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:** Assignation 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.

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?*

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

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

A	B (Mbytes) 32	64	128
1	0.25	0.21	0.15
2	0.52	0.45	0.36
3	0.81	0.66	0.50
4	1.50	1.45	0.70

Two-factor ANOVA

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

Two Factors, *n* Replications

		Factor A					
		1	2	…	j	…	a
Factor B	1	…	…	…	…	…	…
	2	…	…	…	…	…	…
	…	…	…	…	…	…	…
	i	…	…	…	y_{ijk}	…	…
	…	…	…	…	…	…	…
	b	…	…	…	…	…	…

n replications

One-factor ANOVA

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

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

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

$$\alpha_i = \text{effect due to A}$$

$$e_{ij} = \text{measurement error}$$

Two-factor ANOVA

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

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

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

$$\alpha_i = \text{effect due to A}$$

$$\beta_j = \text{effect due to B}$$

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

$$e_{ijk} = \text{measurement error}$$

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

$$\underbrace{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}\left(Y_{ijk}-\bar{Y}_{\cdots}\right)^2}_{SS_{Total}} = \underbrace{r\cdot b\cdot\sum_{i=1}^{a}\left(\bar{Y}_{i\cdot\cdot}-\bar{Y}_{\cdots}\right)^2}_{SS_A} + \underbrace{r\cdot a\cdot\sum_{j=1}^{3}\left(\bar{Y}_{\cdot j\cdot}-\bar{Y}_{\cdots}\right)^2}_{SS_B}$$

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

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

ANOVA table

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

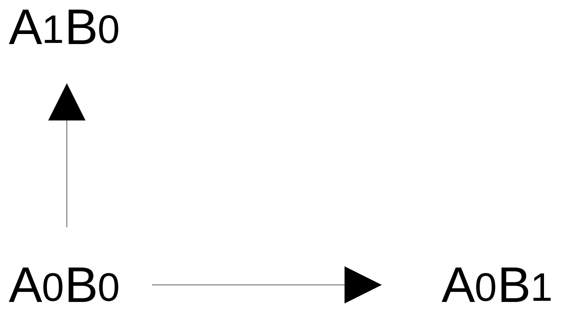
Factorial designs

Explore the landscape

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: A1B0-A0B0.
- Effect B: A0B1-A0B0



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:

$$\frac{A_1B_1 - A_0B_1}{2} - \frac{A_0B_0 - A_1B_0}{2}$$

$$\begin{tikzcd}
A_1B_0 \arrow[r] & A_1B_1 \\
A_0B_0 \arrow[u] \arrow[r] & A_0B_1 \arrow[u]
\end{tikzcd}$$

Factorial designs

- Controlling “k” factors.
- “l” levels for each factor (“li” levels for the l factor).
- $l_1 \cdot l_2 \cdot \ldots \cdot l_k$ experiments
- The easiest factorial design is the 2k with li = 2 ∀i = 1,..,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
- m factors, v levels, n replications

  $\rightarrow n\, v^m$ experiments
- *Example:*
  - $m = 5$ input factors, $v = 4$ levels, $n = 3$
  - $\rightarrow 3(4^5) = 3{,}072$ experiments!

Fractional Factorial Designs: $n2^m$ 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

$n2^m$ Experiments

	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	$F_{[1-\alpha;1,2^m(n-1)]}$	$F_{[1-\alpha;1,2^m(n-1)]}$	$F_{[1-\alpha;1,2^m(n-1)]}$	

Finding Sum of Squares Terms

Sum of *n* measurements with (A,B) = (High, Low)	Factor A	Factor B
y_{AB}	High	High
y_{Ab}	High	Low
y_{aB}	Low	High
y_{ab}	Low	Low

Contrasts for $n2^m$ with $m = 2$ factors -- revisited

Measurements	**Contrast**		
	w_a	w_b	w_{ab}
$\mathbf{y_{AB}}$	+	+	+
$\mathbf{y_{Ab}}$	+	-	-
$\mathbf{y_{aB}}$	-	+	-
$\mathbf{y_{ab}}$	-	-	+

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

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

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

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

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

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

$n2^m$ with $m = 3$ factors

$$SSAC = \frac{w_{AC}^2}{2^3 n}$$

- df(each effect) = 1, since only two levels measured
- SST = SSA + SSB + SSC + SSAB + SSAC + SSBC + SSABC
- df(SSE) = $(n-1)2^3$
- Then perform ANOVA as before
- Easily generalizes to m > 3 factors

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 *m* factors
- Use $n2^m$ design to reduce the number of experiments needed
  - But loses some information
  - Useful to undertint the tendency with economy of experiments.

Yates algorithm

Simplifying the interaction calculus on a 2k factorial design

2k 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.

2k Matrix

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

2k Matrix example

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

Interactions for 2 and 3 factors

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

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

Effects calculus example

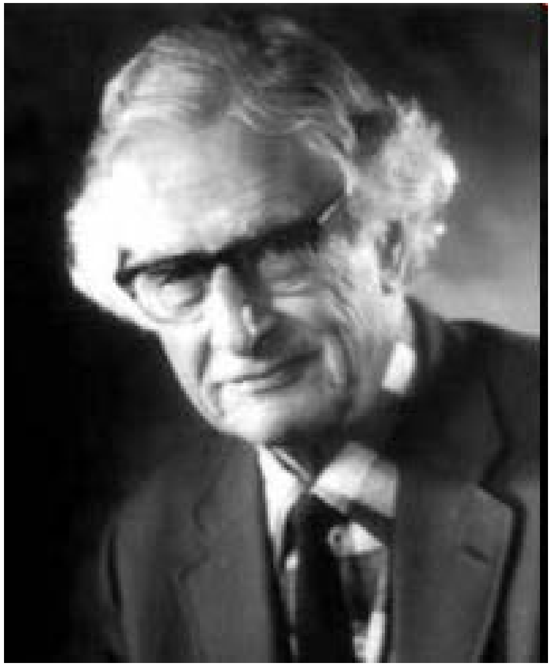
$$Main\ effect = \overline{y}_{+} - \overline{y}_{-}$$

