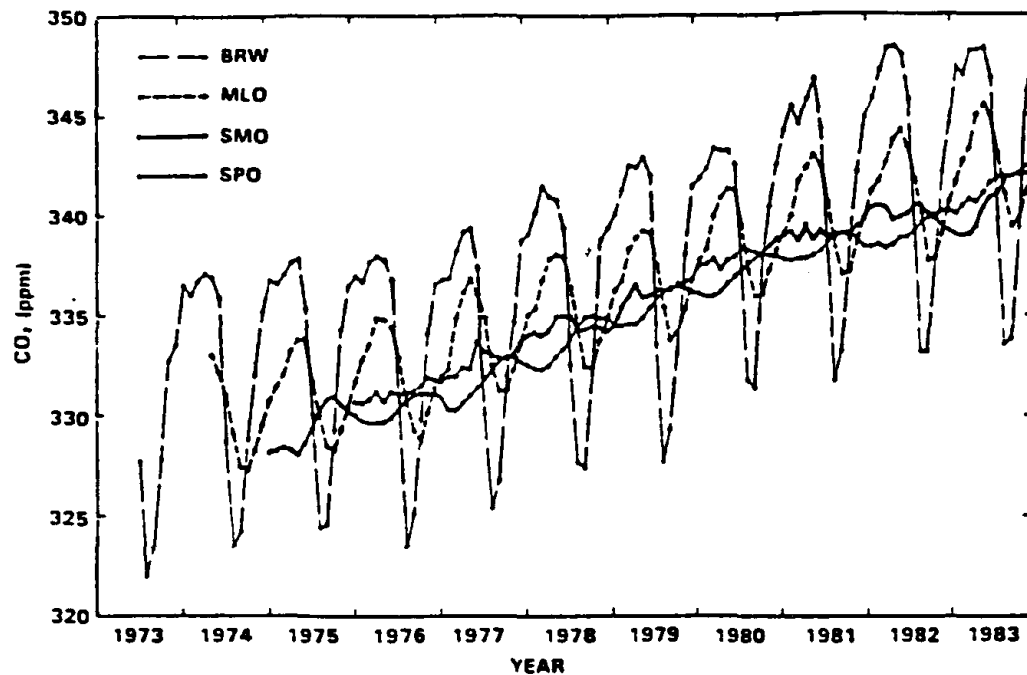


Fig. 1. Selected monthly mean carbon dioxide concentrations from continuous measurements (Barrow, Alaska (BRW); Mauna Loa, Hawaii (MLO); American Samoa (SMO); South Pole (SPO). From: WMO, 1985.

Applicability

	Finite simulations	No finite 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 an specific answer variable, that is represented by its confidence interval, must be adjusted (as possible).

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

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.

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

Common random numbers

- Using the same random number stream for the different configurations.
- Both streams represents “identical conditions” for both configurations.
- Is needed to establish mechanism to synchronize the 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 reduce the difference.



