

El Diseno de Experimentos en la Modelacion de Sistemas Ecologicos: Consideraciones, Problemas y Soluciones.

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Sinopsis

- Planteo del Problema
- Algunas Soluciones
- Ejemplo de Simulacion
- Disenos Experimentales
- Ventajas y resultados
- Problemas y consecuencias
- Otras consideraciones
- Conclusiones

Planteo del Problema

- Dada una red de masas de agua
 - E.g. Grandes Lagos, Puertos Fluviales
- Optimizar las medidas de rendimiento
 - Preservacion; Utilizacion; Exportacion etc.
- Sujetas a un conjunto de restricciones economicas, sociales, laborales, politicas, ambientales, climaticas, culturales, etc.
- Manteniendo Robustez respecto a “ruido”

Metodos de Resolucion

- Teoricos (leyes o relaciones fisicas)
 - Pero, podremos encontrar tal ecuacion?
- Empiricos (e.g. regresion)
 - Encontraremos datos para implementarlo?
- Simulation Discreta
 - No hace falta relajar los supuestos
 - Puede incluir complejas interacciones
 - Tiempos de corrida sumamente largos!

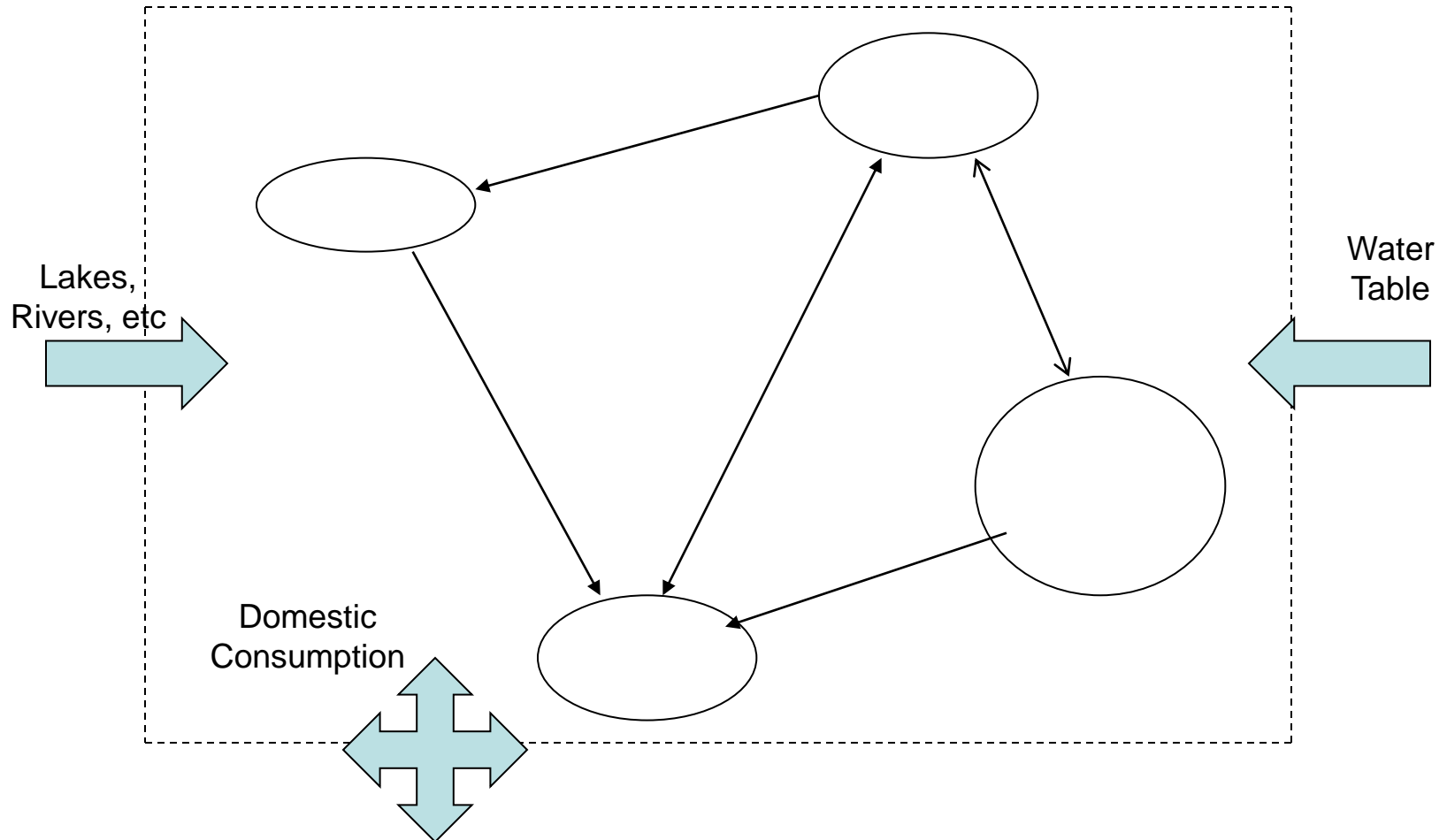
Problemas de Modelizacion

- Un Complejo Modelo de Simulacion
- Principales complicaciones:
 - Demasiadas variables en el sistema
 - Estructura de un “sistema dinamico”
- Solucion propuesta
 - Obtener un Meta Modelo mas sencillo
 - Via Diseno de Experimentos (DOE)
 - Usarlo como sustituto del modelo original

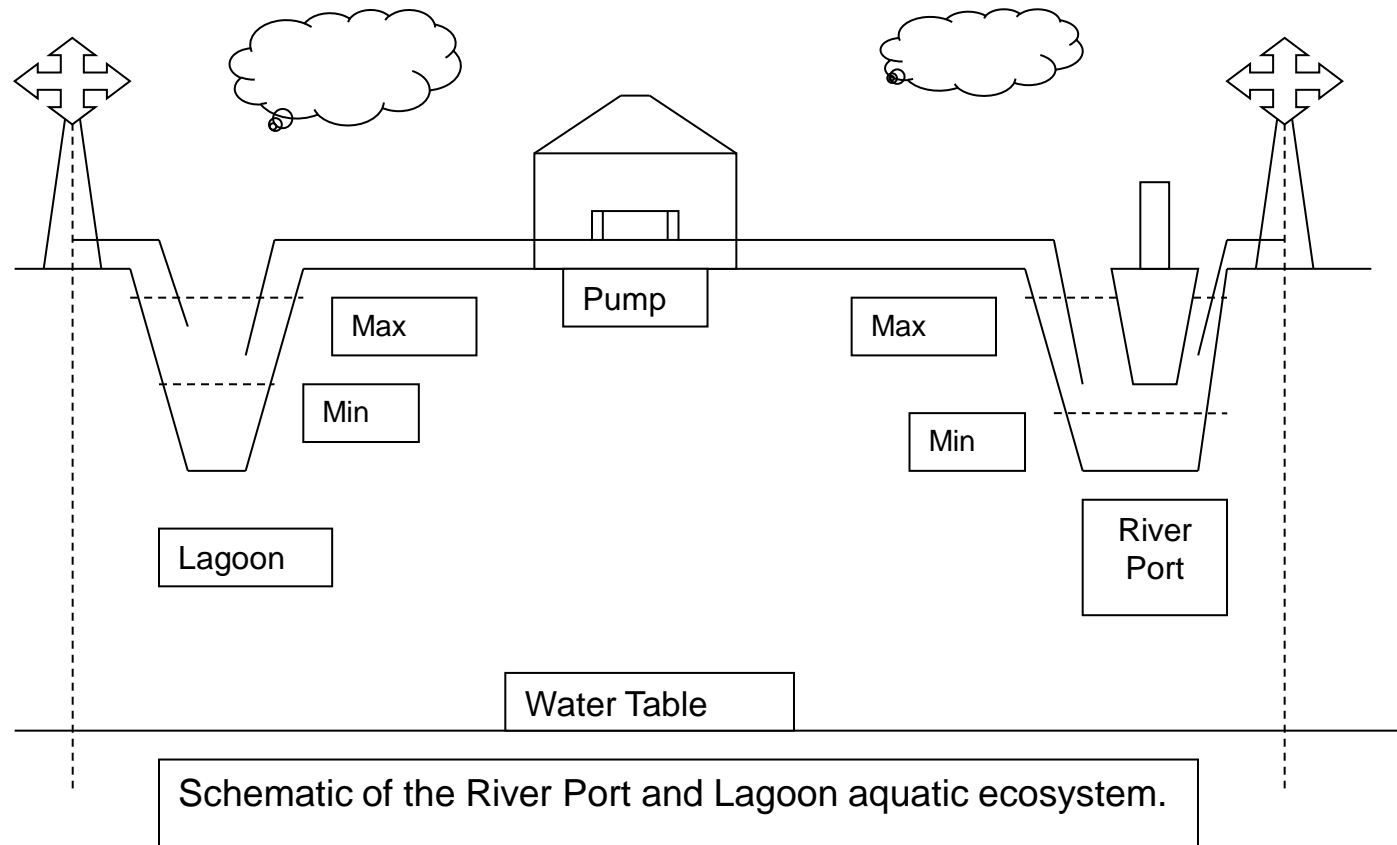
Ejemplo de una Simulacion

- Dada una red de Puerto Fluvial y Laguna
- Optimizar ciertas medidas de rendimiento
 - Del su uso social, comercial o industrial
- Sometidas a restricciones economicas, comerciales, politicas, ambientales etc.
 - Mantener los niveles de produccion,
 - De empleo, ecologicos, sociales etc.
- Robustas a “ruidos” (climaticas etc.)