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

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

$$C = \frac{52+83+45+80}{4} - \frac{60+72+54+68}{4} = 1.5$$

Frank Yates



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

Yates algorithm

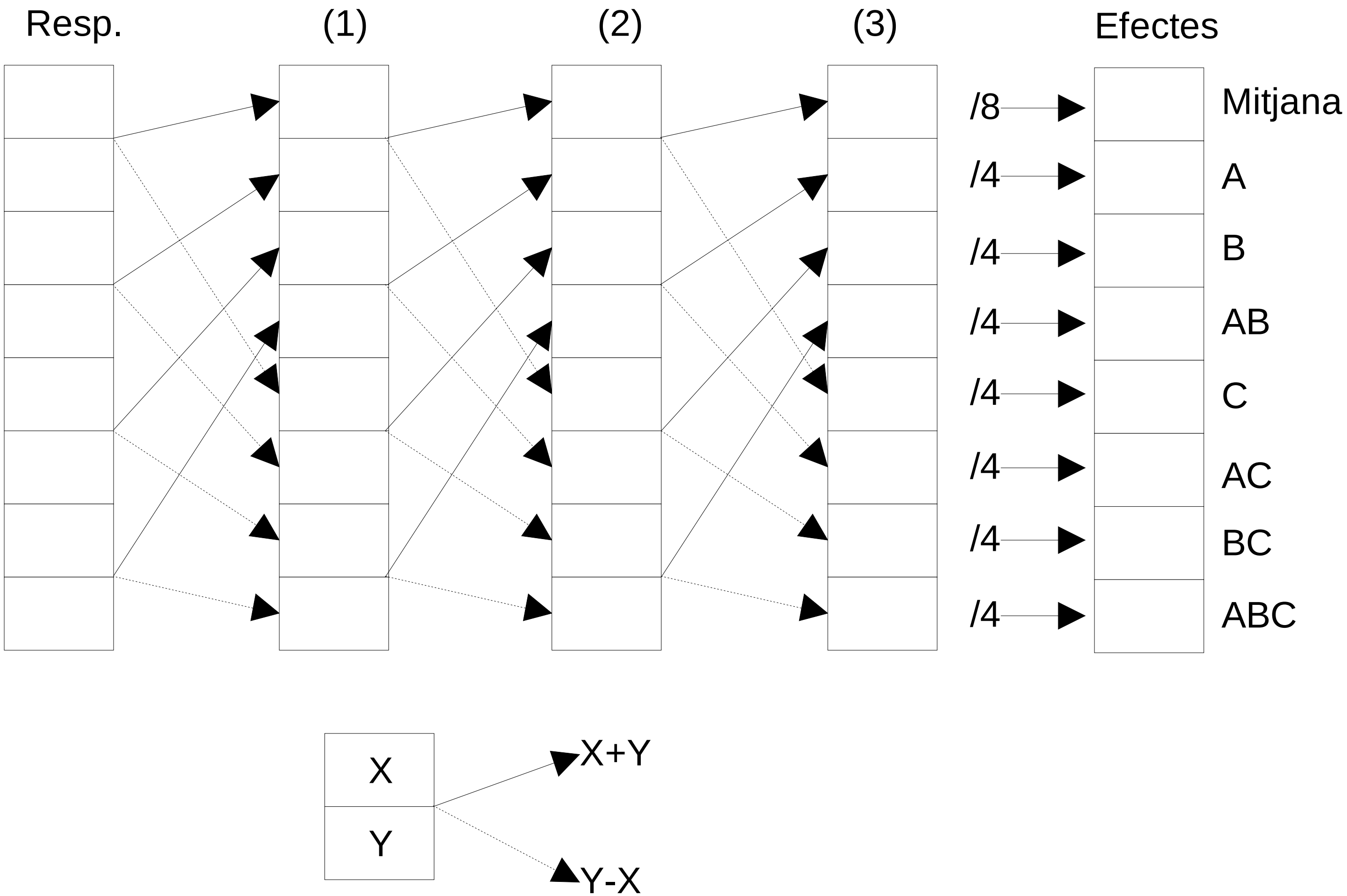
To make systematic the interactions calculus using a table.

- 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 wit two + on A and C corresponds to the interaction of AC, etc.

Yates algorithm



Yates algorithm example

Exp.	A	B	C	Resp	(1)	(2)	(3)	div.	efecte	Id
1	-	-	-	60	132	254	514	8	64.25	Mitja
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 useof 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	Efecte	Descripció
(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

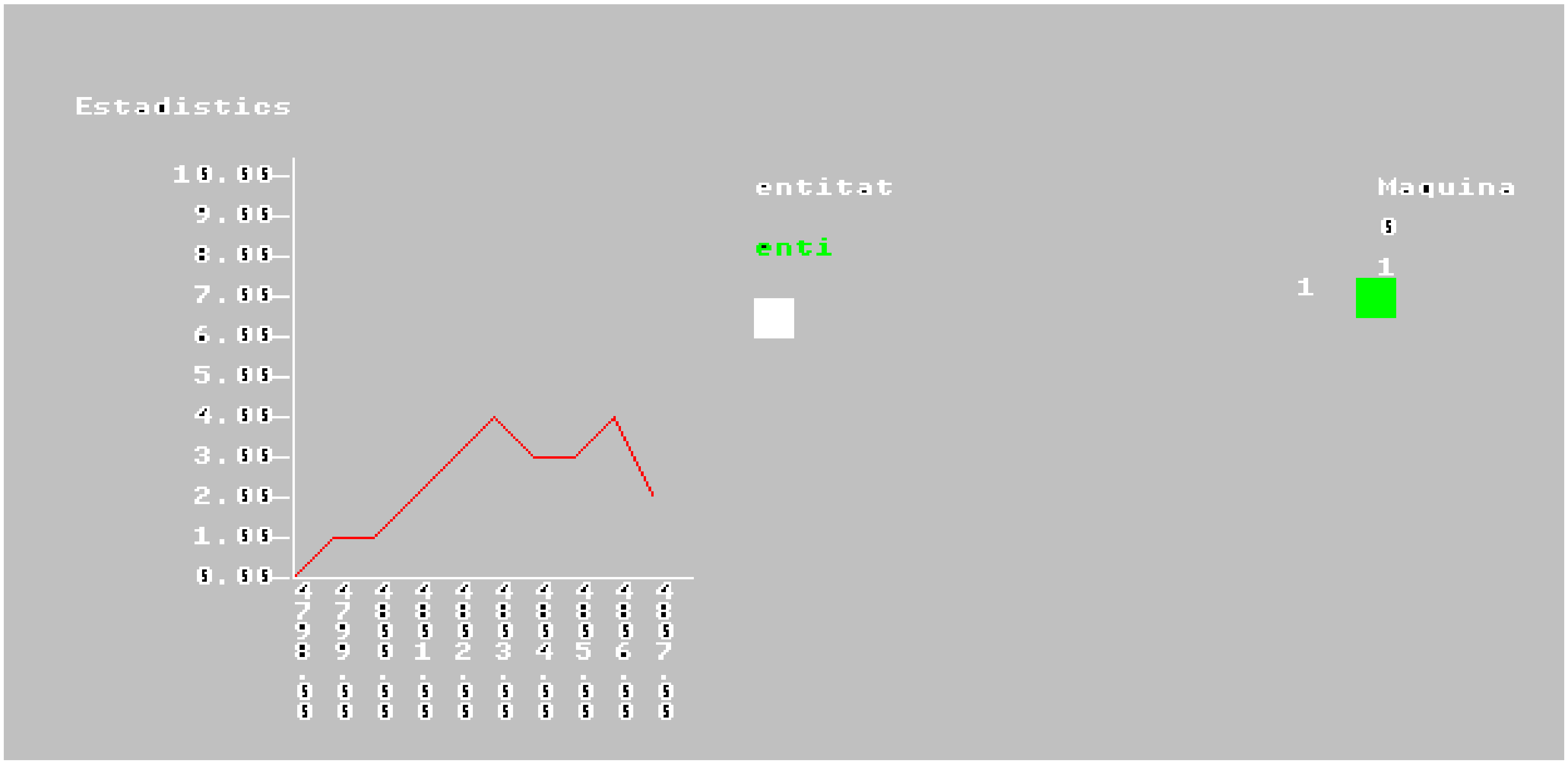
Comb.	obs.	1	2	3	4	Efects	Description
(1)	71	132	304	600	1156	72,25	Mean
a	61	172	296	556	-64	-8	A
b	90	129	283	-32	192	24	B
ab	82	167	273	-32	8	1	AB
c	68	111	-18	78	-18	-2,25	C
ac	61	172	-14	114	6	0,75	AC
bc	87	110	-17	2	-10	-1,25	BC
abc	80	163	-15	6	-6	-0,75	ABC
d	61	-10	40	-8	-44	-5,5	D
ad	50	-8	38	-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

Replications

Number of replications calculus.

