Design of Experiments

Workshop - DAT4.ZERO

February 13th, 2022

Frank Westad

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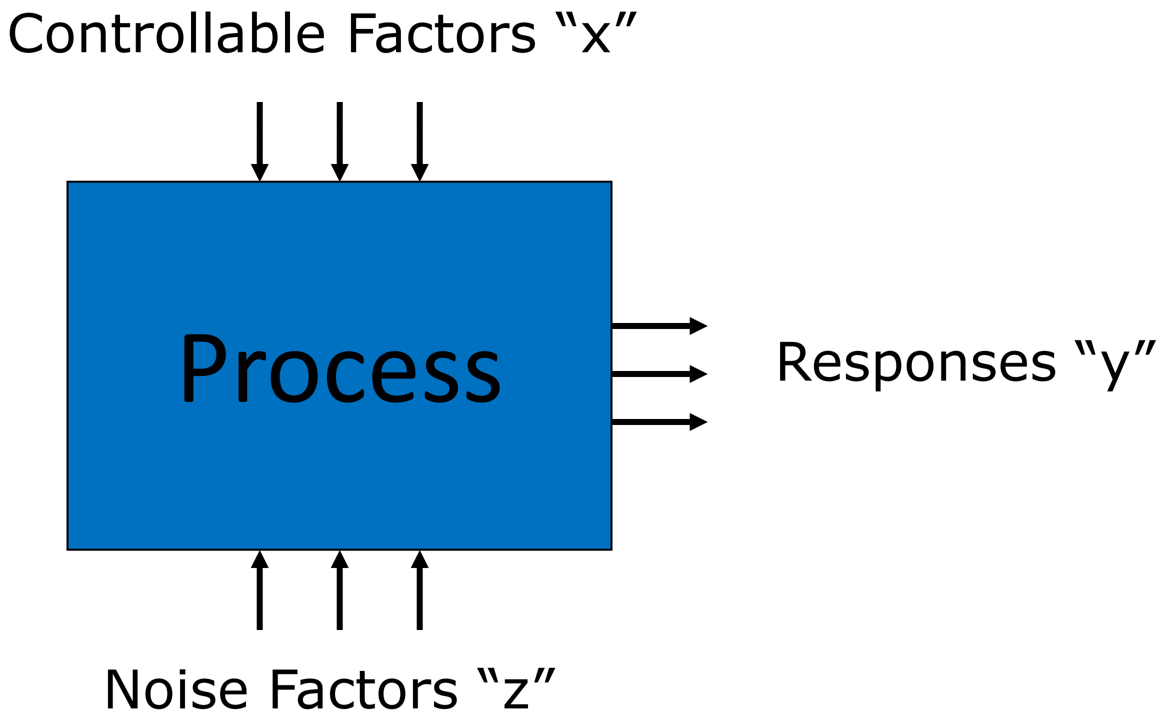
Contents

External

What is Design of Experiments?



DoE (Design of Experiments) is:

“A systematic series of tests, in which purposeful changes are made to input factors, so that you may identify causes for significant changes in the output responses with minimum effort to gain a maximum amount of information.”

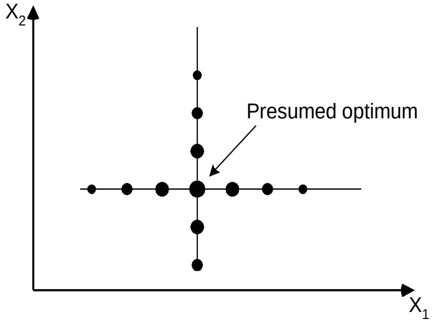
One variable at the time (OVAT)

In order to establish a relationship between cause and effect,
each cause must be investigated separately,
all other conditions being fixed.

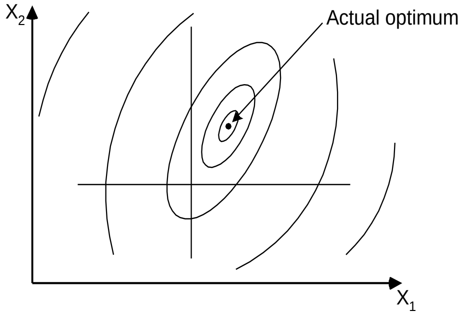
True or false?

How to span the experimental space

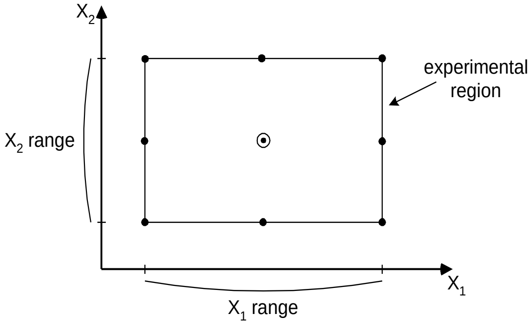
The Classical Approach:
(OVAT)



What can go wrong?



How can we do it better?



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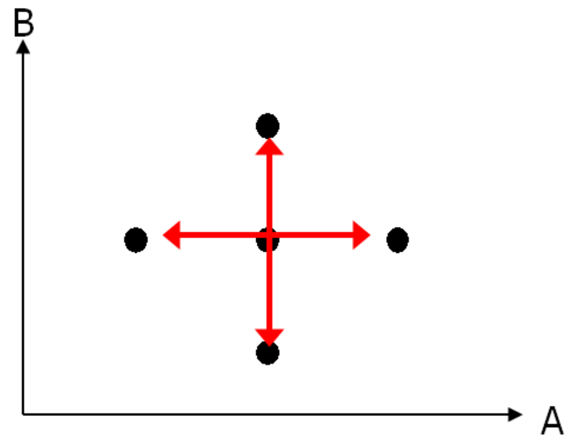
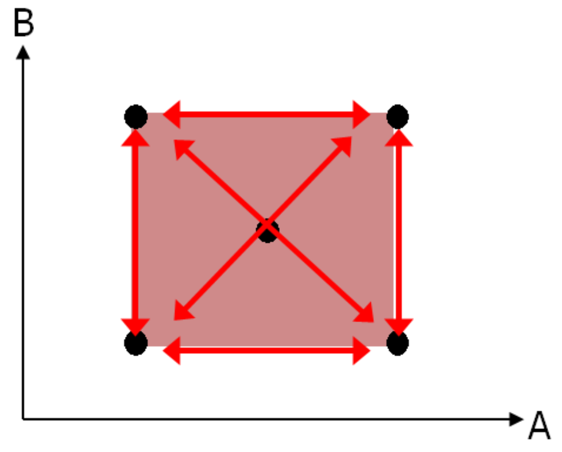
Experimental design versus OVAT