Red de Masas de Agua Interconectadas



Ejemplo: Puerto Fluvial/Laguna



Variables de Decision

- ECONOMICAS
- Niveles de Relleno
- Capacidad de Presa
- Orden de Relleno
- Politicas de Transferencias
- Politicas de Uso
- Politicas de Escasez
- Nivel del Manto
- Condiciones Iniciales
- ECOLOGICAS
- Tierras Humedas
- Temperatura de aguas
- Velocidad de aguas
- Salinidad de aguas
- Nivel de Polucion
- Area/Profundidad
- Poblacion Piscicola
- Poblacion avicola
- Reproduccion

Costos Asociados

- ECONOMICOS
- De bombeo del Manto
- De bombeo entre masas de agua
- De venta a usuarios
- De escasez de agua
- De falta de agua
- Costos Indirectos
- Costos Totales
- ECOLOGICOS
- De Extincion de especies
- De Biodegradacion
- Danos al habitat
- Reacondicionamiento
- Relocalizacion
- Costos Indirectos
- Costos Totales

Variables Libres y Aplicaciones

- *VARIABLES RUIDO*
- Nivel del Manto
- Condiciones Climaticas
- Regimen de Lluvias
- Salinidad de Aguas
- Oxigeno del Agua
- Temperatura
- Evaporacion
- *APLICACIONES*
- Estudio
- Nuevo Diseno
- Optimizacion
- Comparacion de:
 - -estrategias
 - -regulaciones
- Impactos ecologicos
- Mediacion/conflictos

Variables Adicionales

- Political issues
- Labor issues
- Water Theft
- Water Leaks
- Markets
- Financial

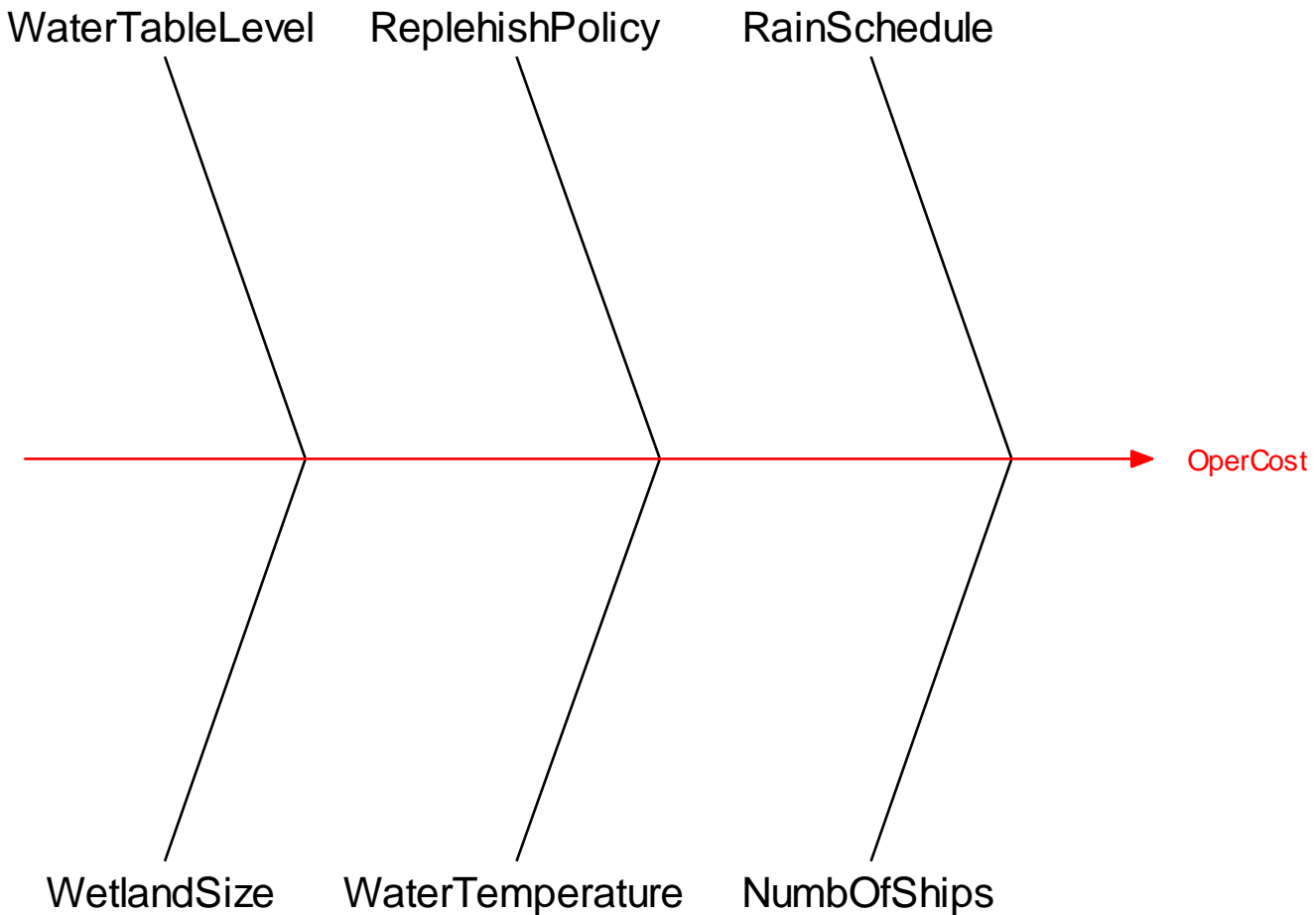
Y sus costos asociados

- Of Importing Water from other places
- Transferring from Social to Economic
- Allocation to various constituencies
- Of Water shortages and rationing
- Indirect costs (labor, political, social)
- Ecological costs (degradation, loss)
- Total costs (compound response)

Usos Adicionales del Modelo

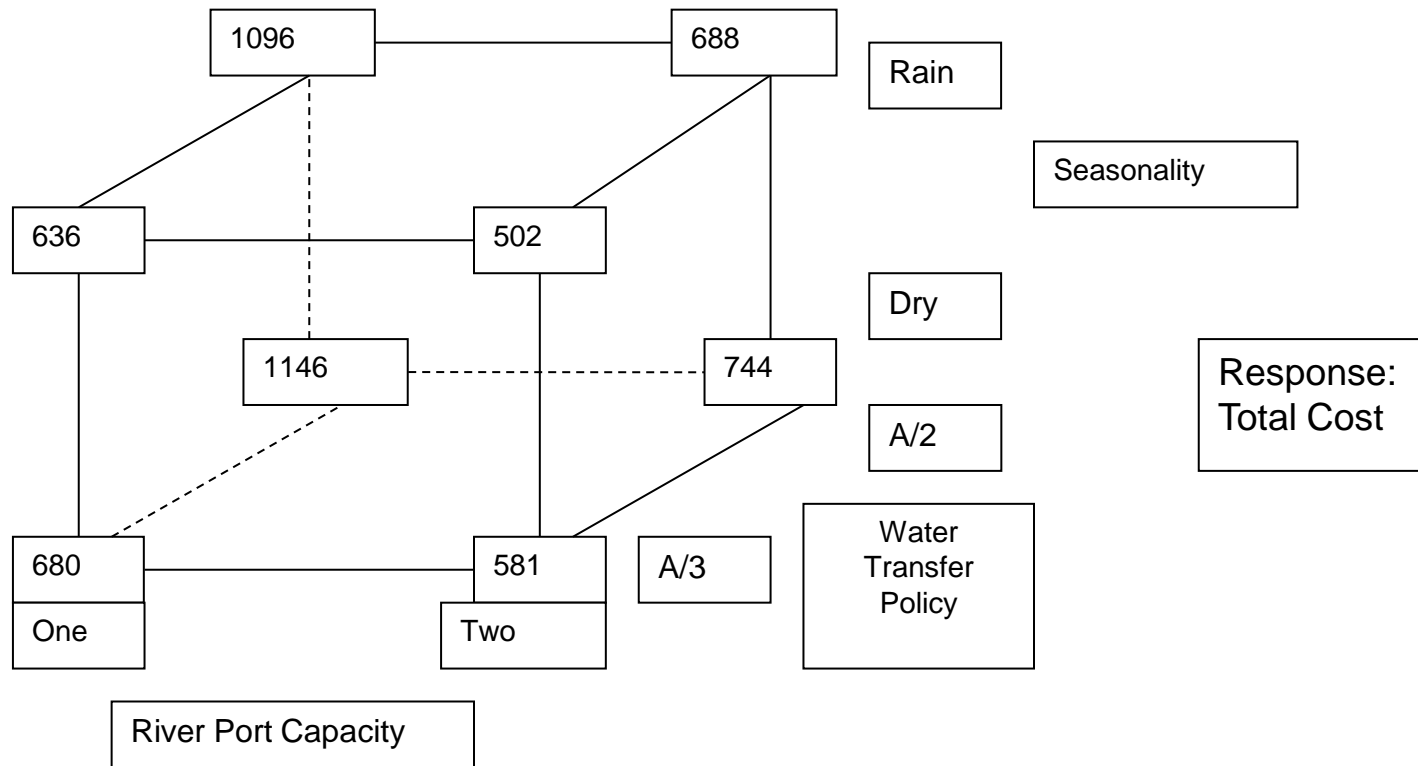
Multi-criteria (ecological, social, economic, etc.) system responses (consolidating elements in the system) can be obtained, by combining (say k) contrasting and competing individual responses into a single, complex one. The linear combinations formed will quantify the contrasting policies and philosophies of different constituencies. This way, comparisons of competing and contrasting policies, produced by the simulation model results, can help diverse constituencies to rationally discuss their differences and better reach a consensus.