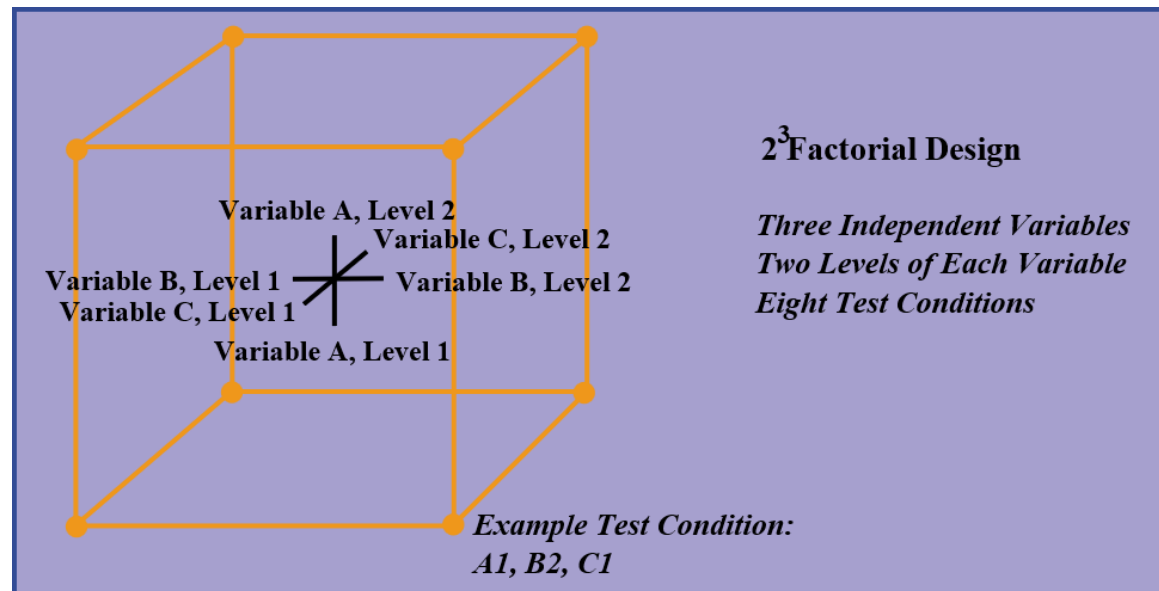
Fractional factorial design

Fractional factorial design

- A factorial experiment in which only an **adequately chosen fraction** of the treatment combinations 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

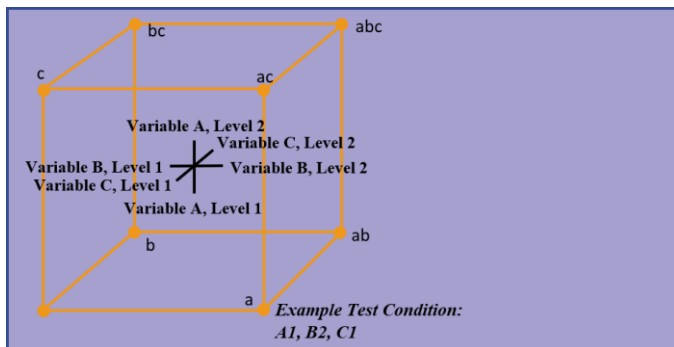
	X1	X2	X3	Y
1	-1	-1	-1	$y_1 = 33$
2	+1	-1	-1	$y_2 = 63$
3	-1	+1	-1	$y_3 = 41$
4	+1	+1	-1	$y_4 = 57$
5	-1	-1	+1	$y_5 = 57$
6	+1	-1	+1	$y_6 = 51$
7	-1	+1	+1	$y_7 = 59$
8	+1	+1	+1	$y_8 = 53$

Computing the effects

- Effect of $C1 = (1/4)(y_2 + y_4 + y_6 + y_8) - (1/4)(y_1 + y_3 + y_5 + y_7)$
- $c1 = (1/4)(63 + 57 + 51 + 53) - (1/4)(33 + 41 + 57 + 59) = 8.5$
- Suppose, however, that we only have enough resources to do four runs. Is it still possible to estimate the main effect for $X1$? 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
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	$y_8 = 53$



Main effects

□ C1 main effect:

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

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

□ C2 main effect

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

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

□ C3 main effect

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

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

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 X_1 and X_2

	X_1	X_2	$X_1 * X_2$
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 $c12$)

Notation

- $X_3 = X_1 * X_2$ can be represented by:
 - $3=12$
- Playing with this
- Multiplying with 3
 - $33=123$, and $33=I$ (identity)
 - $I=123$, $2I=2123$, $2I=2$, $I=22$

3
 - $I=123$ is the design generator
 - $1=23$, $2=13$, $3=12$, $I=123$ aliases

Principal fraction

- We can replace any design generator by its negative counterpart and have an equivalent, but different fractional design.
- The fraction generated by positive design generators is sometimes called the principal fraction.