- One Variable At a Time
  - Pairs of experiments are used to estimate effects of A and B
  - Experimental region is given by the red arrows
- Experimental design
  - All experiments are used to estimate effects of A and B
  - Interactions can be estimated
  - Precision can be estimated
  - Experimental region is given by the red area





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The DoE process

1. Identify opportunity and define objective.
2. State objective in terms of measurable responses.
   a) Define the minimal change (Δy) that is <u>important</u> to detect for each response (signal).
   b) Estimate experimental error (s) for each response (noise).
   c) Use the signal to noise ratio (Δy/s) to estimate power.
3. Select the input factors to study
4. Select a design and:
   a) Evaluate aliases.
   b) Assess power.
   c) Examine the design layout to ensure all the factor combinations are safe to run and likely to result in meaningful information (no disasters).

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Why is not DoE more widely used?

- Perception:
  - The problem is viewed as too big and complicated
  - Training consultants remind everyone that DoE’s are for the “select”
  - Therefore, those who do not receive the training believe, “we can’t do that.”
- Employees who are very reluctant to share knowledge, especially partial knowledge, and those who seek to dominate a problem-solving team, may undermine projects
- Education and knowledge:
  - Lack of education in scientific communities
  - Not supported by management
  - The people involved do not know how to perform a DoE
  - The people involved do not have enough prior knowledge to learn by doing
- Prior experience may be negative, as “we did once but it didn’t work out”

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Advantages of Experimental Design

	OVAT	Experimental Design
Main effects	Not estimated	Estimated
Interactions	Not detected	Detected and estimated
Experimental Variability	100% impact	Reduced impact
Number of experiments	Unknown	Known per step
Best solution **If no solution**	??? ???	Spotted Detected
Several responses	Difficult	As easy as 1 response
New objectives	Start all over again!	Re-use existing results

Main types of designs

Type of design	Objective
• Fractional factorial	Find main effects
• Full factorial	Find main effects and interactions
• Optimization designs	Find optimal settings for a response surface
• Mixture designs	Find the optimal recipe of a mixture
• D-optimal designs	Designs with constraints

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What is Power of a design?

Power = (1–β)*100%

Power is the probability of revealing an active effect of size delta (Δ) relative to the noise (σ) as measured by signal to noise ratio (Δ/σ).

It should be high (at least 80%!) for the effect size of interest.

Effect?		ANOVA says:	
		Retain H_0	***Reject H_0***
Truth:	***No***	OK ☺	Type I Error (alpha) *False Alarm*
	Yes	Type II Error (beta) *Failure to detect*	OK ☺

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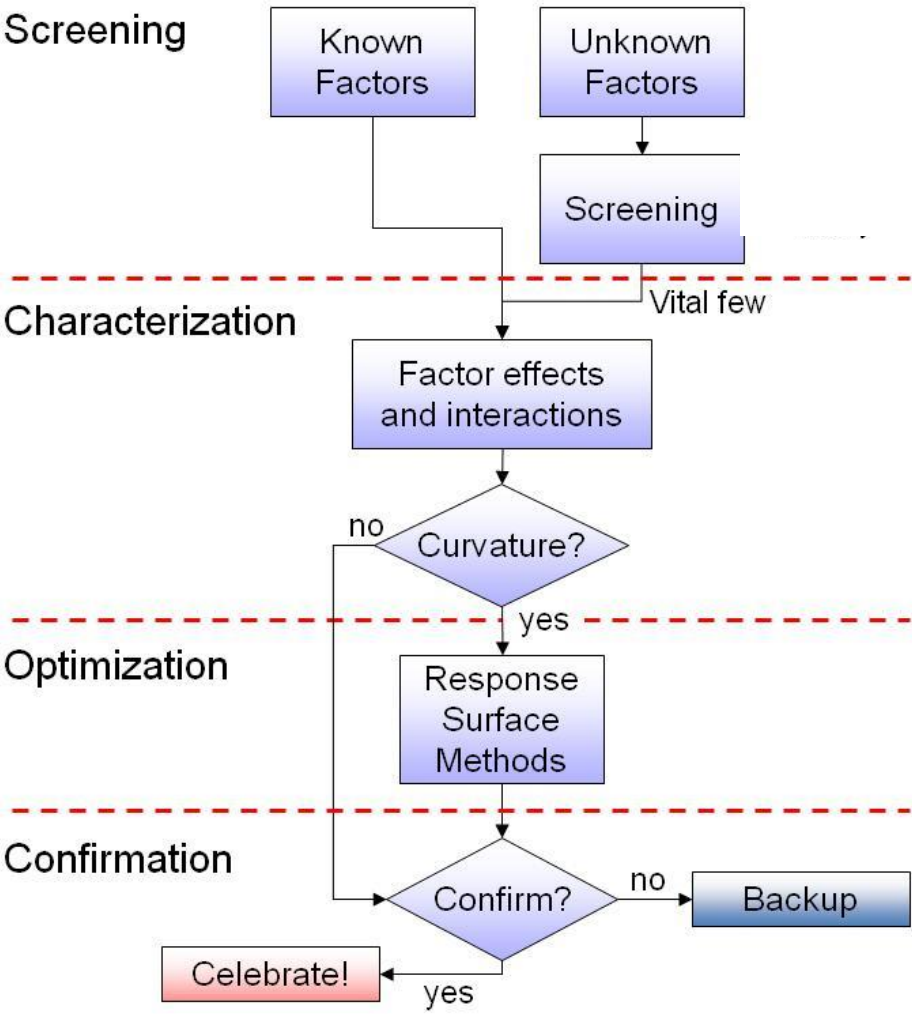
Strategy of Experimentation