Cause-and-Effect Diagram



Ejemplo de DOE Simple

Complete Factorial Experiment for the Simulation



Análisis de los Resultados:

- Variable Respuesta: costo de operacion
- Factores Principales Significativos:
- Capacidad (decrece los costos)
- Transferencias (incrementa los costos)
- Regimen de Lluvias (decrece los costos)
- Interaccion: Capacidad x Transferencias
- Los demas factores no son significativos

Interpretaciones/Extensiones

- Influencia Mayor: capacidad/transferencias
- Influencia Secundaria: regimen de aguas
- Optimo: lago grande/pocas transferencias
- Pesimo: lago chico/grandes transferencias
- Extensiones: definir combinaciones lineales
- Ventajas: contraste/arbitraje de politicas
- Adicional: educacion social en ambientacion

DOE Sumamente Restringido

- Pocas variables ($k=3$)
 - Pues 2^K Factores son generados
- Interaccion Limitada, cuando $k > 3$
 - Si estan presentes, modifica resultados
- Variables de Respuesta Robustas
 - Poco sensitivas a las variables de “ruido”
- Necesidad de Identificar *Grupo Minimo*
 - Para reducir dimension del modelo original

Problemas y Consecuencias

- Fuerte interacción entre los factores
 - consecuencia de la estructura del modelo
- Gran número de factores en el sistema
- Finalidad de uso del modelo creado:
 - Describir/estudiar, pronóstico y control
- Diseño Robusto a Parámetros negativos
 - Resistentes a factores libres o de “ruido”

Algunos DOE aplicables

- Factoriales completos
- Factoriales Fraccionados
- Disenos Plackett-Burnam
- Controlled Sequential Bifurcation
- Muestreo de Latin-Hypercube
- Otros enfoques o tipos de analisis
 - Bayesiano, Jerarquico, Taguchi, CPA.

Factoriales Completos

- Most expensive (time and effort)
 - Prohibitive with large number of factors
- Most comprehensive information
 - Provides info on all factor interactions
- Examples of a 2^3 Full Factorial
 - First case: mild interaction (AB only)
 - Second: strong and complex interaction
 - Notice how the Model-Estimations vary

Ejemplo de Factorial Completo: Variables Usadas

- A = Replenishing Levels (MIN)
- B = Reservoir Capacity (MAX)
 - C = Transfer Policy
- Mild interaction assumed
 - A* B only

Full Factorial Experiment 2³

Run	A	B	C	AB	AC	BC	ABC	Avg.
1	-1	-1	-1	-1	1	1	1	-1.07
2	1	-1	-1	-1	-1	-1	1	3.72
3	-1	1	-1	-1	-1	1	-1	-0.58
4	1	1	-1	-1	1	-1	-1	12.04
5	-1	-1	1	1	1	-1	-1	7.75
6	1	-1	1	1	-1	1	-1	15.45
7	-1	1	1	1	-1	-1	1	11.09
8	1	1	1	1	1	1	1	18.31
TotSum								66.71
Effect	8.08	3.75	9.62	1.84	-0.62	-0.65	-2.08	

Regression Estimations

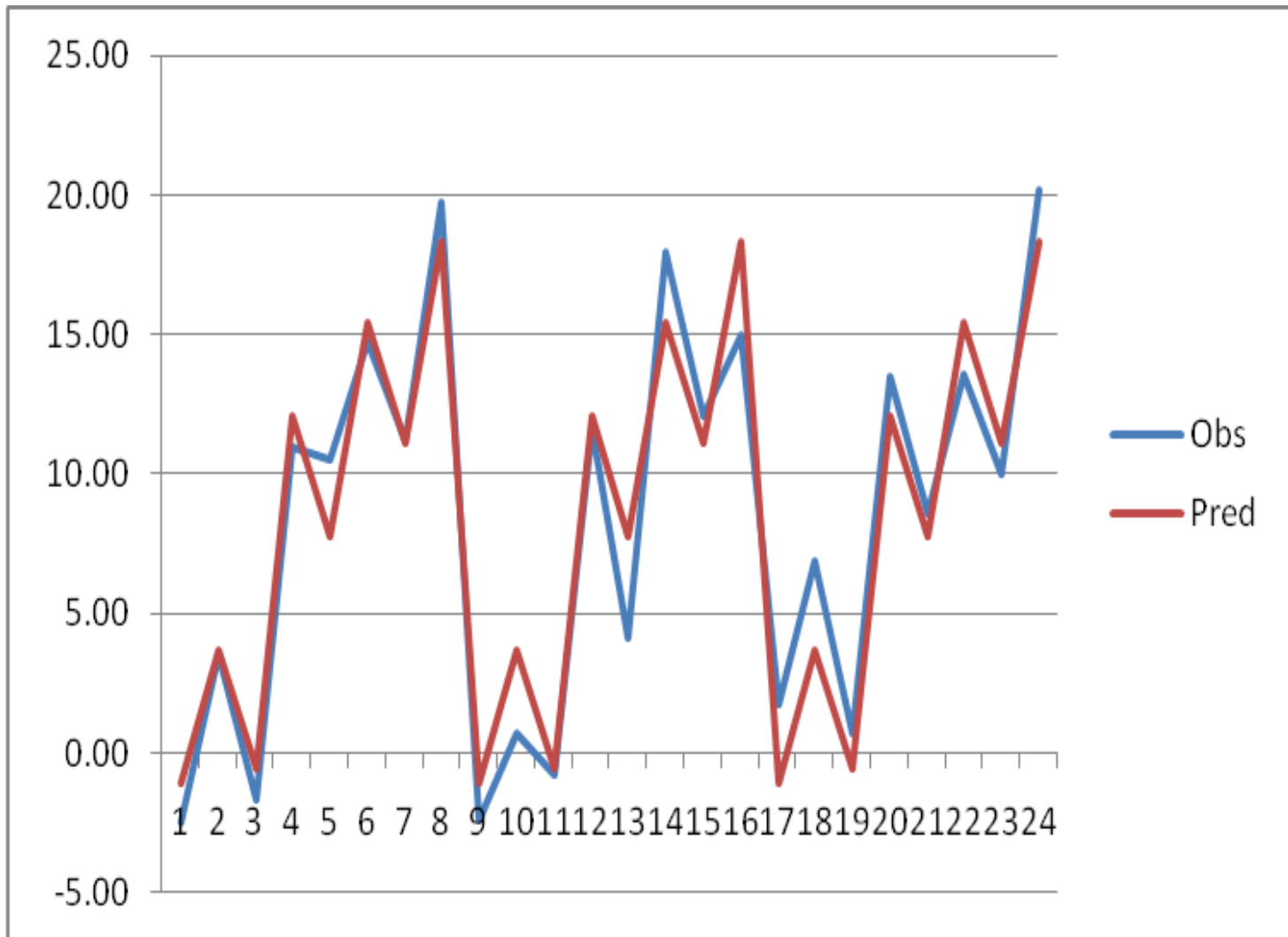
RegCoef	A	B	C	AB	b0
Estimat.	4.04	1.88	4.81	0.92	8.34
TRUE	4	2	5	1	10

Meta Model: $Y_{ijkl} = 8.33 + 4.04A + 1.88B + 4.81C$

True Model: $Y = 10 + 4*A + 2*B + 5*C + AB + \epsilon$

Mild Interaction (AB only)

Meta Model Re-creation ability: mild interaction.