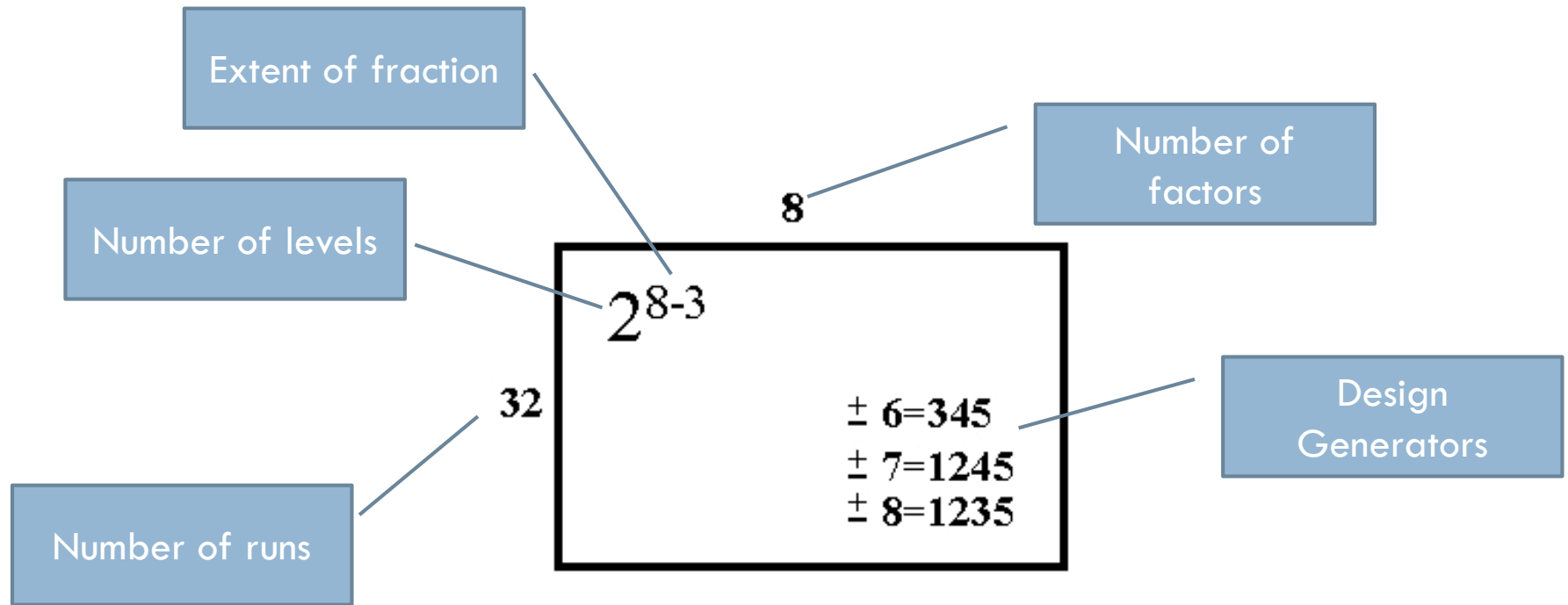
Confounding pattern

- The confounding pattern described by $1=23$, $2=13$, and $3=12$ tells us that all the main effects of 2^{3-1} design are confounded with two-factor interactions.
 - ▣ That is the price we pay for using this fractional design.

Confounding pattern

- In the typical quarter-fraction of a 2^6 design, i.e., in a 2^{6-2} design, main effects are confounded with three-factor interactions (e.g., $5=123$) and so on.
- In the case of $5=123$, we can also readily see that $15=23$ (etc.), which alerts us to the fact that certain two-factor interactions of a 2^{6-2} are confounded with other two-factor interactions.

Definition of the experiment



How to construct this experiment?

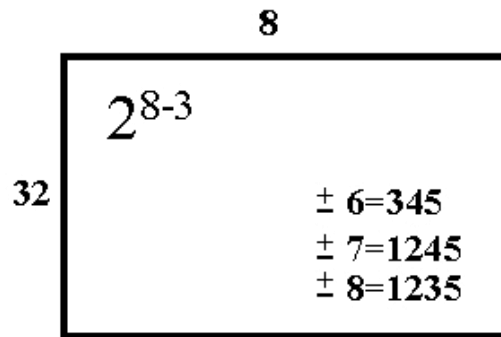
A diagram showing a rectangular box with a thick black border. Above the box is the number 8. To the left of the box is the number 32. Inside the box, in the top-left corner, is the expression 2^{8-3} . In the bottom-right corner of the box, there is a list of three permutations, each preceded by a plus-minus sign (\pm):

- $\pm 6=345$
- $\pm 7=1245$
- $\pm 8=1235$

Construct a Fractional Factorial Design From the Specification

- **Write down a full factorial design** in standard order for $k-p$ factors ($8-3 = 5$ factors for the example above). In the specification above we start with a 2^5 full factorial design. Such a design has $2^5 = 32$ rows.
- **Add a sixth column** to the design table for factor 6, using $6 = 345$ (or $6 = -345$) to manufacture it (i.e., create the new column by multiplying the indicated old columns together).
- **Do likewise** for factor 7 and for factor 8, using the appropriate design generators.
- The resultant design matrix gives the **32 trial runs** for an 8-factor fractional factorial design.