ANalysis Of VAriance (ANOVA)

- ANOVA separates the variance into contributions from structure and noise
- Data = Structure + Noise

  $SS_{Total} = SS_{Model} + SS_{Error}$

  Total variation = Modelled + Not modelled
- The squares sums are calculated from regression coefficients in Multiple Linear Regression (MLR)

Linear model:

$$y = \beta_0 + \sum \beta_i x_i + \varepsilon$$

Linear model with two-variable interactions:

$$y = \beta_0 + \sum \beta_i x_i + \sum \sum \beta_{ij} x_i x_j + \varepsilon$$

ANOVA output (1/2)

- Summary-section:
  - Model (SS_{Model}):
    - Contribution from all terms in model
    - DF given by number of terms (parameters)
  - Error (SS_{Error}):
    - Non-modelled variation or noise
    - DF given by number of runs – number of terms - 1

  - Significance of model estimated from

    $F\text{-}ratio = MS_{Model} / MS_{Error}$

ANOVA output (2/2)

- Variables-section
  - The significance of each model parameter is estimated
- Model check-section
  - Sums the contribution from linear terms, interaction terms, etc. to decide on the most appropriate model
- Lack of Fit-section
  - Total error may be divided into
    - Pure error: Spread between replicates
    - Lack of fit: Modelled values vs. Mean of replicates

ANOVA Table

Analysis of variance table

Source	**Sum of Squares**	**df**	**Mean Square**	**F Value**	**p-value Prob > F**	
Model	5535.81	5	1107.16	56.74	< 0.0001	significant
A-Temperature	*1870.56*	*1*	*1870.56*	*95.86*	*< 0.0001*	
B-Concentration	*390.06*	*1*	*390.06*	*19.99*	*0.0012*	
C-Stir Rate	*855.56*	*1*	*855.56*	*43.85*	*< 0.0001*	
AB	*1314.06*	*1*	*1314.06*	*67.34*	*< 0.0001*	
AC	*1105.56*	*1*	*1105.56*	*56.66*	*< 0.0001*	
Residual	195.12	10	19.51			
Total	5730.94	15				

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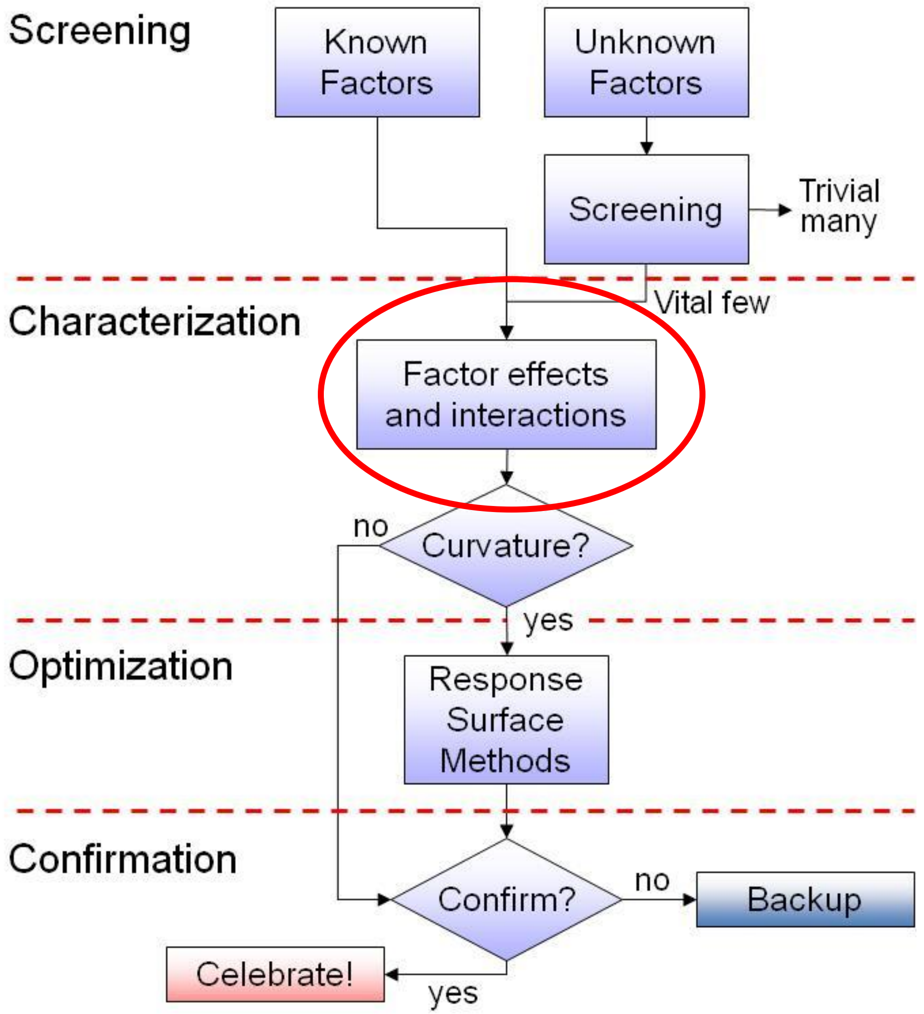
Strategy of Experimentation