Factoriales Fraccionados

- Analyzes only a Fraction of the Full
 - Reduces substantially time/effort
 - Confounding of Main Effects/Interactions
 - If Interactions present, this is a problem
 - Only for Powers of Two (no. of runs)
- Numerical Example: half fractions
 - Of the previous Full Factorial –and others
 - Assess Model-Estimation agreement

Factoriales Fraccionados

First Fraction: L1

Run	A	B	C=AB	Avg.
1	1	-1	-1	-0.33
2	-1	1	-1	-0.33
3	-1	-1	1	-0.33
4	1	1	1	1.00
TotSum				0.00
Effect	7.429	3.130	11.460	
Signif.	No	No	Yes	

$$Y_1 = 7.3 + 3.71A + 1.57B + 5.73C^*$$

C *: Factor C is confounded with AB

Second Fraction: L2

Run	A	B	C=AB	Avg.
1	-1	-1	-1	-1.00
2	1	1	-1	0.33
3	1	-1	1	0.33
4	-1	1	1	0.33
TotSum				0.00
Effect	8.728	4.375	7.784	
Signif.	Yes	No	Yes	

$$Y_2 = 8.33 + 4.36A + 2.18B + 3.89C^*$$

Untangling the Confounded Structure

(L1+L2)/2	8.079	3.753	9.622
(L1-L2)/2	-0.649	-0.623	1.838
Effects	8	4	10

Notice how, by averaging both Half Fraction results, we obtain the Full Factorial results again.

$$\text{True Model: } Y = 10 + 4^*A + 2^*B + 5^*C + AB + \varepsilon$$

Otro Ejemplo Factorial Completo: Mismas Variables, pero ahora con Fuerte Interaccion

- A = Replenishing Levels (MIN)
- B = Reservoir Capacity (MAX)
 - C = Transfer Policy
- Strong interaction assumed
 - A*B, A*C, B*C
 - Overall: A*B*C

Factorial Completo: Complex, Strong Interaction

Model Parameters							
Variables	A	B	C	AB	AC	BC	ABC
RegCoef	3	-5	1	-12	8	-10	-15
RegEstim	1.94	-4.38	1.73	-12.14	7.34	-10.52	-15.26
MainEffEst	3.88	-8.76	3.47	-24.28	14.68	-21.05	-30.51
MainEffects	6	-10	2	-24	16	-20	-30
Var. of Model	12.5173		StdDv		3.53799		
Var. of Effect	2.0862		StdDv		1.44437		
Student T (0.025DF)	2.47287						
C.I. Half Width	3.57177						
Factor	A	B	C	AB	AC	BC	ABC
Signific.	Yes	Yes	No	Yes	Yes	Yes	Yes

True Model and Estimated Meta Model:

$$Y = 3A - 5B + C - 12AB + 8AC - 10BC - 15ABC$$

RegEstim	1.94	-4.38	1.73	-12.14	7.34	-10.52	-15.26
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Corresponding Half Fractions

Run	Half			Analysis:						
	A	B	Fraction First C=AB	Half(a)			Avg.	Var	Model	
2	1	-1	-1	Y1	Y2	Y3	-15.87	0.59	-14	
3	-1	1	-1	7.18	9.21	5.28	7.22	3.87	6	
5	-1	-1	1	-16.75	-19.75	-22.02	-19.51	6.97	-22	
8	1	1	1	-31.61	-27.62	-33.04	-30.76	7.89	-30	
TotSum				-56.21	-54.7	-65.82	-58.91	19.32		
Effect	-17.17	5.92	-20.81		ModlVar.	4.83	StdDev=	2.2	EffVar	
Signif.	Yes	Yes	Yes		T(.975,df)	2.75	CI-HW=	3.49	StdDev	
Run	Second			Half(b)						
	A	B	C=-AB	Y1	Y2	Y3	Avg.	Var	Model	
1	-1	-1	-1	-5.64	-0.28	9.43	1.17	58.32	2	
4	1	1	-1	4	1.47	2.49	2.65	1.62	2	
6	1	-1	1	49.73	54.94	56.86	53.84	13.62	54	
7	-1	1	1	5.99	7.88	2.56	5.48	7.26	2	
TotSum				54.08	64.01	71.34	63.14	80.82		
Effect	24.92	-23.44	27.75		ModlVar.	20.2	StdDev=	4.49	EffVar	
Signif.	Yes	Yes	Yes		T(.975,df)	2.75	CI-HW=	7.14	StdDev	
(a+b)/2	3.88	-8.76	3.47	MainEff	"C"					
(a-b)/2	-21.05	14.68	-24.28	Interact	C=AB					
Coefs	6	-10	2							

NOTE: FRACTIONAL FACTORIAL RESULTS, GIVEN THE STRONG INTERACTIONS, ARE POOR.

Plackett-Burnham DOEs

- Tipo Especial Factorial Fraccionado (FF)
- Analiza “espacios” entre FF adyacentes
- Reduce considerablemente tiempo/effort
- Confounding of Main Effects/Interactions
- Numerical Example: 11 main effects
 - Compare to a 2^{11} Full Factorial effort
- Counter Example: strong interactions

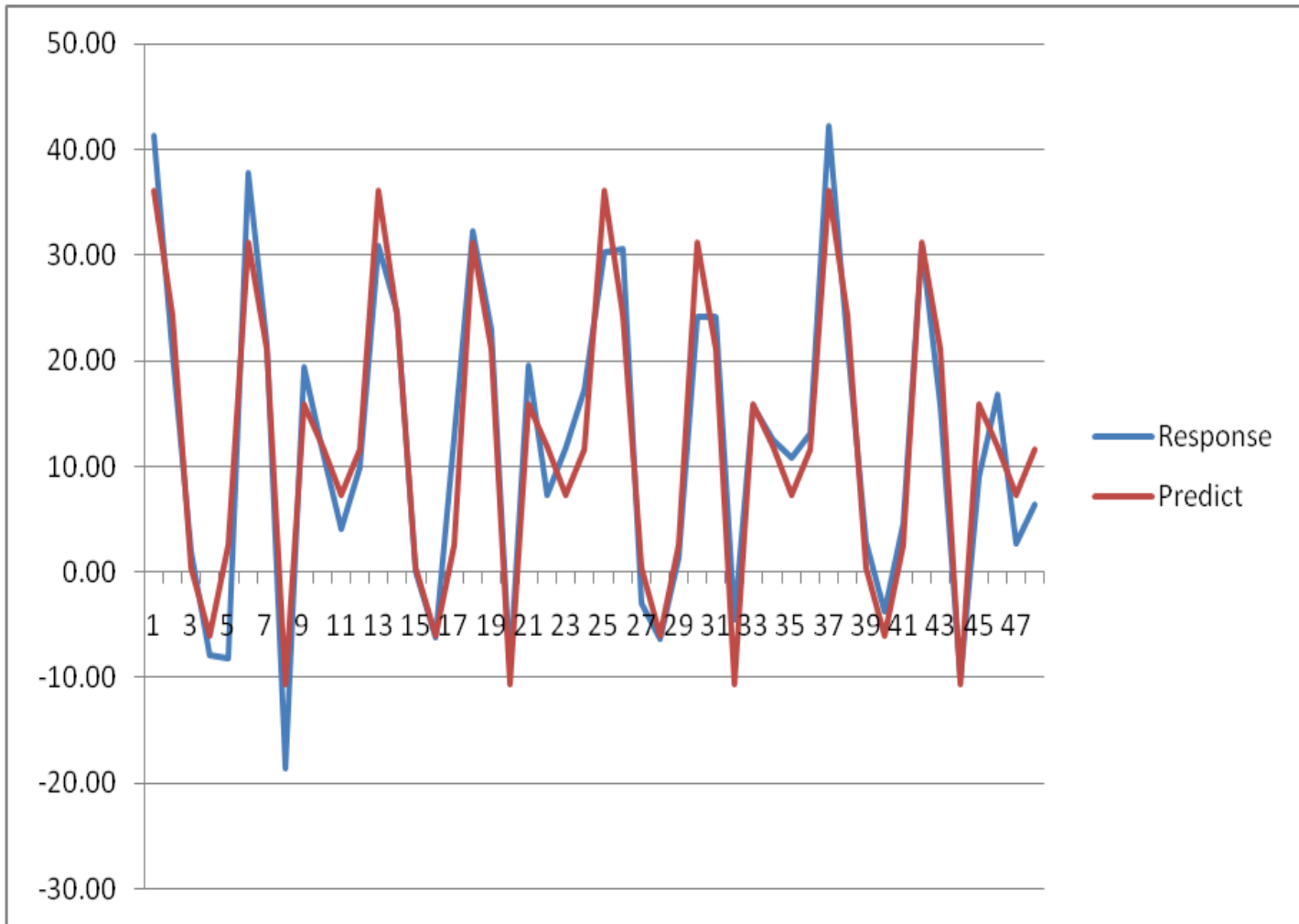
Plackett-Burnam sin Interaccion

- A=Replenishing Levels (MIN)
- B=Reservoir Capacity (MAX)
 - C=Ordering Schedule
 - D=Transfer Policy
- E=Allocation to social sector
 - F=Size of the Reservoirs
- G=Generation of electricity
 - H=Hospitals and schools
 - I=Wetland size
 - J=Water Table
 - K=Fish/Foul Population