Methods to perform the replications.

Interest variable calculus



Experimentation

- Be x an interest variable

  x11,...x1i,...,x1m

  x21,...x2i,...,x2m

  ....

  xn1,...xni,...,xnm

- *n* is the number of replications.
- *xi* is the value of each one of the replications.

Sample mean μ

$$\overline{X} = \frac{\sum_{i=1}^{n} x_i}{n}$$

Sample variance σ2

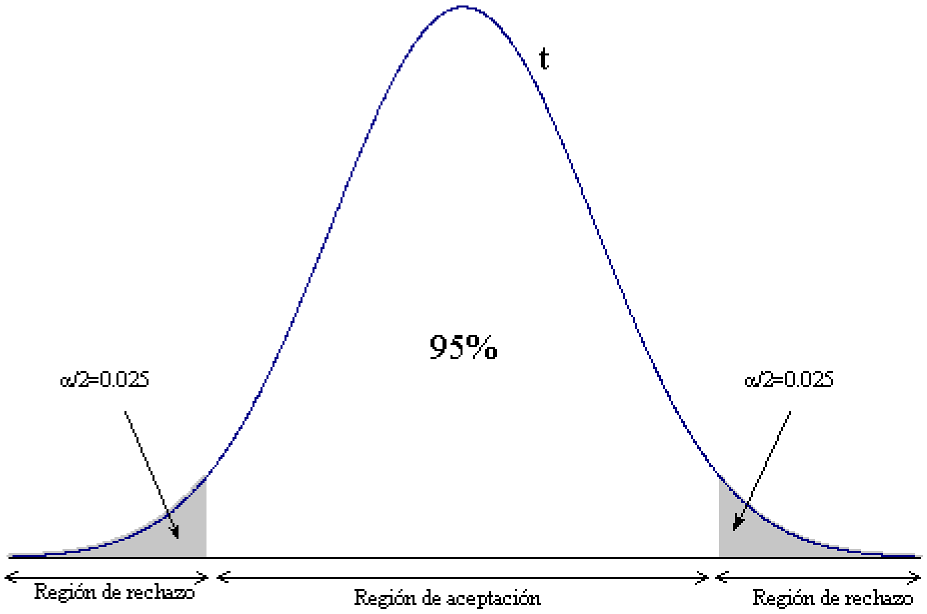
$$S^2 = \frac{\sum_{i=1}^{n} x_i - \overline{X}}{n-1}$$

Confidence interval

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

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

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 an X

$$\overline{X} = 32.4818$$

$$S = 3.5149$$

Calculus of the self-confidence interval

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

$t_{9,0.975} = 2,26$
$h = 2,512$

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

- on:
- 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...

Rèplica	Mesura de rendiment
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

$$\overline{X} = 32.1094$$

$$S = 3.1903$$

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

Replications

Methods to execute the replications.