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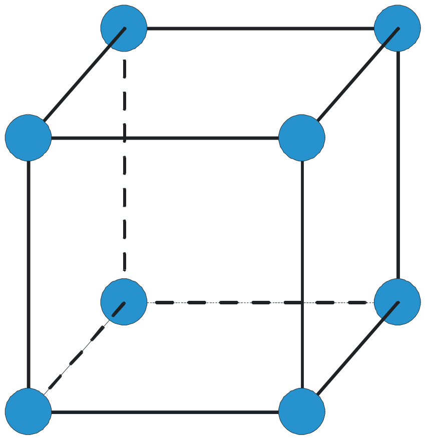
The full factorial design

- Motivation for use:
  - Simplest design situation
  - Basis for many other designs
  - Optimal for detecting main effects and their interactions



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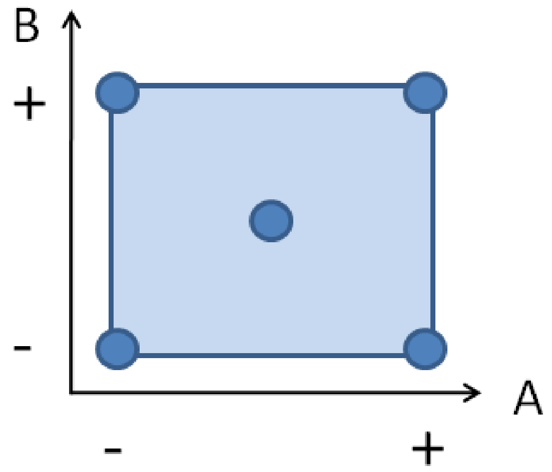
2-level full factorial designs

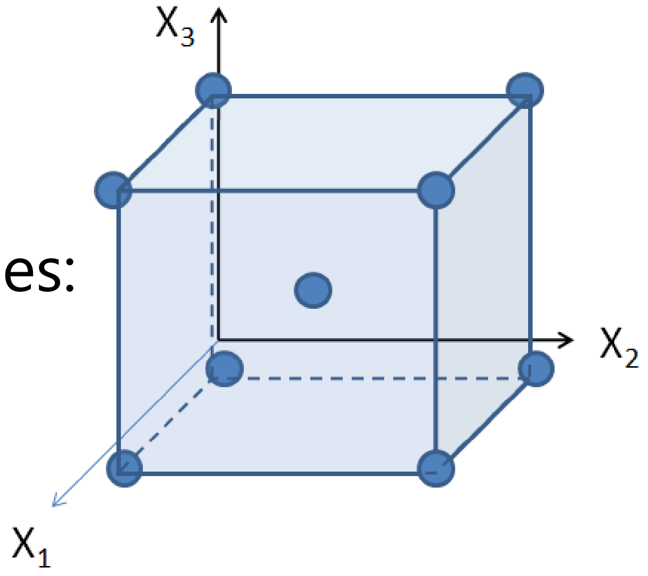
2 X-variables:



run #	X_1	X_2
2	-	-
4	-	+
6	+	-
1	+	+
3	0	0
5	0	0

- 2^2 experiments (+ centre samples)

3 X-variables:



run #	X_1	X_2	X_3
2	-	-	-
11	-	-	+
5	-	+	-
8	-	+	+
4	+	-	-
1	+	-	+
9	+	+	-
7	+	+	+
3	0	0	0
6	0	0	0
10	0	0	0

2^3 experiments (+ centre samples)

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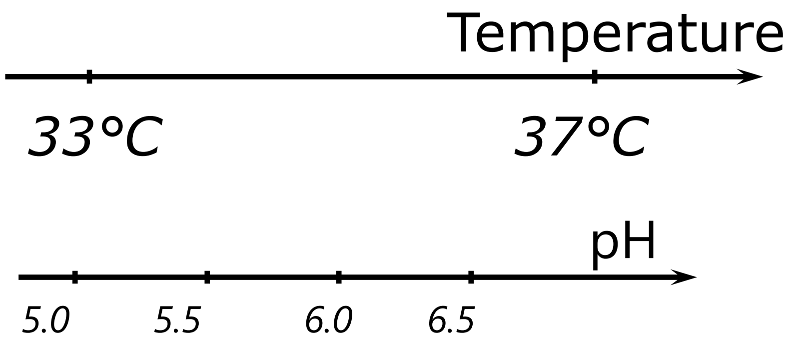
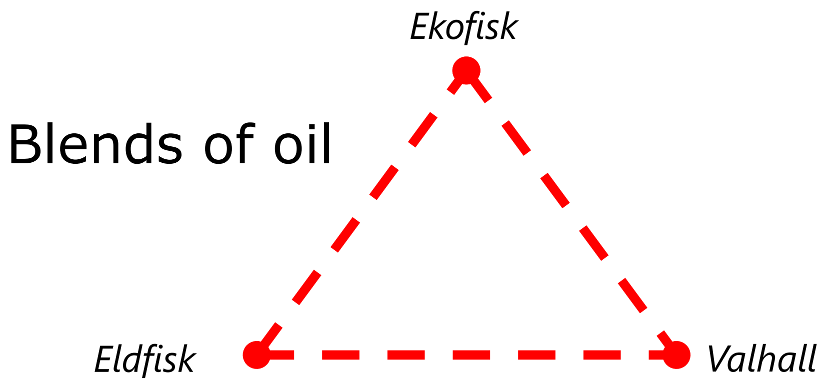
Levels of Design Variables