Example: 2^{8-3}



X1	X2	X3	X4	X5	X6	X7	X8
-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	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	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	1			
1	-1	1	1	1			
-1	1	1	1	1			
1	1	1	1	1			

2⁸⁻³

8

2⁸⁻³

± 6=345
± 7=1245
± 8=1235

X1	X2	X3	X4	X5	X6	X7	X8
-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
-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
-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
-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
-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
-1	1	1	1	1	1	-1	-1
1	1	1	1	1	1	1	1

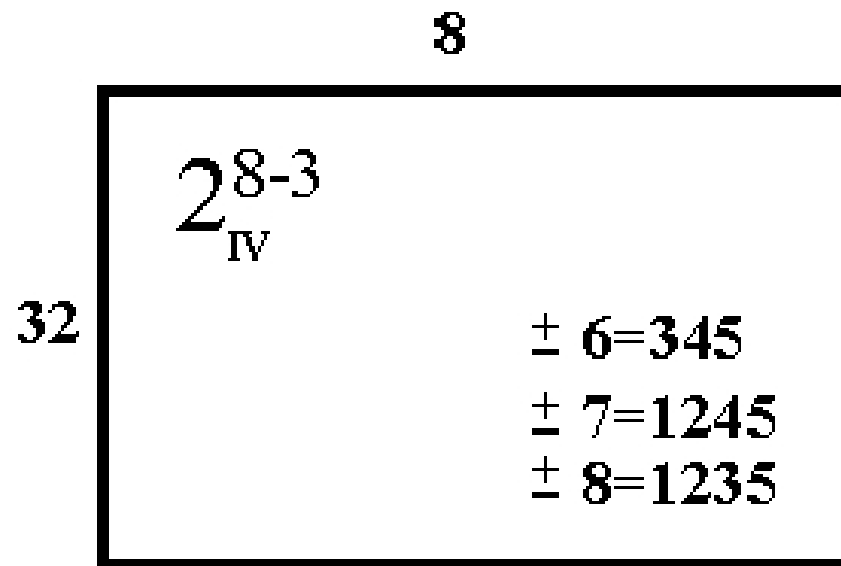
Words

- There are seven "words", or strings of numbers, in the defining relation for the 2^{8-3} design, starting with the original three generators and adding all the new "words" that can be formed by multiplying together any two or three of these original three words. These seven turn out to be $I = 3456 = 12457 = 12358 = 12367 = 12468 = 3478 = 5678$.
- In general, there will be $(2^p - 1)$ words in the defining relation for a 2^{k-p} fractional factorial.

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.

Complete definition of the DOE



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	BUSH	BUCHANAN	NADER	BROWNE	HAGELIN	HARRIS	MCREYNOLDS	MOOREHEAD	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 four variables to be confounded using the first 6 variables.

Answer

9

64

2^{9-3}
VI

$\pm 7 = 123456$

$\pm 8 = 12345$

$\pm 9 = 12346$



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): C, D, E, F, G, A and B.

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=S0104-66322003000300010

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 ₂	r	r
Bornite	Cu ₅ FeS ₄	r	r
Chalcocite	Cu ₂ S	rr	rr
Covelite	CuS	rr	rr
Cuprite	Cu ₂ O	t	-
Malachite	Cu ₂ (CO ₃)(OH) ₂	t	-
Goethite/Limonite	HFeO ₂ /Fe ₂ O ₃ .H ₂ O	26	21
Iron oxide	Fe ₂ O ₃ , Fe ₃ O ₄	8	7
Clorite	(Mg,Al,Fe) ₁₂ [(Si,Al) ₈ O ₂₀](OH) ₁₆	33	35
Quartz	SiO ₂	26	33

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

Latin squares

More than two levels.



Fisher window
Anders Sandberg

When to apply?

- Latin square designs are used when the factors of interest have more than two levels (k).
- We have three factors.
- There are no (or only negligible) interactions between factors.

Pros and cons

□ PROS:

- ▣ They handle the case when we have several nuisance factors and we either cannot combine them into a single factor or we wish to keep them separate.
- ▣ They allow experiments with a relatively small number of runs.

□ CONS:

- ▣ The number of levels of each blocking variable must equal the number of levels of the treatment factor.
- ▣ The Latin square model assumes that there are no interactions between the blocking variables or between the treatment variable and the blocking variable.

Example

- What is the best (fast) browser depending on the OS and the computer?
- Browsers are labeled by A,B, C and D.

Computer	OS			
	1	2	3	4
I3	A	B	C	D
I5	B	C	D	A
I7	C	D	A	B
XEON	D	A	B	C

Terminology

- A Latin Square is a **Standard Latin Square** when the letters of the first row and first column are arranged in alphabetical order (the previous example).
- Exists an unique standard 3×3 Latin Square, however there are four standard 4×4 Latin Square.