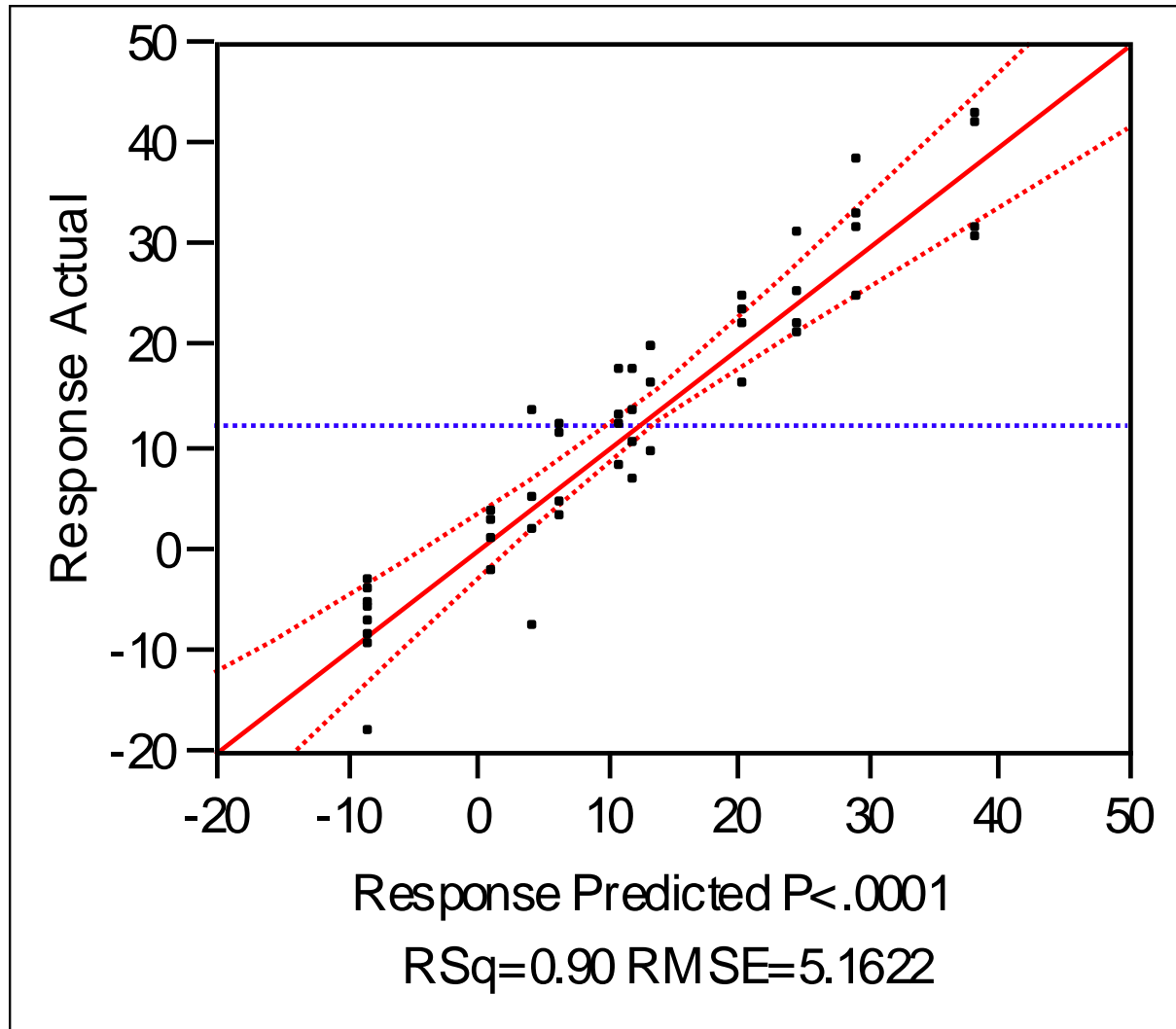
Diseno Plackett-Burnam (sin interaccion)

Run	A	B	C	D	E	F	G	H	I	J	K	Avg	
1	1	-1	1	-1	-1	-1	-1	1	1	1	-1	1	36.14
2	1	1	-1	1	-1	-1	-1	-1	1	1	1	-1	24.39
3	-1	1	1	-1	1	-1	-1	-1	-1	1	1	1	0.5
4	1	-1	1	1	-1	1	-1	-1	-1	-1	1	1	-5.96
5	1	1	-1	1	1	-1	-1	1	-1	-1	-1	1	2.62
6	1	1	1	-1	1	1	1	-1	1	-1	-1	-1	31.26
7	-1	1	1	1	-1	1	1	1	-1	1	-1	-1	21.12
8	-1	-1	1	1	1	1	-1	1	1	-1	1	-1	-10.54
9	-1	-1	-1	1	1	1	1	-1	1	1	-1	1	15.92
10	1	-1	-1	-1	-1	1	1	1	-1	1	1	-1	12.02
11	-1	1	-1	-1	-1	-1	1	1	1	-1	1	1	7.33
12	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	11.66
Factors	A	B	C	D	E	F	G	H	I	J	K	Bo	
RegCoef	6	2	0	-4	-6	0	-2	4	8	-8	0	12	
RegEst.	4.5	2.3	-0.1	-4.3	-3.6	1.4	-0.8	5.2	6.1	-7.6	-2.8	12.2	
MainEff	12	4	0	-8	-12	0	-4	8	16	-16	0	n/a	
EstimEff	9.1	4.7	-0.2	-8.6	-7.2	2.8	-1.5	10.4	12.3	-15.2	-5.6	12.2	
Signific.	Yes	Yes	No	Yes	Yes	No	No	Yes	Yes	Yes	Yes	Yes	

Capacidad del Meta Model para Pronosticos



Actual by Predicted Plot



Plackett-Burnam con Interaccion

- A=Replenishing Levels (MIN)
- B=Reservoir Capacity (MAX)
 - C=Ordering Schedule
 - D=Transfer Policy
- E=Allocation to each sector
 - F=Size of the Reservoirs
- G=Generation of electricity
- H=Hospitals and schools
 - I=Wetland size
 - J=Water Table
- K=Fish/Foul Population

Modelo PB con Interaction Moderada:

Factors	A	B	C	D	E	F	G	H	I	J	K	Bo
RegCoef	6	2	0	-4	-6	0	-2	4	8	-8	0	12

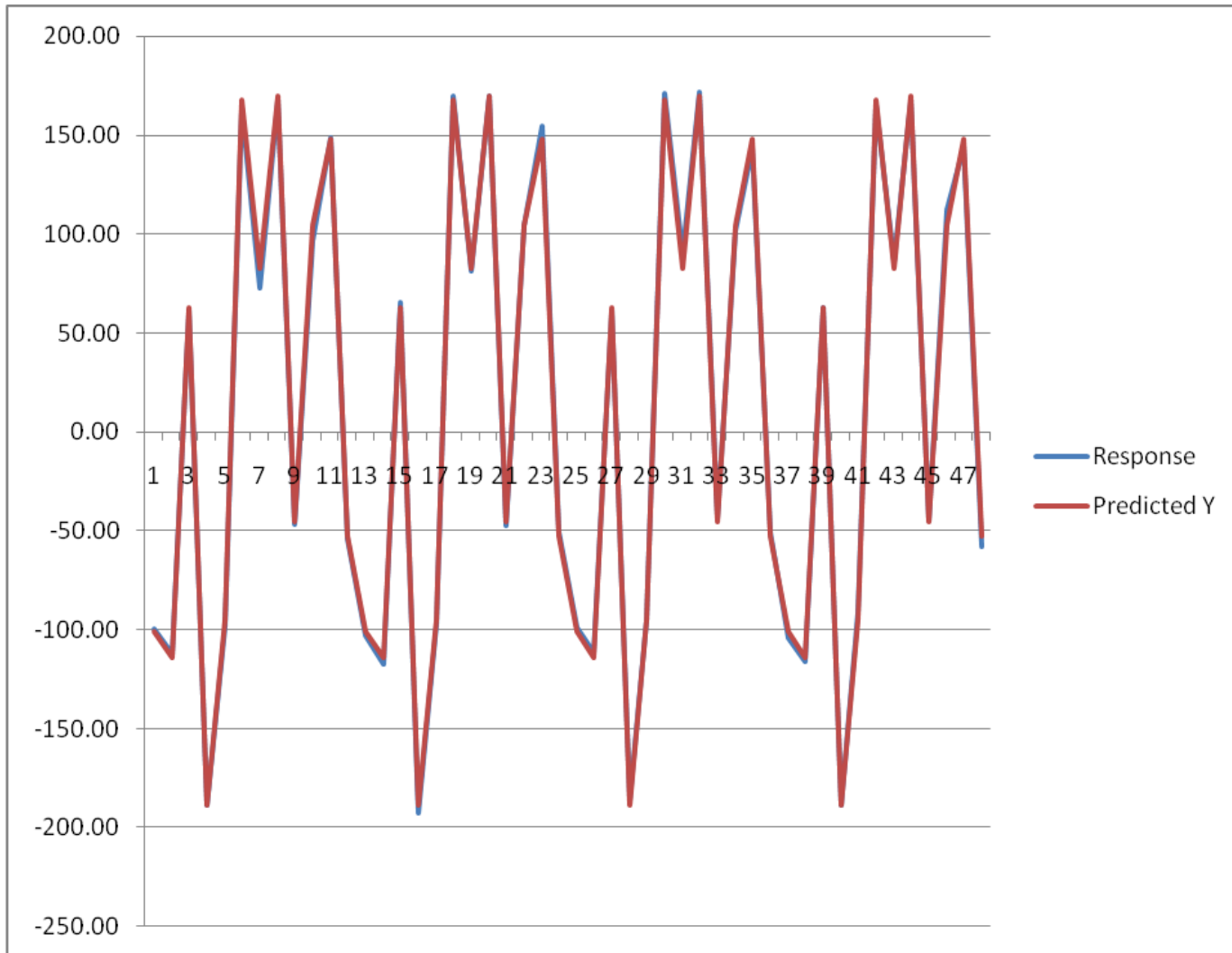
Interaction: $2*A*B-4*H*I+G*J+D*E$

Plackett-Burnam (n=12 rows) Analysis Results:

Factors	A	B	C	D	E	F	G	H	I	J	K
MainEff	12	4	0	-8	-12	0	-4	8	16	-16	0
FacEstim	-98.6	61.1	41.3	-86.5	98.4	66.4	79.7	51.8	-26.6	37.6	-96.0
RegPar.	6	2	0	-4	-6	0	-2	4	8	-8	0
RegEstim	-49.3	30.5	20.6	-43.2	49.2	33.2	39.8	25.9	-13.3	18.8	-48.0
Signific.	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

Results are totally confounded and numerically erroneous.

Capacidad del Meta Model para Pronosticos



Controlled Sequential Bifurcation

- Identifies significant Main Effects
- Requires prior knowledge of Effect signs
 - To ensure all effects are in same direction
 - Something unrealistic in most cases
- Branch and Bound-like approach
 - Top-Down approach most often
- Numerical Example: assess estimations

Identificar dos grupos de variables
via el DOE Plackett-Burnam:
Positivas: B, C, E, F, G, H, J;
Negativas: A, D, I, K.

Implementando Resolution IV FF
a c/uno de estos dos grupos

Ejemplo de Plackett-Burnam con Variables Positivas:

B, C, E, F, G, H, J;

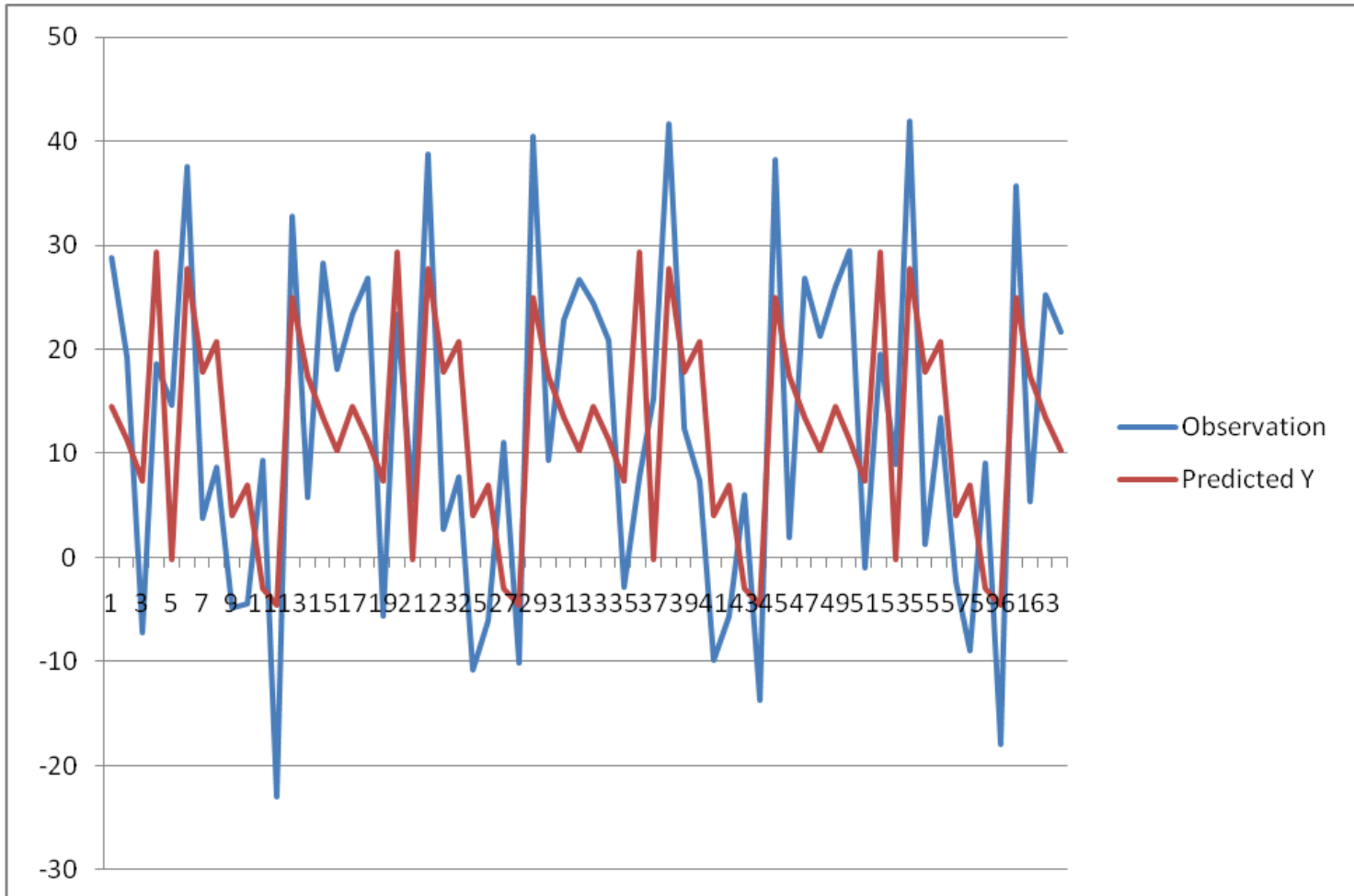
- B=Reservoir Capacity (MAX)
 - C=Ordering Schedule
- E=Allocation to each sector
 - F=Size of the Reservoirs
- G=Generation of electricity
 - H=Hospitals and schools
 - J=Water Table

Implementando Resolution IV FF en el Grupo Positivo: B, C, E, F, G, H, J

Factors	B	C	E	F	G	H	J	Bo
TRUE	12	4	0	-8	-12	0	-4	12
EffectEstim	12.14	2.53	1.17	-7.20	-11.82	0.39	-3.49	13.59
RegCoef	6	2	0	-4	-6	0	-2	12
RegEst.	6.07	1.26	0.59	-3.60	-5.91	0.19	-1.75	6.80
Signific.	Yes	Yes	No	Yes	Yes	No	Yes	

Notice how, once all the Plackett-Burnam (erroneously estimated) variables of the “same sign” were re-analyzed as a sub-group, estimations became closer to True values, both in sign and in magnitude.

Capacidad Descriptiva del modelo aumenta;
Pero su capacidad de pronostico disminuye.



Muestreo Latin Hypercube

- Multiple regression analysis approach
 - Sampling at “best” points in sample space
- Regression selection methods
 - To obtain most efficient Meta Model
- Provides a list of alternative Meta Models
 - Some, not as efficient but close enough
 - Factors can be controlled by model user
- Implements Super-Saturated Models.