- Continuous variables
  - Range: Low to high



- Category variables



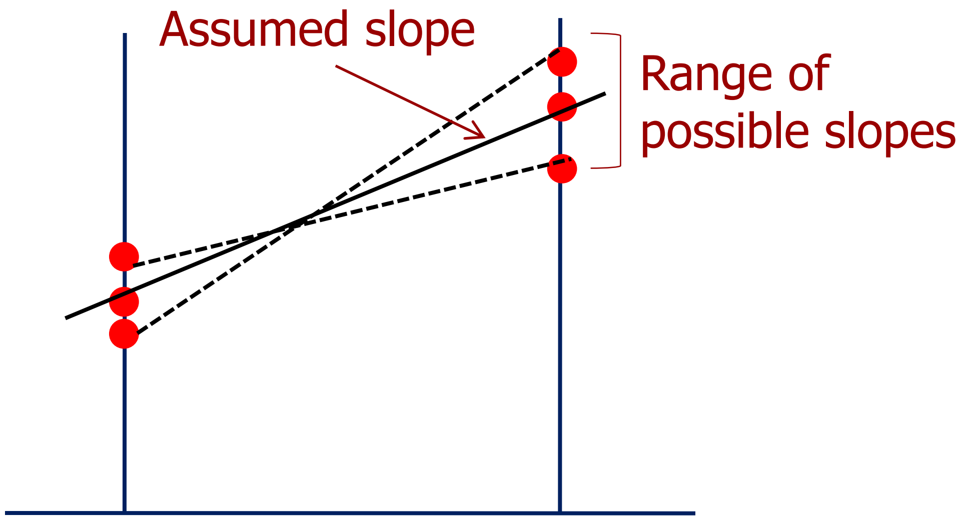
Additional experiments

- Center samples
  - To detect curvature
  - To estimate error variance
  - Category?
    - One center point at each level

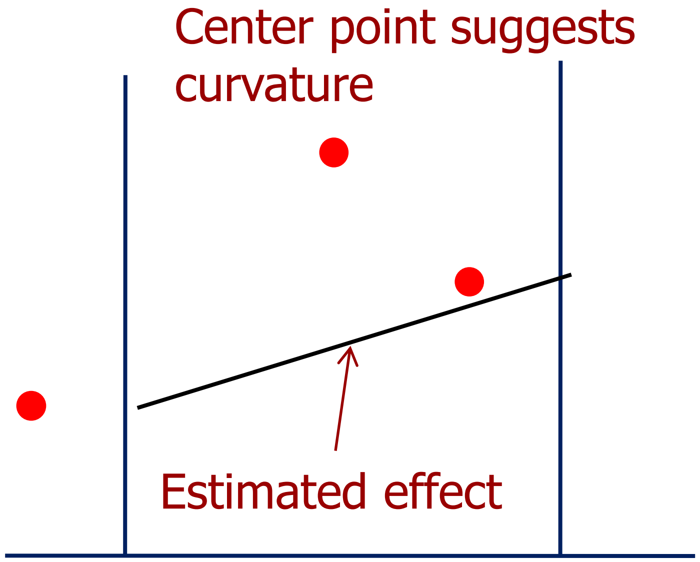
- Replicated samples
  - Replication of the factorial points
  - More precise estimates of error variance

Replicates and center samples

Replicates :



Center samples :



Precision

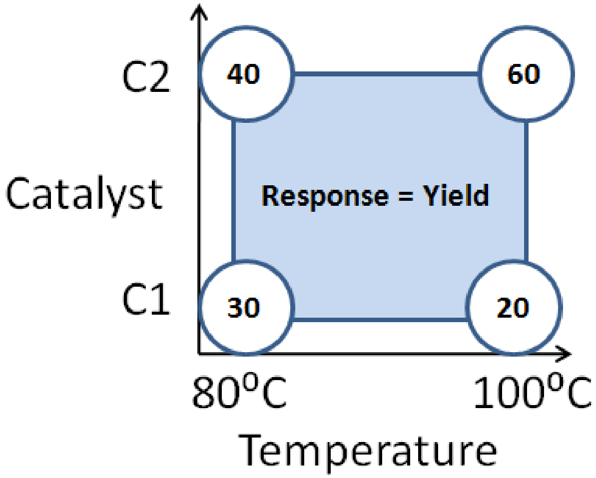
$SD_{\text{repl. samples}} << SD_{\text{whole design}}$?

Curvature check

$\bar{Y}_{\text{center samples}} = \bar{Y}_{\text{design}}$?

Main Effects

A simple experimental design:



Average of T at Low Level = (30+40)/2 =**35**

Average of C at High Level = (20+60)/2 =**40**

Main Effect of Temperature =40-35 = +5

Main effect: Temperature on Yield

Main effect: Catalyst on Yield

Average of C at High Level = (40+60)/2 =**50**

Average of C at Low Level = (30+20)/2 =**25**

Main Effect of Catalyst

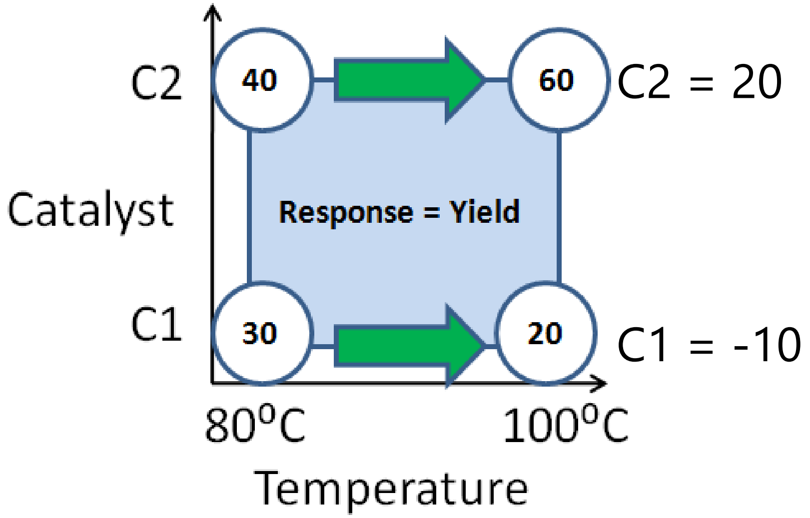
=50-25

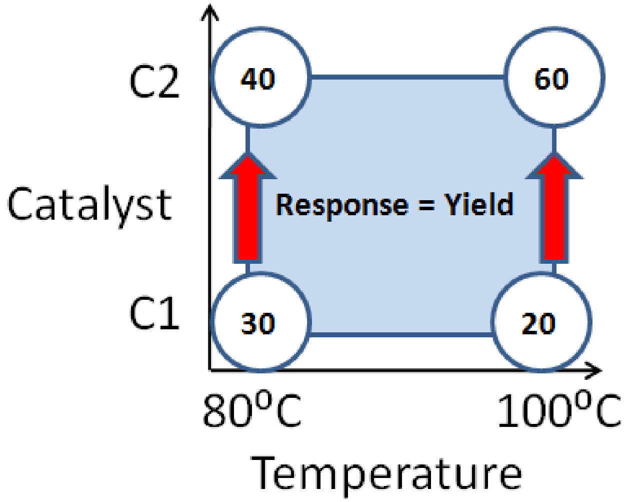
= +25

The Main Effects indicate what the overall effect a single variable has on the overall response