Square 1				Square 2				Square 3				Square 4			
A	B	C	D	A	B	C	D	A	B	C	D	A	B	C	D
B	C	D	A	B	A	D	C	B	A	D	C	B	D	A	C
C	D	A	B	C	D	A	B	C	D	B	A	C	A	D	B
D	A	B	C	D	C	B	A	D	C	A	B	D	C	B	A

Creating a Latin Square design

- Write down any Latin square of the required size (it could be a standard Latin square).
- And randomize:
 - ▣ Randomize the order of the rows.
 - ▣ Randomize the order of the columns.
 - ▣ Randomize the allocation of treatments to the letters of the square.

The model

- $Y_{ijt} = \mu + R_i + C_j + T_k + \varepsilon_{ijk}$
- Where
- Y_{ijt} denoting any observation for which
 - ▣ $X_1 = i, X_2 = j, X_3 = k$
 - ▣ X_1 and X_2 are blocking factors
 - ▣ X_3 is the primary factor (treatment).
- μ denoting the general location parameter
- R_i denoting the effect for block “i”
- C_j denoting the effect for block “j”
- T_k denoting the effect for treatment “k”

Calculating the model

- Estimate for μ : \bar{Y} = the average of all the data
- Estimate for R_i : $\bar{Y}_i - \bar{Y}$
 - ▣ \bar{Y}_i = average of all Y for which $X_1 = i$
- Estimate for C_j : $\bar{Y}_j - \bar{Y}$
 - ▣ \bar{Y}_j = average of all Y for which $X_2 = j$
- Estimate for T_k : $\bar{Y}_k - \bar{Y}$
 - ▣ \bar{Y}_k = average of all Y for which $X_3 = k$
- Estimate for ε_{ijk}
 - ▣ $\varepsilon_{ijk} = (y_{ijk} - \bar{y}_i - \bar{y}_j - \bar{y}_k + 2\bar{y})$

The ANOVA table

Source	SS	df (N-1)=k ² -1	MS	F
Row	SSROW	k-1	MSROW = SSROW / df	MSROW / MSE
Column	SSCOL	k-1	MSCOL = SSCOL / df	MSCOL / MSE
Treatments	SSTR	k-1	MSTR = SSTR / df	MSTR / MSE
Error	SSE	(k-1)(k-2)	MSE = SEE / df	

$$\begin{aligned}
 \underbrace{\sum_{j=1}^k \sum_{i=1}^k (y_{ijt} - \bar{y})^2}_{\text{TSS}} &= \underbrace{k \sum_{i=1}^k (\bar{y}_{i..} - \bar{y})^2}_{\text{SSROW}} + \underbrace{k \sum_{j=1}^k (\bar{y}_{.j.} - \bar{y})^2}_{\text{SSCOL}} + \underbrace{k \sum_{t=1}^k (\bar{y}_{..t} - \bar{y})^2}_{\text{SSTR}} + \\
 &\quad + \underbrace{\sum_{i=1}^k \sum_{j=1}^k \sum_{t=1}^k (y_{ijt} - \bar{y}_{i..} - \bar{y}_{.j.} - \bar{y}_{..t} + 2\bar{y})^2}_{\text{SSE}}
 \end{aligned}$$

Example

- A courier company is interested in deciding between five brands (D,P,F,C and R) of car for its next purchase of fleet cars.
 - ▣ The brands are all comparable in purchase price.
 - ▣ The company wants to carry out a study that will enable them to compare the brands with respect to operating costs.
 - ▣ For this purpose they select five drivers (Rows).
 - ▣ In addition the study will be carried out over a five week period (Columns = weeks).

Example

- Each week a driver is assigned to a car using randomization and a Latin Square Design.
- The average cost per mile is recorded at the end of each week and is tabulated below:

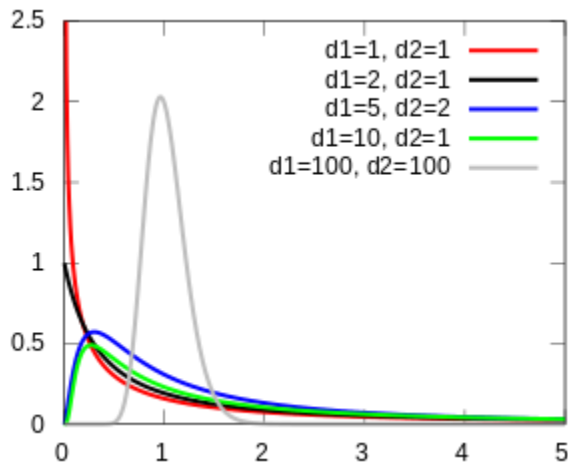
	Week					
		1	2	3	4	5
Drivers	1	5.83	6.22	7.67	9.43	6.57
		D	P	F	C	R
	2	4.80	7.56	10.34	5.82	9.86
		P	D	C	R	F
	3	7.43	11.29	7.01	10.48	9.27
		F	C	R	D	P
	4	6.60	9.54	11.11	10.84	15.05
		R	F	D	P	C
	5	11.24	6.34	11.30	12.58	16.04
		C	R	P	F	D