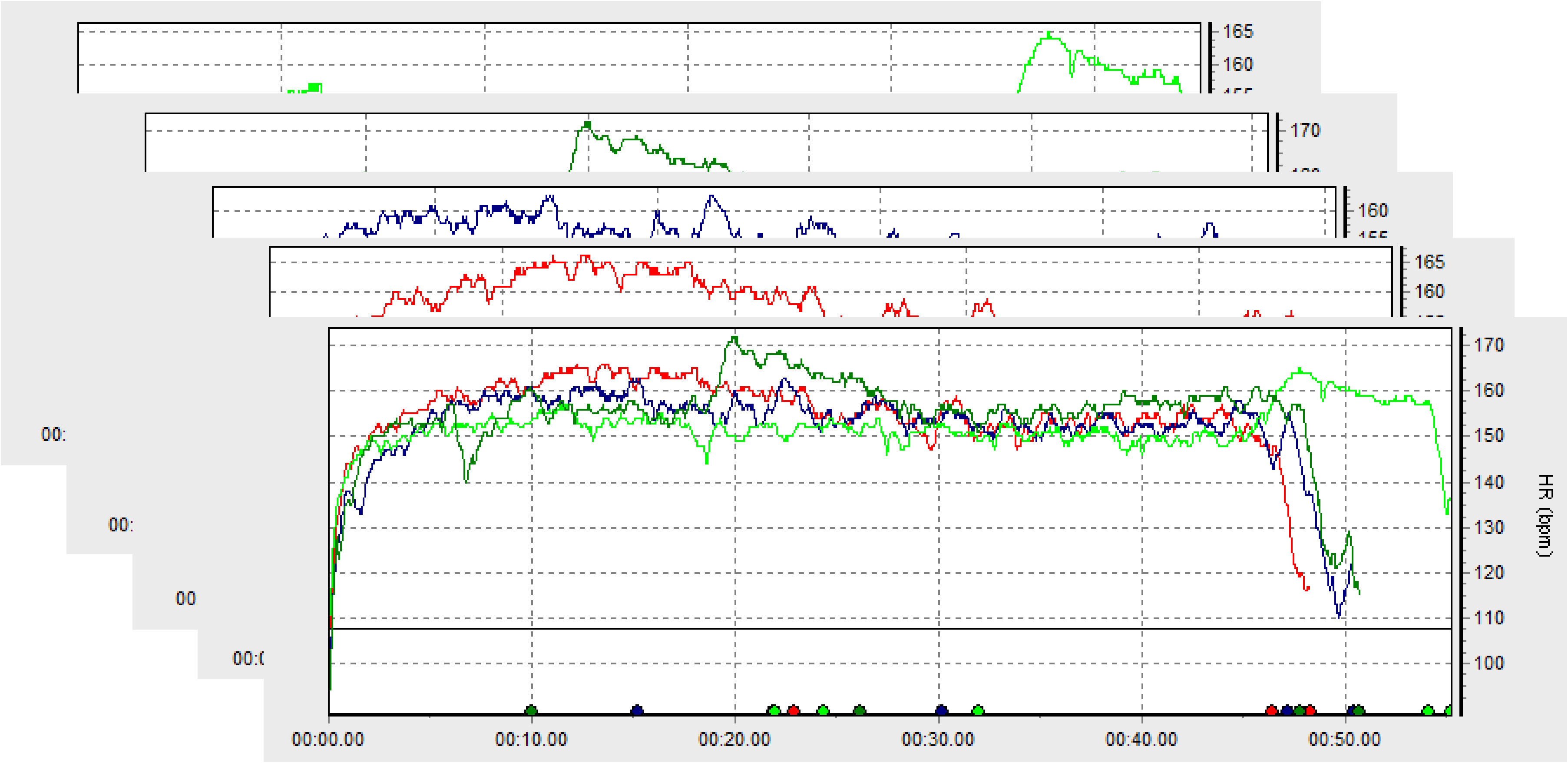
Kind of simulations

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

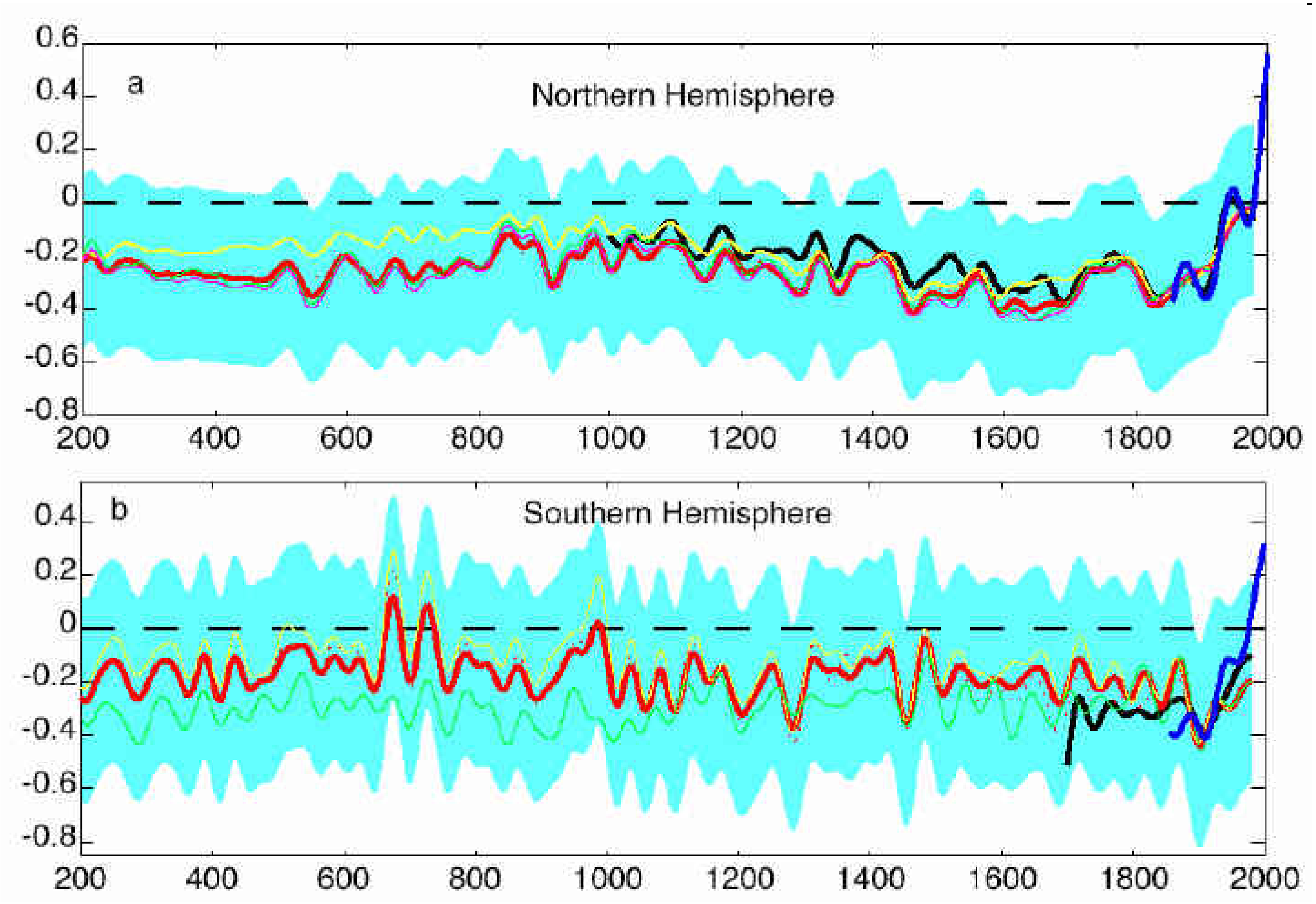
Independent repetitions

- From the same initial state of the model, that means, with the same parameterizations and behavior, only random numbers to be used un 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).