Interactions

Interaction: Catalyst*Temperature





Effect of Temperature on Catalyst

C2 = 60 – 40 =20
C1 = 20 – 30 = -10

Interaction = (20 – (-10))/2 **= +15**

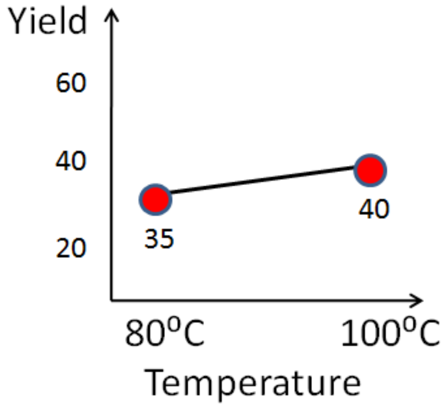
Effect of Catalyst on Temperature

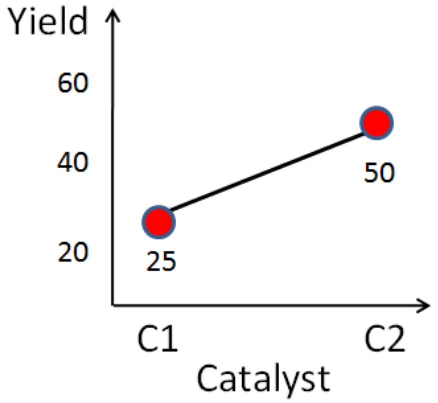
T2 = 60 – 20 =40
C1 = 40 – 30 =10

Interaction = (40 – 10)/2 **= +15**

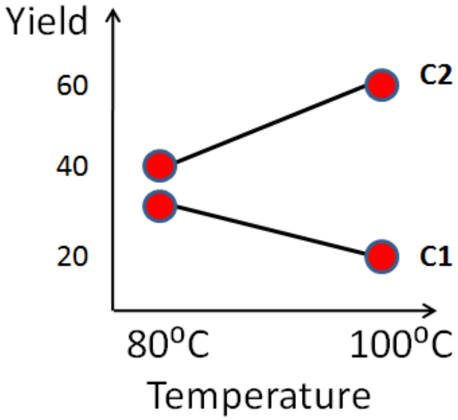
Interpreting Effects

Main effects

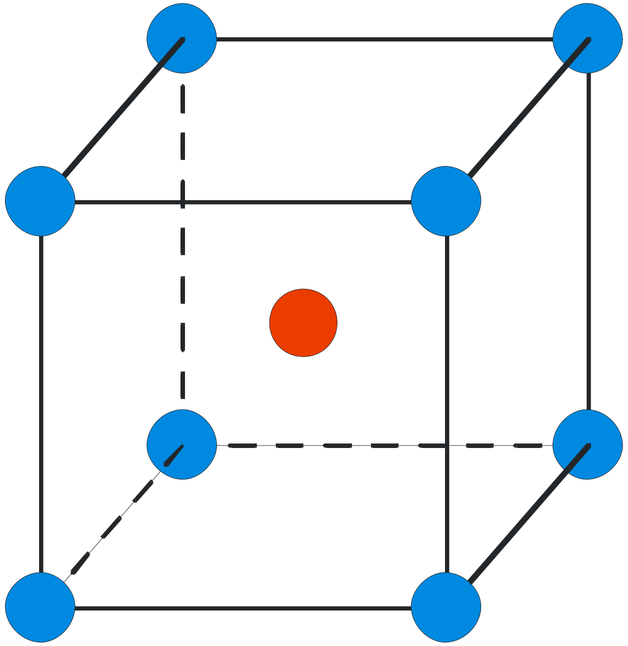




Interactions

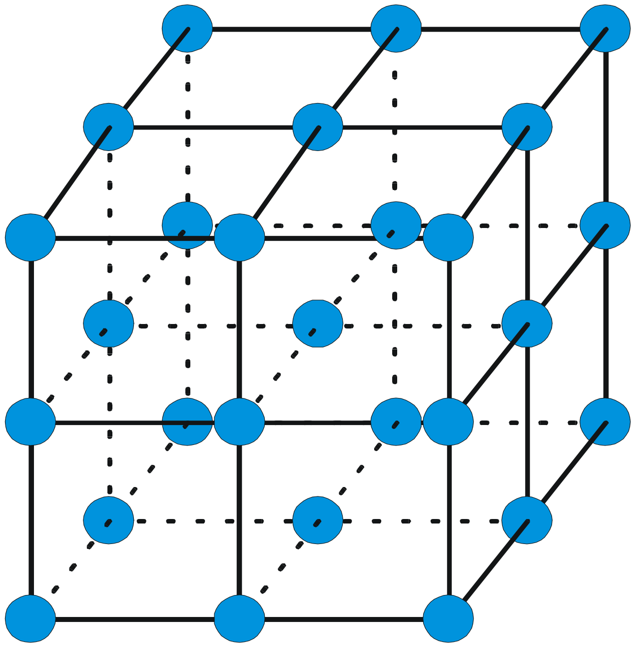


Center Points in Factorial Designs



2^3 factorial with center point

(8 runs plus 4 cp’s = 12 pts)