Example

□ The Anova Table for Example

Source	S.S.	d.f.	M.S.	F ratio	F (table $\alpha=0.05\%$)
Week	51.17887	4	12.79472	16.06	F(4,12)=3.25
Driver	69.44663	4	17.36166	21.79	
Car	70.90402	4	17.72601	22.24	
Error	9.56315	12	0.79693		
Total	201.09267	24			

F-table

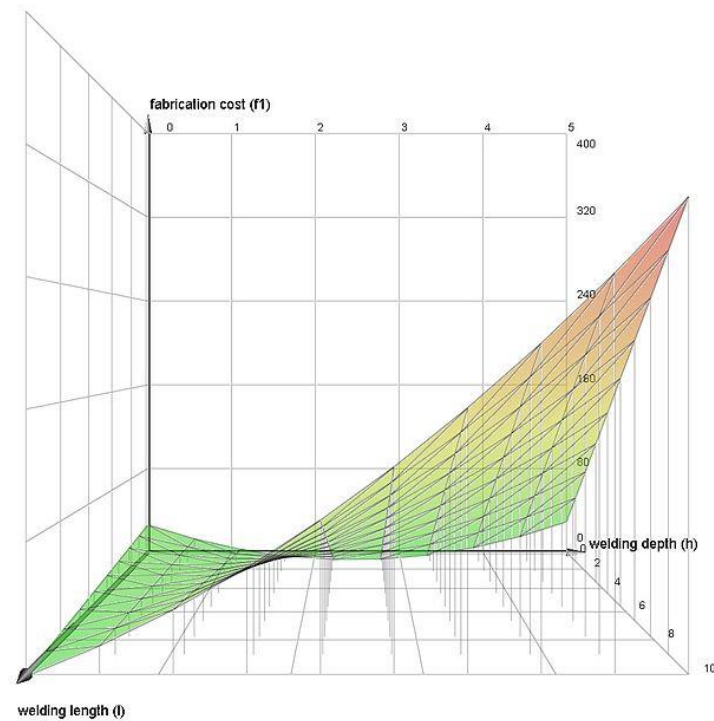
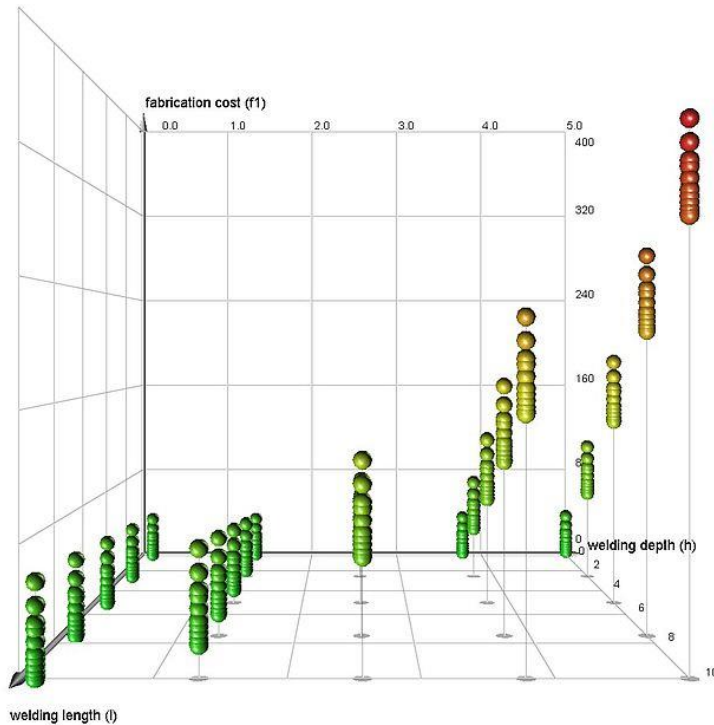


	Numerator df: df_B				
df_W	1	2	3	4	5
5 5%	6.61	5.79	5.41	5.19	5.05
1%	16.3	13.3	12.1	11.4	11.0
10 5%	4.96	4.10	3.71	3.48	3.33
1%	10.0	7.56	6.55	5.99	5.64
12 5%	4.75	3.89	3.49	3.26	3.11
1%	9.33	6.94	5.95	5.41	5.06
14 5%	4.60	3.74	3.34	3.11	2.96
1%	8.86	6.51	5.56	5.04	4.70



Response surface methods

From full factorial design to the surface



Steps

1. Set objectives
2. Select process variables
3. Select an experimental design
4. Execute the design
5. Check that the data are consistent with the experimental assumptions
6. Analyze and interpret the results
7. Use/present the results (may lead to further runs or DOE's).