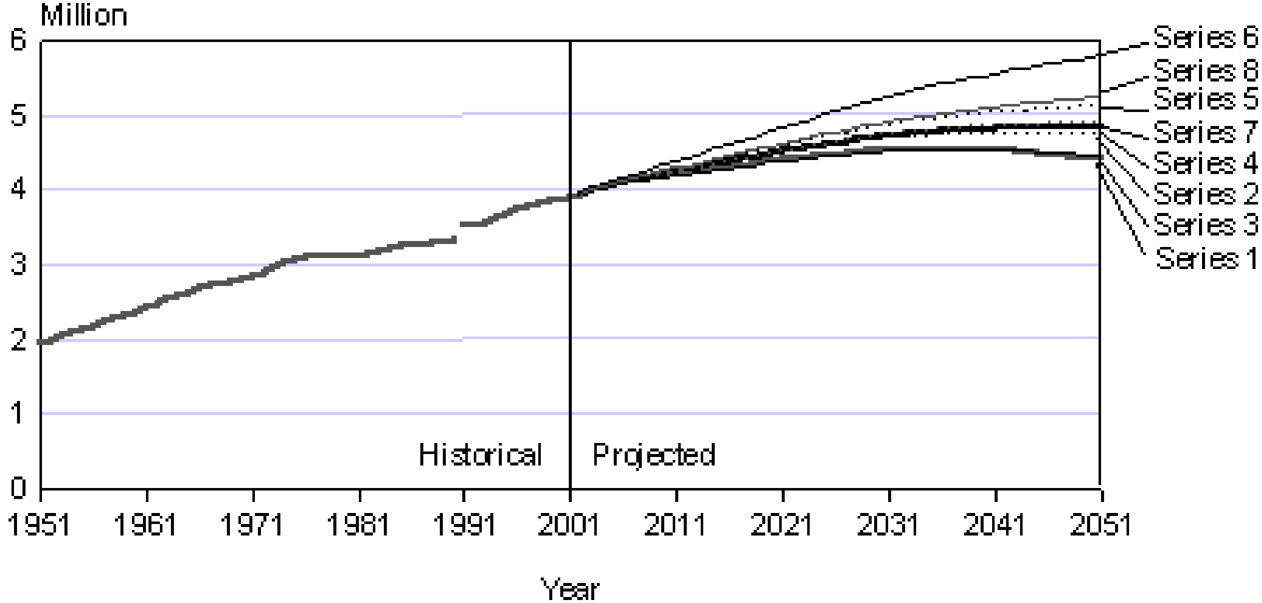
Independent repetitions



Independent repetitions



Independent repetitions

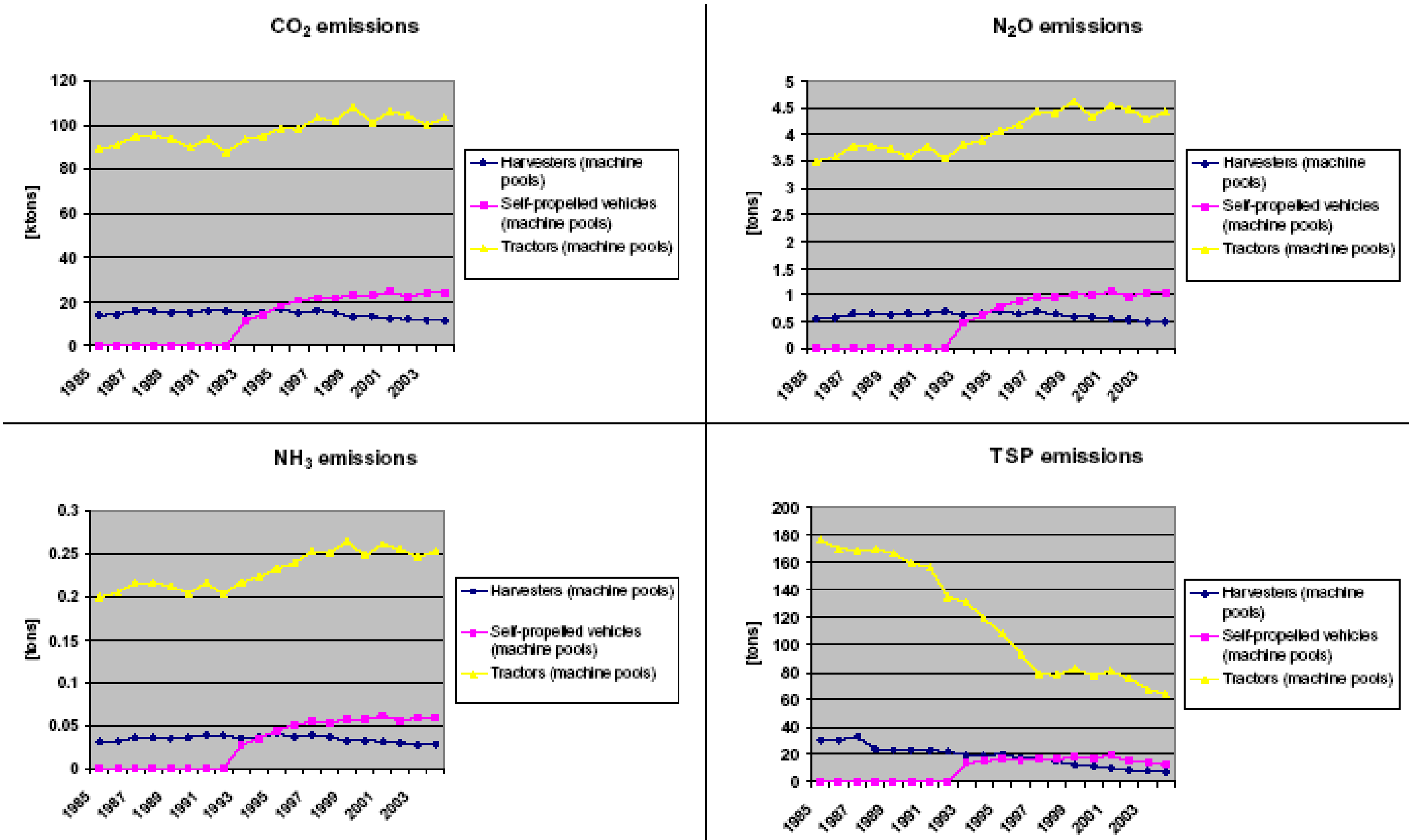


Note: The break in series between 1990 and 1991 denotes a change from the de facto population concept to the resident population concept.

Batch means

- Execute a long simulation and then divide it in different blocks, or execution bags.
  - We work with the mean values of these observations.
- 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