Ejemplo de Muestreo Latin Hypercube

Assume we have a three dimensional ($p = 3$) problem in variables B, I, J (reservoir capacity; wetland size and water table use) and that these are respectively distributed Normal, Uniform and Exponential,. Assume that we want to draw a random sample of size $n = 10$. Divide each variable, according to its probability distribution, into ten equi-probable segments (Prob. = $0.1 = 1/10$), identifying each segment with integers 1 through 10. Then, draw a random variate (r.v.) from each of the ten segments, for each of the three variables B, I, J. Finally, obtain the $10!$ permutations of integers 1 through 10. Randomly assign one of such permutations (e.g. segments 2,1,5,4,6,9,8,10,7 for B), to each of the variables, select the corresponding segment r.v., and form the vector sample, as below:

Example of Latin Hypercube Sampling Segments

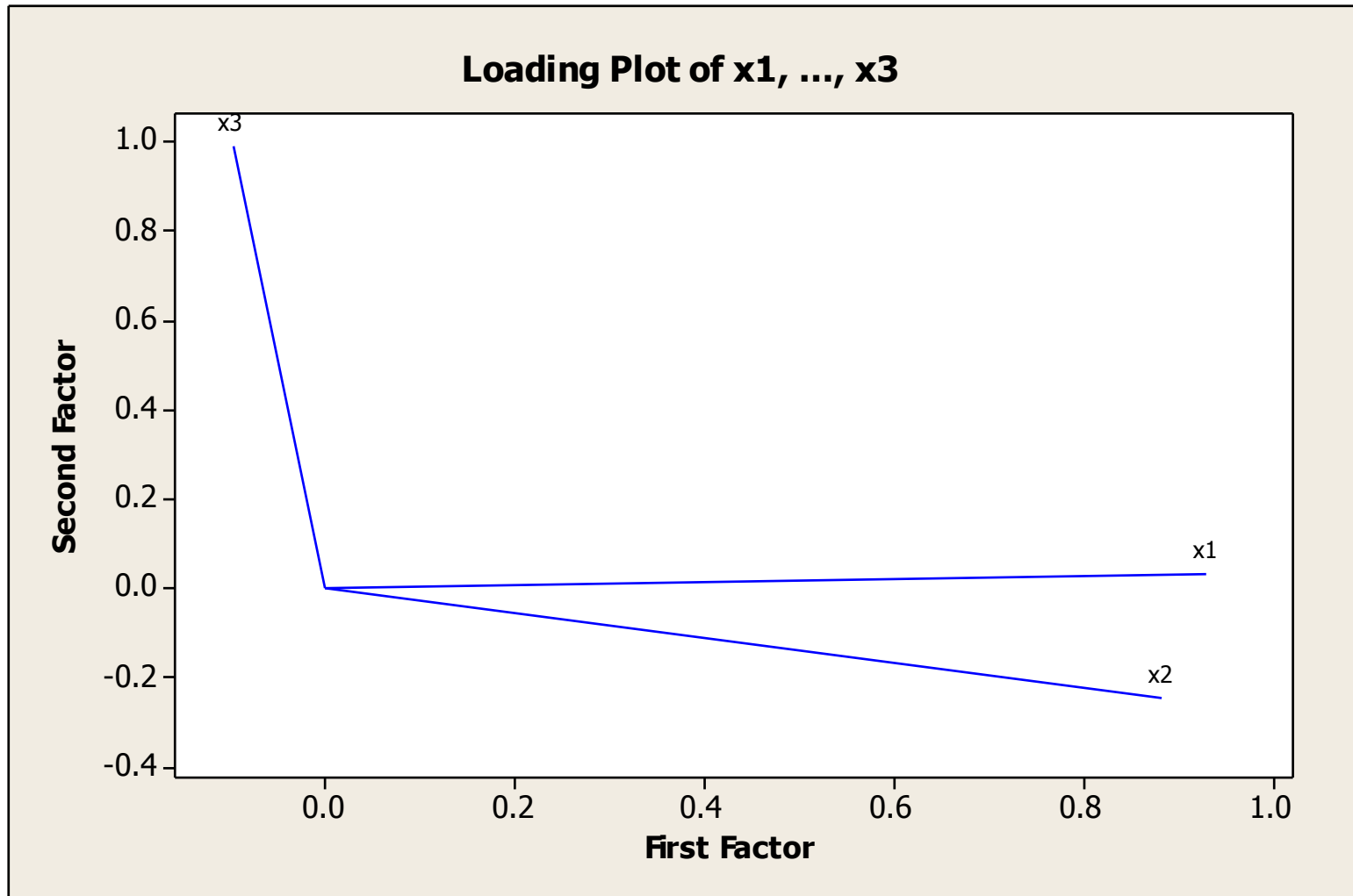
Sample	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th
B	2	3	1	5	4	6	9	8	10	7
I	4	2	7	1	5	9	10	8	6	3
J	8	6	2	7	1	5	4	3	9	10

Componentes Principales (CPA)

- Can be used with Latin Hypercube
 - For now, variables are not uncorrelated
 - Alternative dimension reduction technique
- Main problem: how to interpret it:
 - To identify Key variables through loadings?
 - To use the PCA Main Factors, instead?
 - Alternative approaches?
- Needs evaluation and comparison w/DOE

Example of Varimax Factor Rotation :
Project Variables X1 and X2 on F1
Then, Project Variable X3 on Factor 2.

Variable	Factor1	Factor2
x1	0.930	0.030
x2	0.883	-0.249
x3	-0.097	0.989



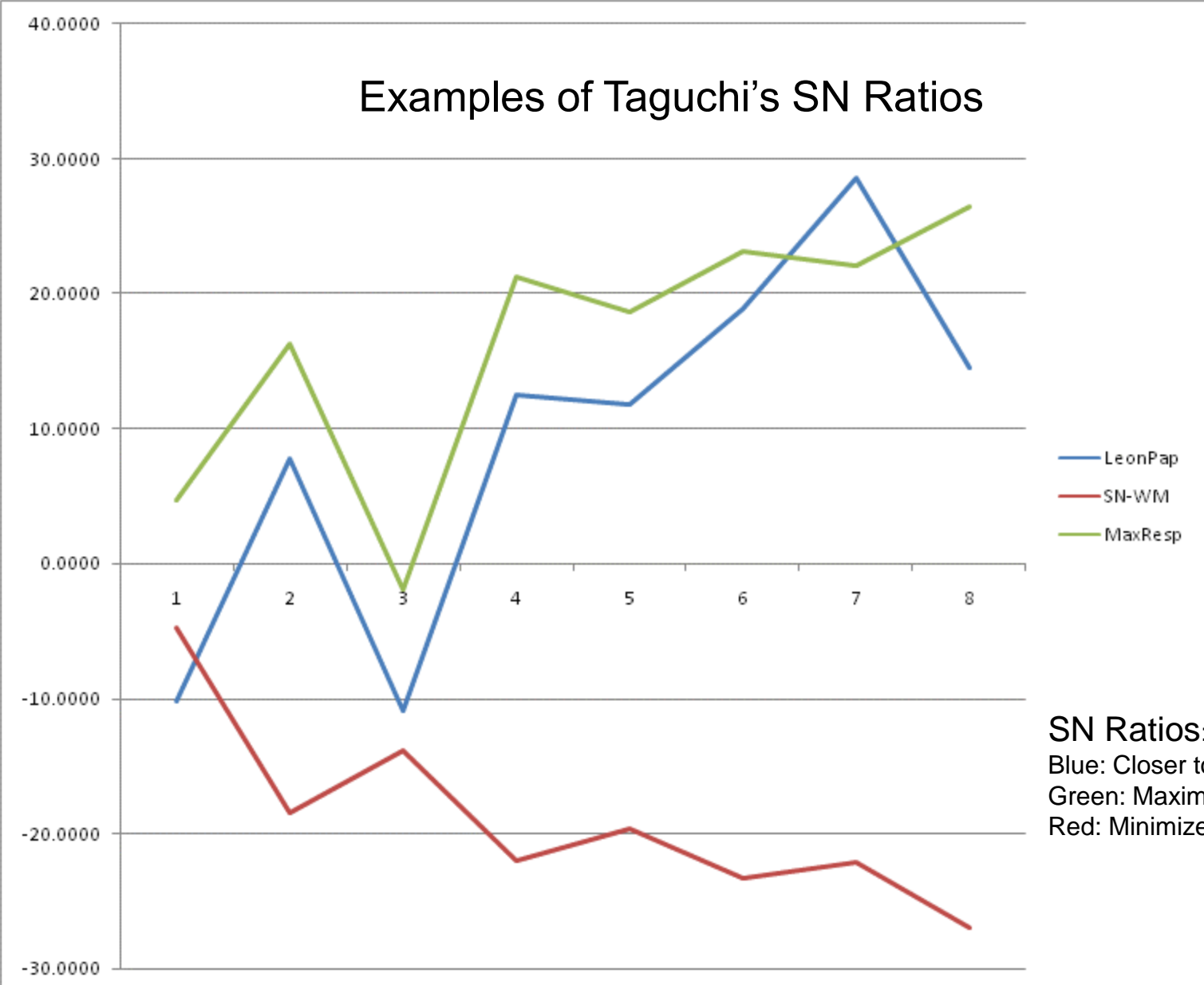
Otros Enfoques y Analisis

- Bayesian
 - Assume a prior on Meta Model terms
- Hierarchical
 - Sub-model output yields upper level input
- Taguchi
 - Derive results resilient to “noise” parameters
 - Parameters representing “uncontrolled” vars
 - Provides many conceptual DOE ideas.