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.



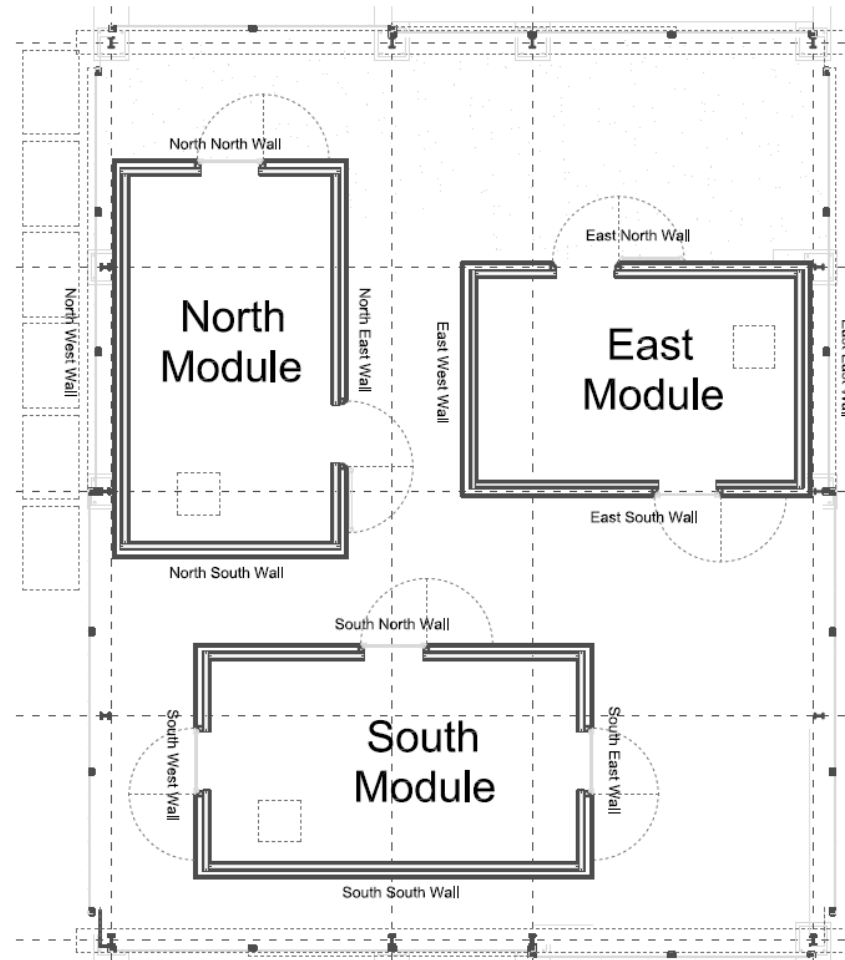
Case study

DOE applied to construction problems

Solar Decathlon Europe, LOW3



Solar Decathlon Europe, LOW3

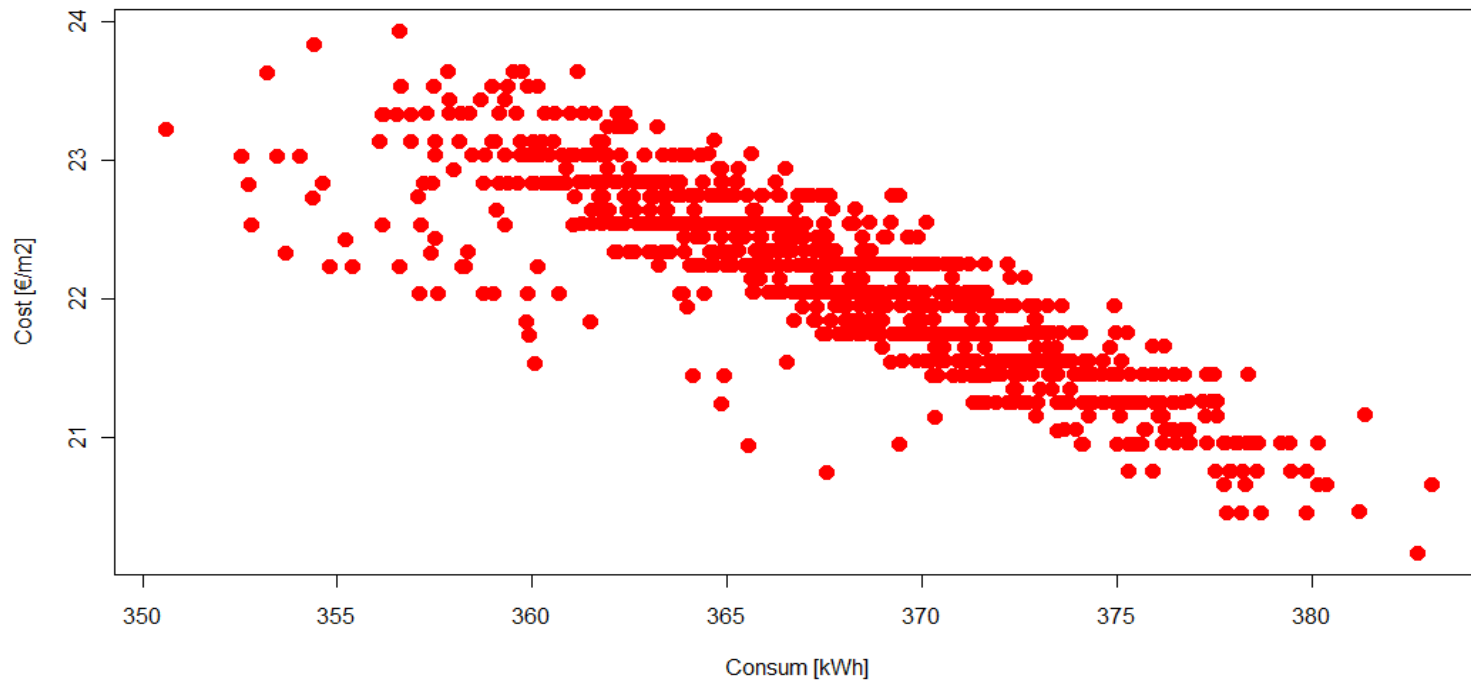


Solar Decathlon Europe, LOW3

	North MODULE				South MODULE				East MODULE			
U (W/m ² K)	North Wall	West Wall	South Wall	East Wall	North Wall	West Wall	South Wall	East Wall	North Wall	West Wall	South Wall	East Wall
s1	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212
s2	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,174
s3	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,174	0,212
s4	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,212	0,174	0,212	0,212
...
S4096	0,174	0,174	0,174	0,174	0,174	0,174	0,174	0,174	0,174	0,174	0,174	0,174

	North MODULE				South MODULE				East MODULE				Results
U (W/m ² K)	North Wall	West Wall	South Wall	East Wall	North Wall	West Wall	South Wall	East Wall	North Wall	West Wall	South Wall	East Wall	KWh