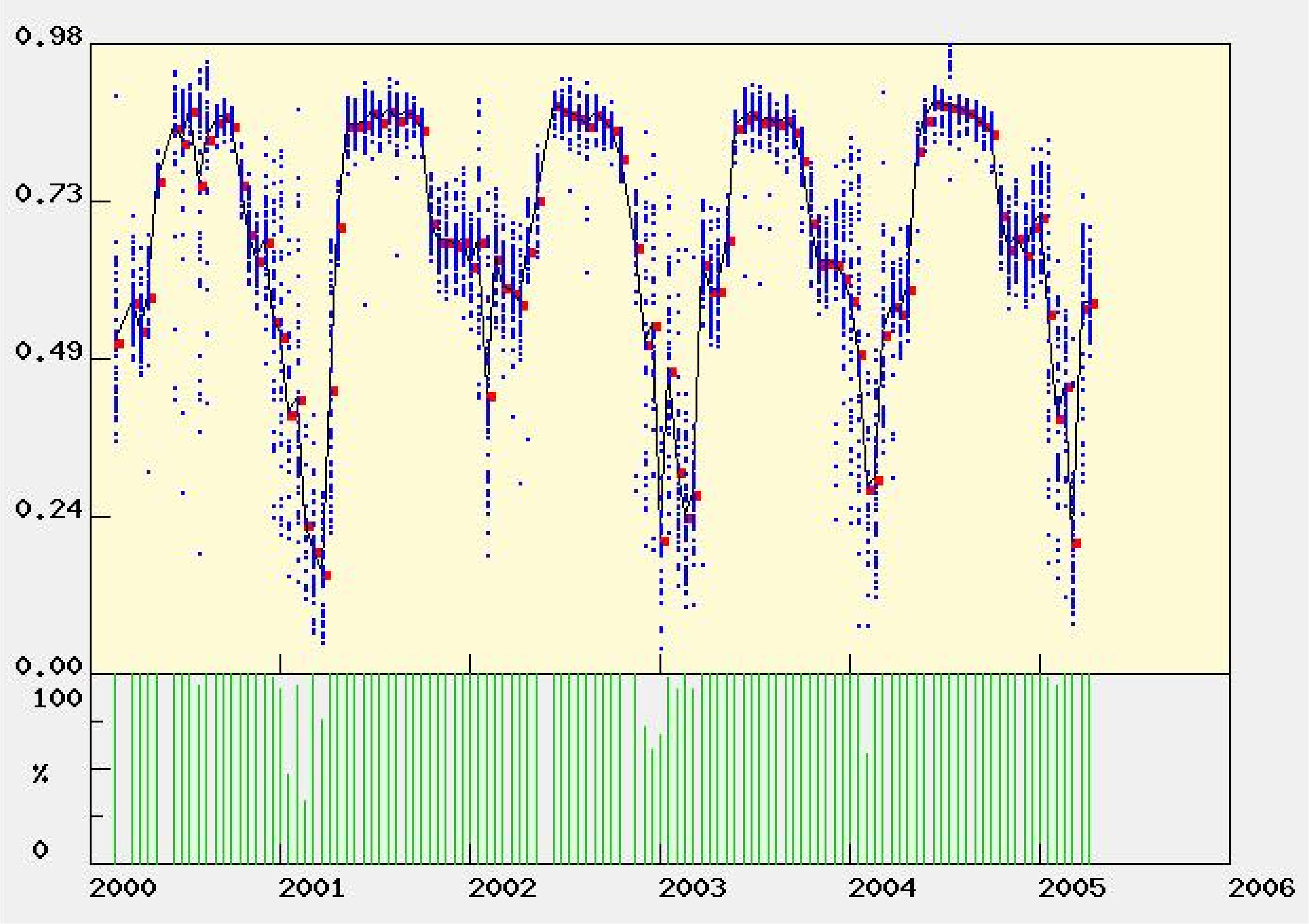


CO$_2$ emissions
[ktons]
120
100
80
60
40
20
0
1985
1987
1989
1991
1993
1995
1997
1999
2001
2003
Harvesters (machine pools)
Self-propelled vehicles (machine pools)
Tractors (machine pools)
N$_2$O emissions
[tons]
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
1985
1987
1989
1991
1993
1995
1997
1999
2001
2003
Harvesters (machine pools)
Self-propelled vehicles (machine pools)
Tractors (machine pools)
NH$_3$ emissions
[tons]
0.3
0.25
0.2
0.15
0.1
0.05
0
1985
1987
1989
1991
1993
1995
1997
1999
2001
2003
Harvesters (machine pools)
Self-propelled vehicles (machine pools)
Tractors (machine pools)
TSP emissions
[tons]
200
180
160
140
120
100
80
60
40
20
0
1985
1987
1989
1991
1993
1995
1997
1999
2001
2003
Harvesters (machine pools)
Self-propelled vehicles (machine pools)
Tractors (machine pools)

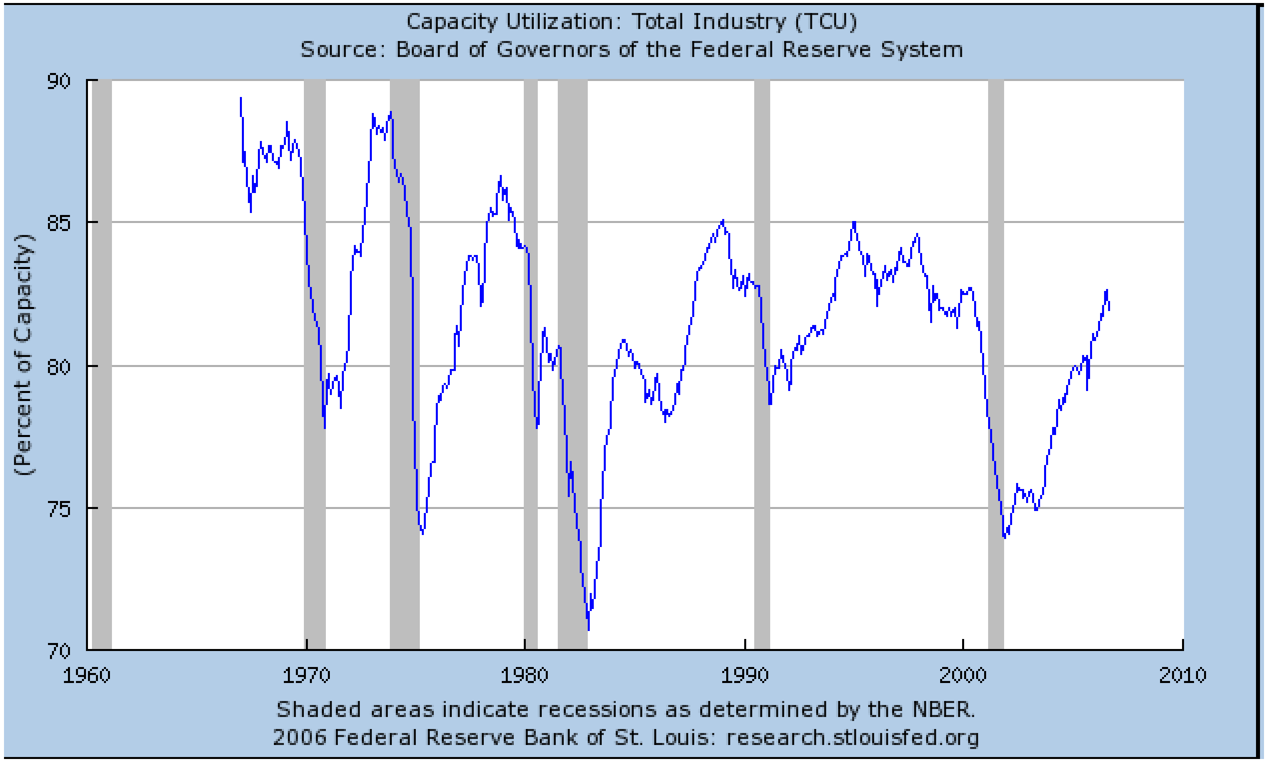
Regenerative methods

- 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



Regenerative methods

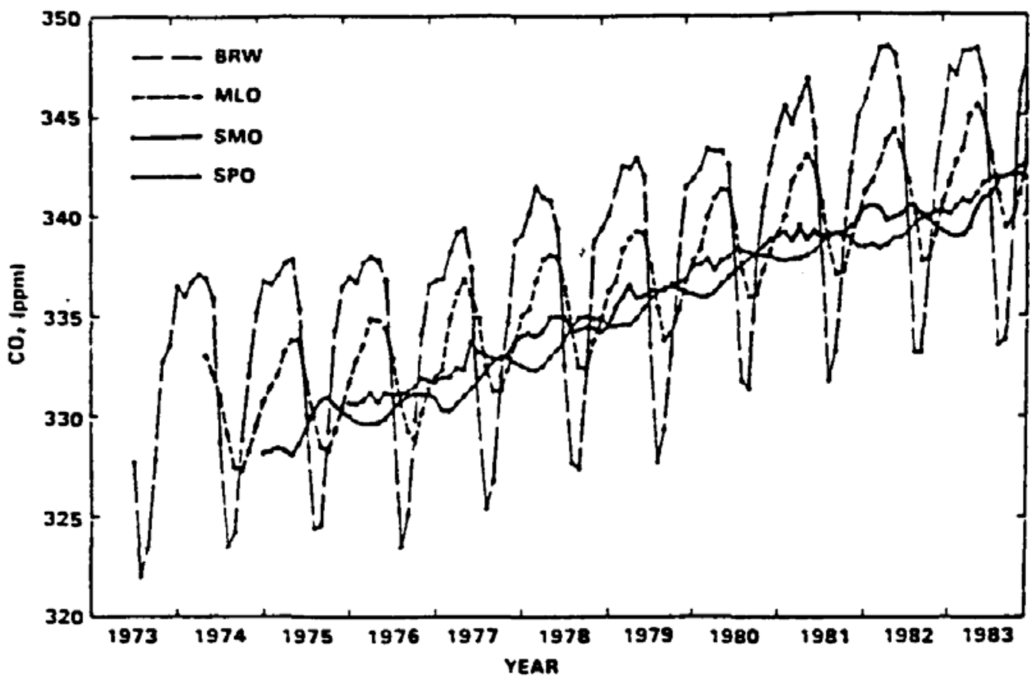


Fig. 1. Selected monthly mean carbon dioxide concentrations from continuous measurements (Barrow, Alaska (BRW); Mauna Loa, Hawaii (MLO); American Samoa (SMO); South Pole (SPO). From: WMO, 1985.