3^3 Three-level factorial

(27 runs + 5 cp’s = 32 pts)

Not used in practice

Factorial designs - ANOVA

- Additive treatment effects
  - *Factorial: An interaction model will adequately represent response behavior*
- Independence of errors
  - *Knowing the residual from one experiment gives no information about the residual from the next*
- Residuals N(0,s^2):
  - ✓ Normally distributed
  - ✓ Mean of zero
  - ✓ Constant variance

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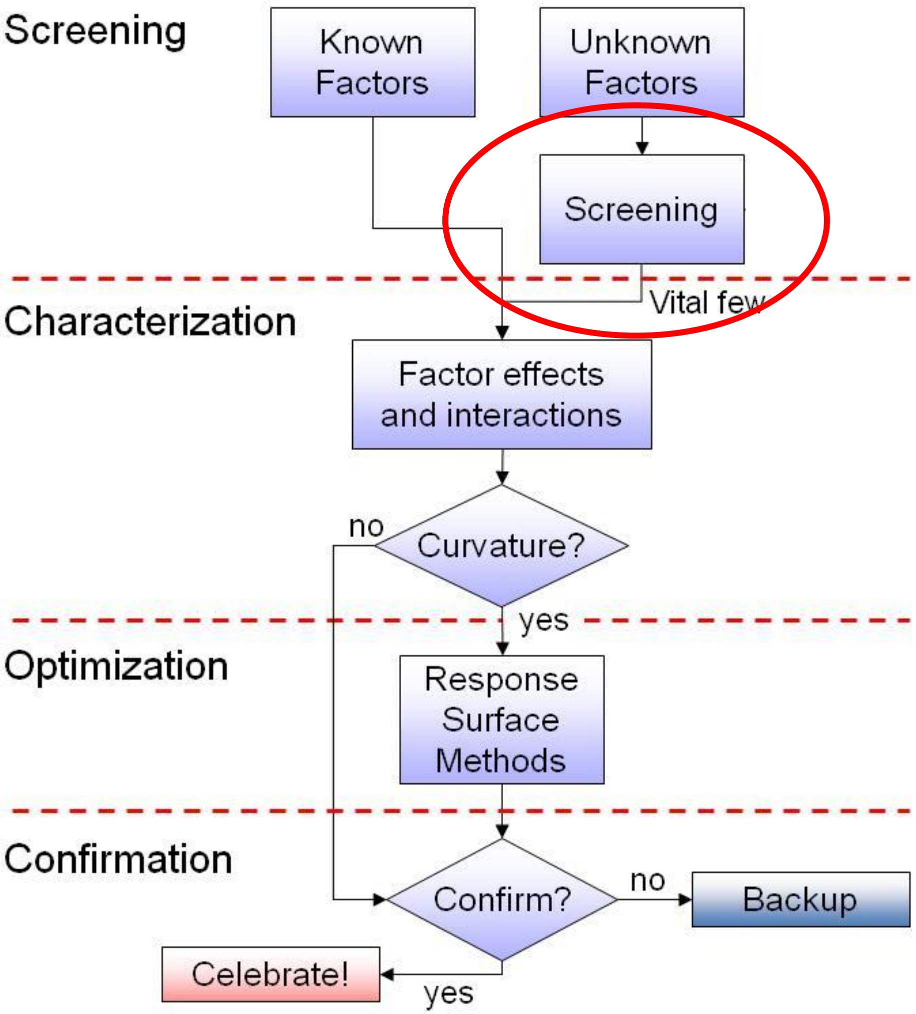
Strategy of Experimentation



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Fractional factorial designs

- Full factorial designs are expensive if many variables
- Often higher order interactions can be neglected → Fractional factorial design
- Subset of the full factorial design
- Experiments are systematically chosen to cover the widest possible design space
- Introduces confounding between the model terms -> not all effects can be estimated independently of other terms
- The degree of confounding is described by the confounding pattern and the resolution

Purposes of screening designs

- **Sort out** between many potentially influential variables
- Describe the **main effects** of several predictors on one or several responses
- Describe the **main effects** and **interactions** of several predictors on one or several responses
- Generate a **structured data table**
- Do all this **cost-efficiently**

2-level Fractional factorial design

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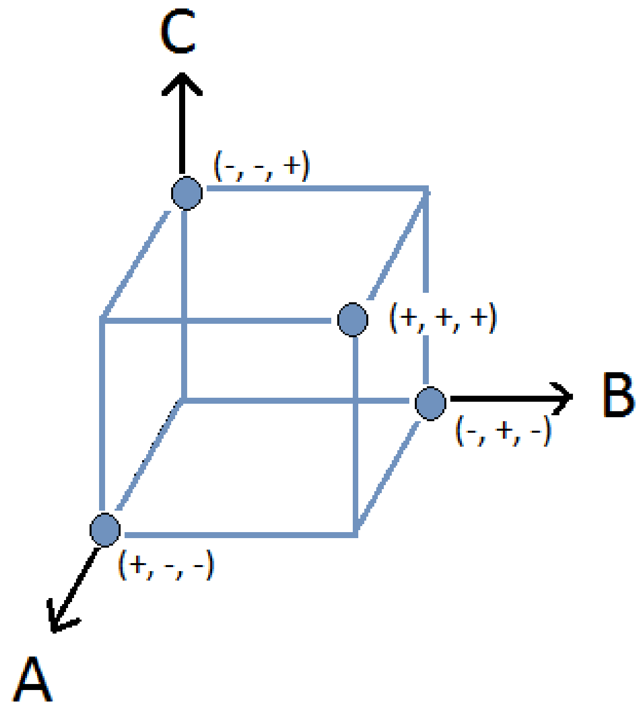
- 3 design variables A, B, C:
- 2^{3-1} design, C = AB
- All main effects estimated in 2^{3-1} = 4 runs
- Main effect C confounded with interaction AB



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Constructing a 2-level Fractional Factorial design: Confounding