Modelos de Taguchi

- Analyzes both Location and Variation
 - Of the performance measure of interest
- Best combination of both these together
 - To obtain most efficient Meta Model
- Optimize Location, resilient to Variation
- Minimize Variation, resilient to Location
- Determine regions of joint optimality
- Determine Variation is Not an issue
- Can be equivalently implementing w/DOE

Examples of Taguchi's SN Ratios



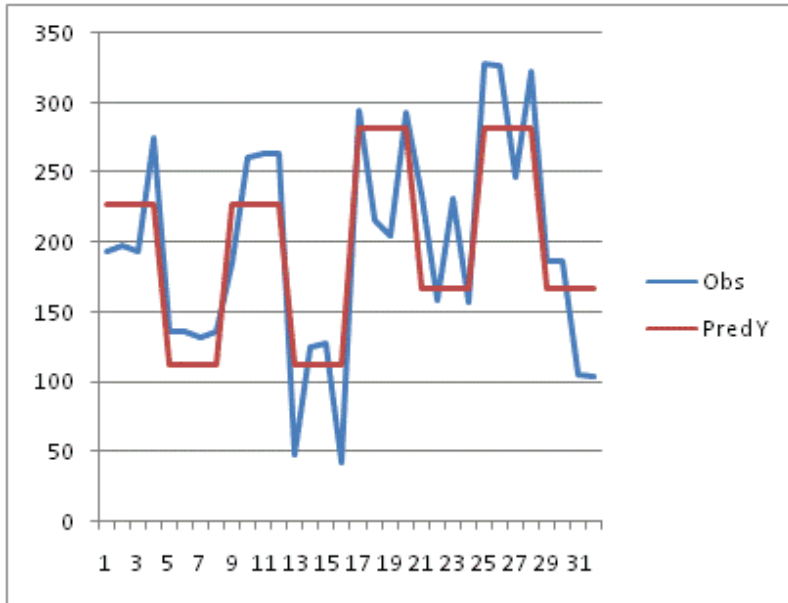
SN Ratios:
Blue: Closer to Target
Green: Maximize Yield
Red: Minimize Yield

Ejemplo: Variable de Respuesta es el tamaño del área húmeda

- X_1 =Reservoir Capacity (MAX)
- X_2 =Generation of electricity
 - X_3 =Hospital Capacity
 - X_4 =Social Services
- X_5 =Fish/Foul Population

Comparison of *Combined* DOE and Taguchi's Approach

X1	X3	X2	X4	X5	1	2	3	4	Var	LnVar	Average	TagMinim
1	1	1	-1	-1	194	197	193	275	1616.25	7.39	214.75	-46.75
1	1	-1	1	1	136	136	132	136	4.00	1.39	135.00	-42.61
1	-1	1	-1	1	185	261	264	264	1523.00	7.33	243.50	-47.81
1	-1	-1	1	-1	47	125	127	42	2218.92	7.70	85.25	-39.51
-1	1	1	1	-1	295	216	204	293	2376.67	7.77	252.00	-48.15
-1	1	-1	-1	1	234	159	231	157	1852.25	7.52	195.25	-45.97
-1	-1	1	1	1	328	326	247	322	1540.25	7.34	305.75	-49.76
-1	-1	-1	-1	-1	186	187	105	104	2241.67	7.71	145.50	-43.59

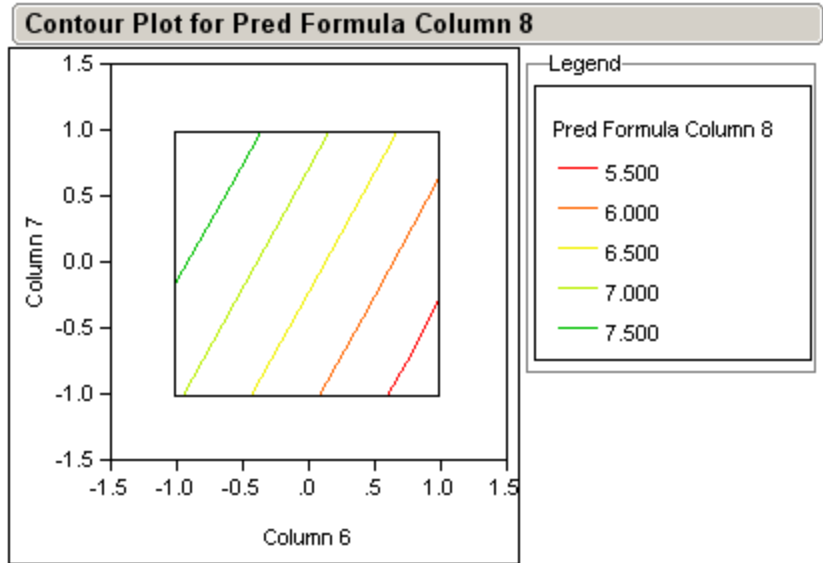
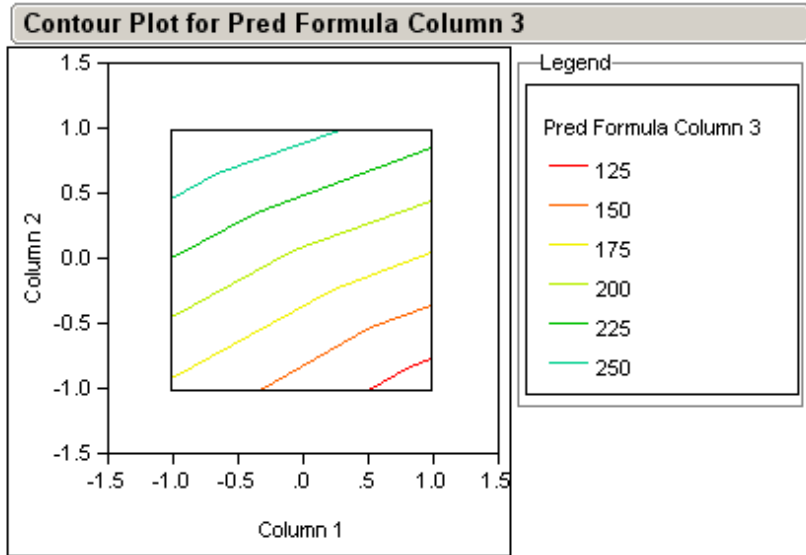


Regression Analysis for the Main Effect influence

	Coef	Std Err	t Stat	P-value	Lower 95	Upper 95
Intrcpt	197.13	7.88	25.01	0.00	181.00	213.25
X Var 1	-27.50	7.88	-3.49	0.00	-43.62	-11.38
X Var 2	56.88	7.88	7.21	0.00	40.75	73.00

Regression Analysis for the Variance Influence

	Coef	Std Err	t Stat	P-value	Lower 95	Upper 95
Intrcpt	6.77	0.78	8.70	0.00	4.77	8.77
X Var 1	-0.82	0.78	-1.05	0.34	-2.82	1.18
X Var 2	0.69	0.78	0.88	0.42	-1.31	2.69



Optimal Solution:

Overlaying both plots (for location and variation) we seek to Minimize both Yield (Errors) and Variation.

Jointly applying the two above (cols. 3 & 8).

The Optimum is around (1, -1), yielding

Estimated Minimum Output = 113; Min Variation = 5.3

Estimated Yield:

$$Y = 197.12 + 27.5X_1 - 56.9X_3$$

$$Y(1, -1) = 112.72$$

Estimated Variation:

$$Y = 6.77 + 0.82X_1 - 0.69X_3$$

$$Y(1, -1) = 5.26$$

Alternative *Combined* DOE Approach

Algunas Aplicaciones

- Reduccion de la dimension del modelo
- Evaluation of Decisions and Strategies
- Evaluation of Robust Strategies
- Trade-offs and Sensitivity analyses
- What-if, time to catastrophic fails, etc.
- Design and Optimization of Systems
- Study of key Factors on a System
- Arbitration and Conflict Resolution

Ejemplo de uso del Enfoque

- Reduce Model to Key Variables to:
- Minimize Total Water Operations Cost
- Subject to:
 - Maintaining specified labor levels
 - Reducing pollution to specified levels
 - Maintaining specified social levels
 - Maintaining specified consumption levels
 - Increasing overall health indices

Trade-Off Examples

Scenario	Ecologic	Health	Industry	Education	Recreation	Other
Best Ecologic	X1	Y1	Z1	W1	L1	M1
Best Health	X2	Y2	Z2	W2	L2	M2
Best Industry	X3					
Best Education	X4					
Best Recreation	X5					
Best Other	X6					

Analyze Maxi-min and Mini-max results

Conclusiones

- Es un problema sumamente complejo
 - Dimension del modelo e interacciones
- Los metodos existentes se quedan cortos
 - Mas pueden encontrarse adaptaciones
- Meta Modelos extremadamente utiles
 - Para decisiones estrategicas y tacticas
 - En una crisis -o para evitarlas y prevenirlas
 - En estudios teoricos de sistemas.