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).

$$(\bar{x} - k\, {}^{s}\!/_{\sqrt{n}},\ \bar{x} + k\, {}^{s}\!/_{\sqrt{n}})$$

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.

$$s \big/ \sqrt{n}$$

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.

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 it's 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 reduce the difference.

Fractional factorial designs

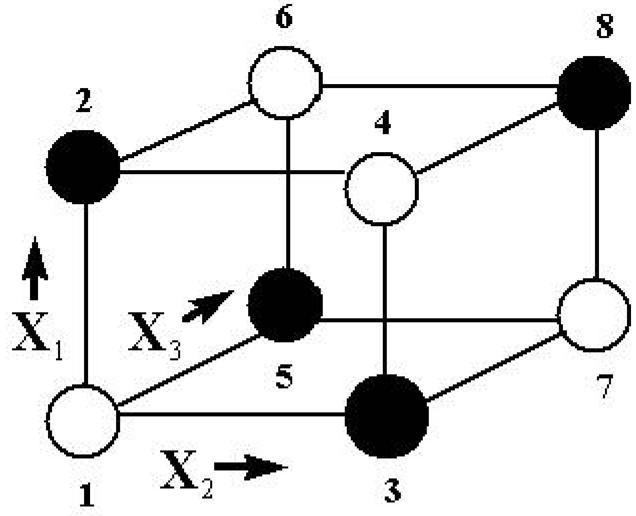
Still Too Many Experiments with $n2^m$!

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

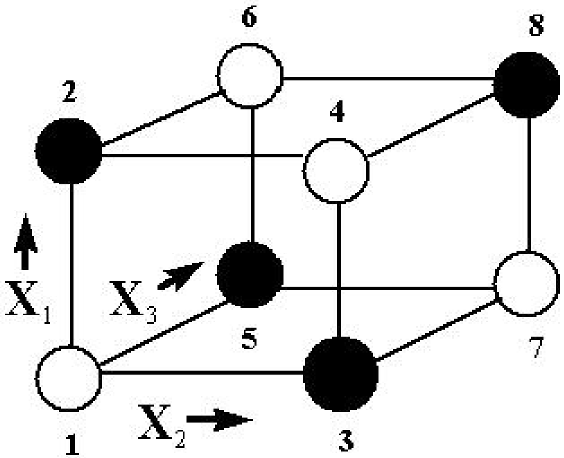
	X1	X2	X3	Y
1	-1	-1	-1	$y_1 = 33$
2	+1	-1	-1	$y_2 = 63$
3	-1	+1	-1	$y_3 = 41$
4	+1	+1	-1	$Y_4 = 57$
5	-1	-1	+1	$y_5 = 57$
6	+1	-1	+1	$y_6 = 51$
7	-1	+1	+1	$y_7 = 59$
8	+1	+1	+1	$y_8 = 53$

Computing the effects

- Effect of C1= (1/4)(y2 + y4 + y6 + y8) - (1/4)(y1 + y3 + y5 + y7)
- 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

	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	$y_8 = 53$



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)

Notation

- X3 = X1*X2 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

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

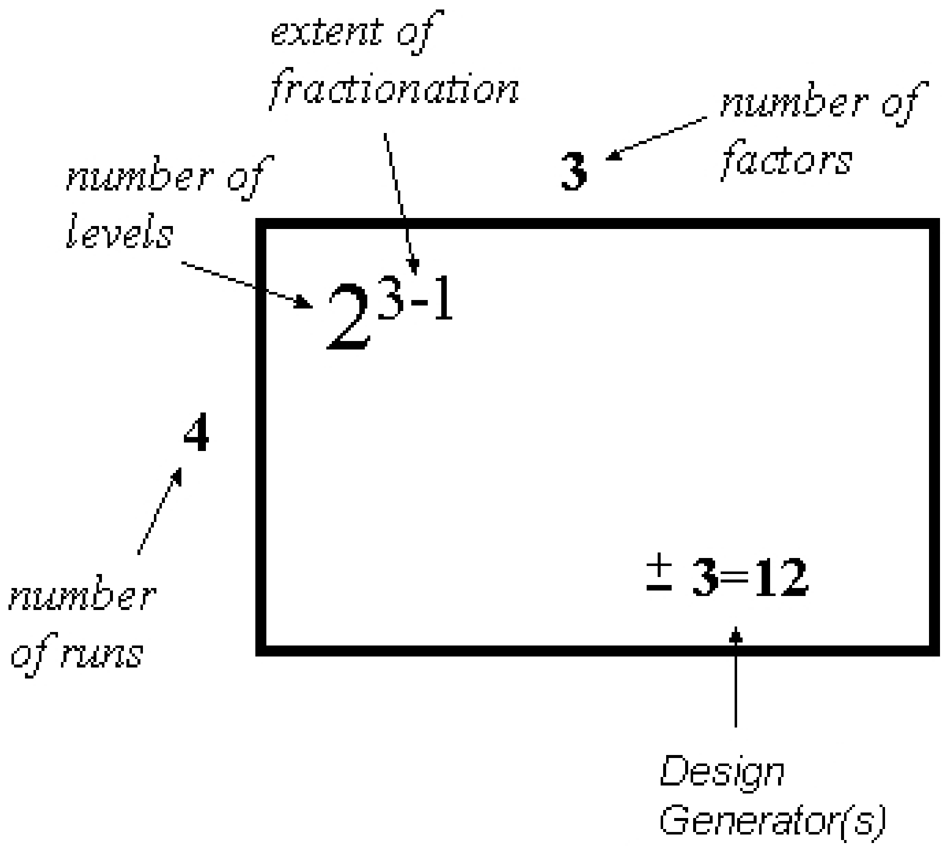
Principal fraction

- 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 the 2^{3-1} design are confounded with two-factor interactions.
  - That is the price we pay for using this fractional design.
- 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?

8

32

2^{8-3}

$\pm 6 = 345$

$\pm 7 = 1245$

$\pm 8 = 1235$

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.

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
-1	-1	1	-1	1	1	-1	1
1	-1	1	-1	1	-1	1	1
-1	1	1	-1	1	-1	1	-1
1	1	1	-1	1	1	-1	-1
-1	-1	-1	1	1	-1	1	1
1	-1	-1	1	1	1	-1	1
-1	1	-1	1	1	1	-1	-1
1	1	-1	1	1	-1	1	-1
-1	-1	1	1	1	1	1	-1
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 aliased (or confounded) 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

8

32

$$2^{8-3}_{IV}$$

$\pm$ 6=345

$\pm$ 7=1245

$\pm$ 8=1235

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(2m) or O(vm)

Plackett and Burman Designs

- PB designs exist only in sizes that are multiples of 4
- Requires X experiments for m parameters
  - X = 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	9
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	9
2	-1	+1	+1	+1	-1	+1	-1	11
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	9
2	-1	+1	+1	+1	-1	+1	-1	11
3	-1	-1	+1	+1	+1	-1	+1	2
4	+1	-1	-1	+1	+1	+1	-1	1
5	-1	+1	-1	-1	+1	+1	+1	9
6	+1	-1	+1	-1	-1	+1	+1	74
7	+1	+1	-1	+1	-1	-1	+1	7
8	-1	-1	-1	-1	-1	-1	-1	4
Effect								