1	0	0	0	0	0	0	0	0	0	0	0	0	386,99
2	0	0	0	0	0	0	0	0	0	0	0	1	383,30
3	0	0	0	0	0	0	0	0	0	0	1	0	383,71
4	0	0	0	0	0	0	0	0	0	0	1	1	378,86
5	0	0	0	0	0	0	0	0	0	1	0	0	381,82
6	0	0	0	0	0	0	0	0	0	1	0	1	380,42
7	0	0	0	0	0	0	0	0	0	1	1	0	379,96
8	0	0	0	0	0	0	0	0	0	1	1	1	375,42

Solar Decathlon Europe, LOW3



Solar Decathlon Europe, LOW3

□ Using Yates

Module	Wall	Effects	Mean
East	East Wall	4,35	3,34
	South Wall	3,09	
	West Wall	3,26	
	North Wall	2,66	
South	East Wall	2,23	2,54
	South Wall	2,16	
	West Wall	3,44	
	North Wall	2,35	
North	East Wall	2,74	3,46
	South Wall	4,65	
	West Wall	1,60	
	North Wall	4,86	

Solar Decathlon Europe, LOW3

- To know more:

- ▣ Fonseca i Casas, P., Fonseca i Casas, A., Garrido-Soriano, N., & Casanovas, J. (2014). Formal simulation model to optimize building sustainability. *Advances in Engineering Software*, 69, 62–74.
doi:10.1016/j.advengsoft.2013.12.009