PB Design Matrix

Config	Input Parameters (factors)							Response
	A	B	C	D	E	F	G	
1	+1	+1	+1	-1	+1	-1	-1	9
2	-1	+1	+1	+1	-1	+1	-1	11
3	-1	-1	+1	+1	+1	-1	+1	2
4	+1	-1	-1	+1	+1	+1	-1	1
5	-1	+1	-1	-1	+1	+1	+1	9
6	+1	-1	+1	-1	-1	+1	+1	74
7	+1	+1	-1	+1	-1	-1	+1	7
8	-1	-1	-1	-1	-1	-1	-1	4
Effect	16.25							

$$16.25 = (+1(9) + 1(1) + 1(74) + 1(7))/4 - (1(11) + 1(2) + 1(9) + 1(4))/4$$

PB Design Matrix

Config	Input Parameters (factors)							Response
	A	B	C	D	E	F	G	
1	+1	+1	+1	-1	+1	-1	-1	9
2	-1	+1	+1	+1	-1	+1	-1	11
3	-1	-1	+1	+1	+1	-1	+1	2
4	+1	-1	-1	+1	+1	+1	-1	1
5	-1	+1	-1	-1	+1	+1	+1	9
6	+1	-1	+1	-1	-1	+1	+1	74
7	+1	+1	-1	+1	-1	-1	+1	7
8	-1	-1	-1	-1	-1	-1	-1	4
Effect	16,25	-11,25	18,75	-18,75	-18,75	18,25	16,75	

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

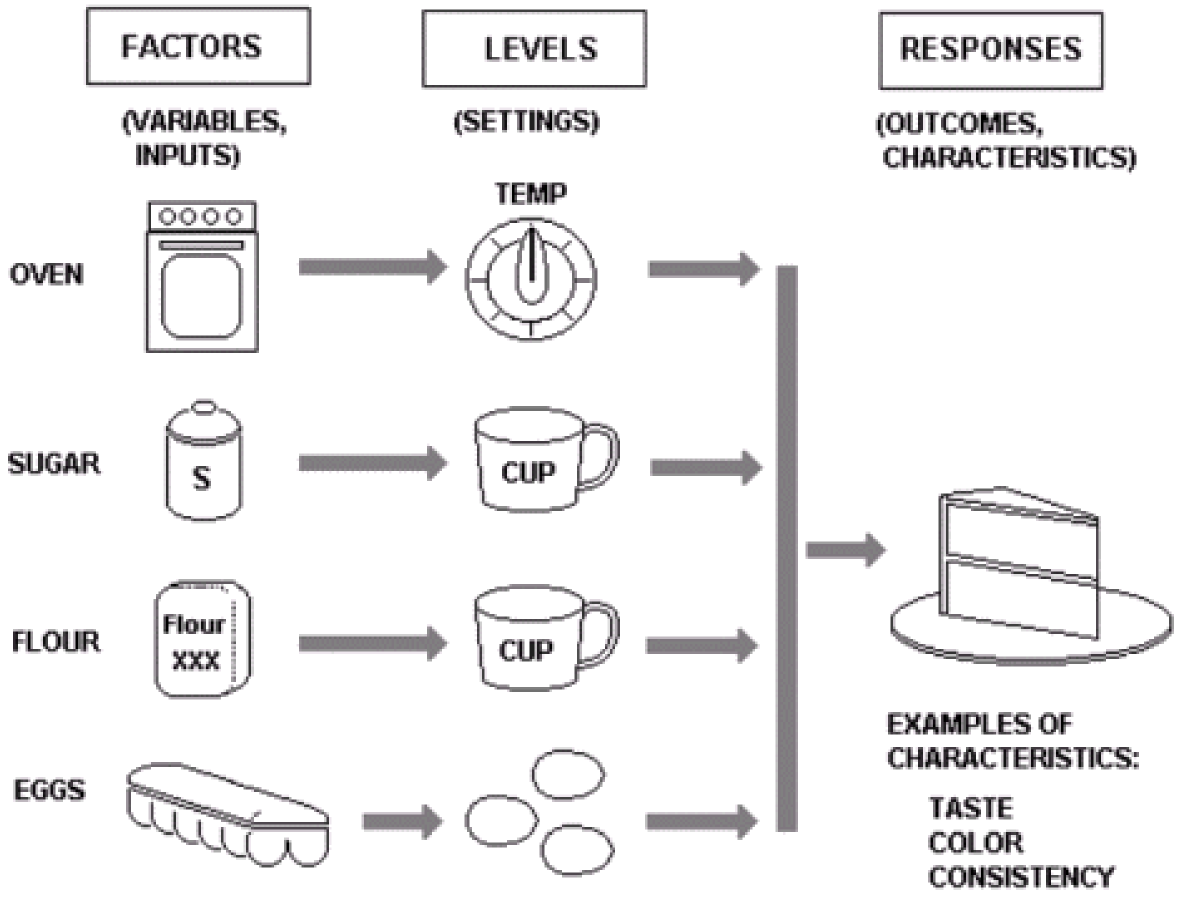
Minerals	Molecular formulae	Assay (%)	
		Transition ore	Leach residue
Native Cu	Cu	0.39	0.30
Chalcopyrite	$CuFeS_2$	r	r
Bornite	Cu_5FeS_4	r	r
Chalcosite	Cu_2S	rr	rr
Covelite	CuS	rr	rr
Cuprite	Cu_2O	t	-
Malachite	$Cu_2(CO_3)(OH)_2$	t	-
Goethite/Limonite	$HFeO_2$ / $Fe_2O_3.H_2O$	26	21
Iron oxide	Fe_2O_3, Fe_3O_4	8	7
Clorite	$(Mg,Al,Fe)_{12}[(Si,Al)_8O_{20}](OH)_{16}$	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%

Table 5: Matrix for twelve replicated experiments based on the Plackett-Burman method and their respective copper extraction responses (R_1, R_2)

Test	Variable											Response (%)	
	A	X1	B	C	D	X2	E	F	G	X3	X4	R_1	R_2
1	+	+	-	+	+	+	-	-	-	+	-	70.5	71.8
2	+	-	+	+	+	-	-	-	+	-	+	77.6	77.4
3	-	+	+	+	-	-	-	+	-	+	+	67.2	68.2
4	+	+	+	-	-	-	+	-	+	+	-	73.2	74.4
5	+	+	-	-	-	+	-	+	+	-	+	77.0	76.8
6	+	-	-	-	+	-	+	+	-	+	+	76.5	77.9
7	-	-	-	+	-	+	+	-	+	+	+	74.0	73.5
8	-	-	+	-	+	+	-	+	+	+	-	59.9	59.9
9	-	+	-	+	+	-	+	+	+	-	-	73. 9	73.9
10	+	-	+	+	-	+	+	+	-	-	-	80.2	78.0
11	-	+	+	-	+	+	+	-	-	-	+	66.5	64.9
12	-	-	-	-	-	-	-	-	-	-	-	69.3	68.0

Your exercise



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.