- Example: Constructing the 2^{4-1} Design from a 2^3 Design
- Write out the full 2^3 Design

A	B	C	AB	AC	BC	ABC
-	-	-	+	+	+	-
+	-	-	-	-	+	+
-	+	-	-	+	-	+
+	+	-	+	-	-	-
-	-	+	+	-	-	+
+	-	+	-	+	-	-
-	+	+	-	-	+	-
+	+	+	+	+	+	+

Define I = ABCD

and

let D = ABC

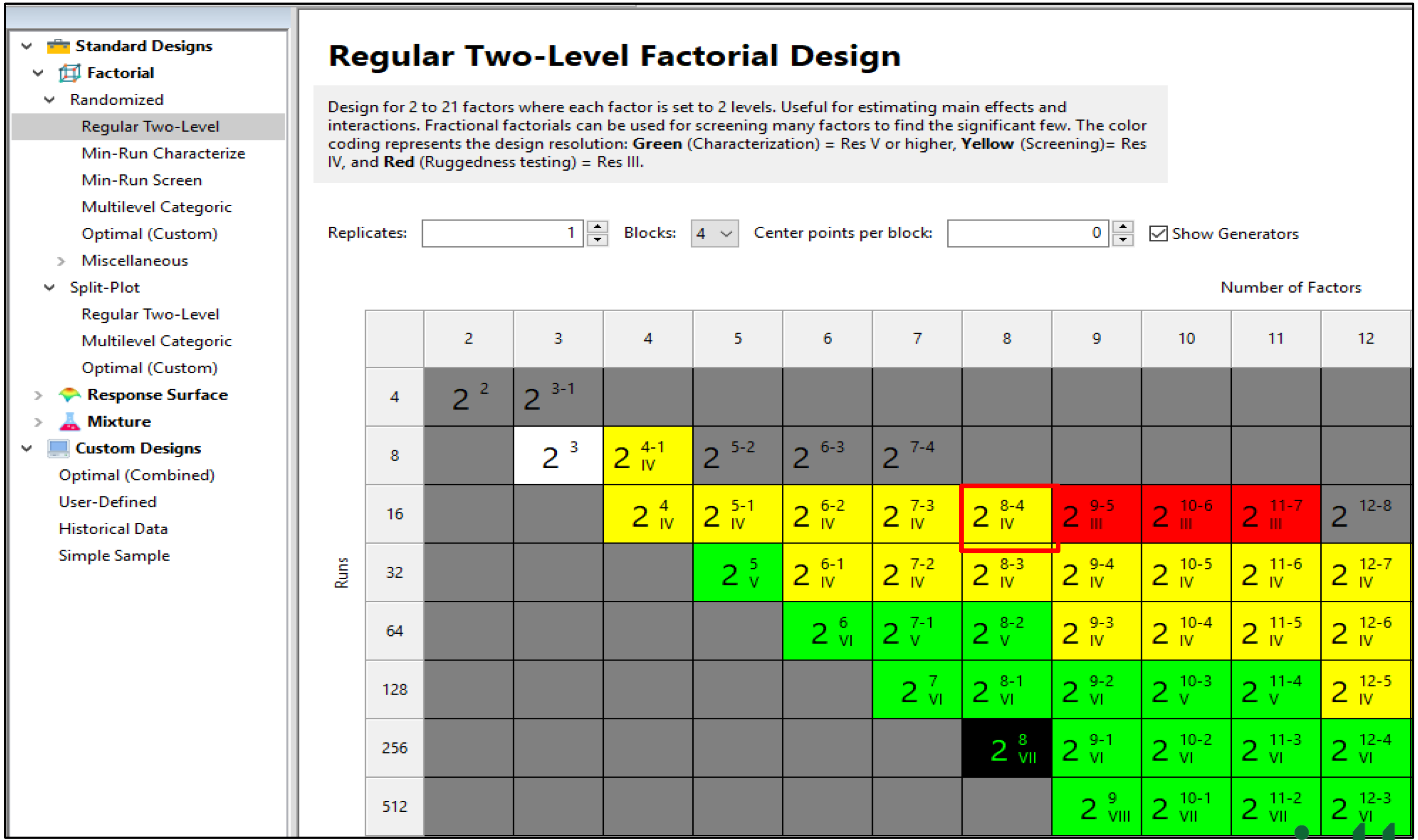
All interactions can be easily calculated to produce the interaction patterns

Fractional Factorial designs - resolution

- Resolution V: Main effects confounded with 3-way interactions
- Resolution IV: 2-way interactions are confounded with each other
- Resolution III: Main effects are confounded with 2-way interactions

	Resolution		
Factors	Full	V	Runs
5	32	16	$^1/_2$
6	64	32	$^1/_2$
7	128	64	$^1/_2$
8	256	64	$^1/_4$
9	512	128	$^1/_4$
10	1,024	128	$^1/_8$
11	2,048	128	$^1/_{16}$
12	4,096	256	$^1/_{16}$
13	8,192	256	$^1/_{32}$
14	16,384	256	$^1/_{64}$
15	32,768	256	$^1/_{128}$

Fractional Factorial designs – resolution, overview



Runs	2	3	4	5	6	7	8	9	10	11	12
4	2^{2}	2^{3-1}									
8		2^{3}	2^{4-1}_{IV}	2^{5-2}	2^{6-3}	2^{7-4}					
16			2^{4}_{IV}	2^{5-1}_{IV}	2^{6-2}_{IV}	2^{7-3}_{IV}	2^{8-4}_{IV}	2^{9-5}_{III}	2^{10-6}_{III}	2^{11-7}_{III}	2^{12-8}
32				2^{5}_{V}	2^{6-1}_{IV}	2^{7-2}_{IV}	2^{8-3}_{IV}	2^{9-4}_{IV}	2^{10-5}_{IV}	2^{11-6}_{IV}	2^{12-7}_{IV}
64					2^{6}_{VI}	2^{7-1}_{V}	2^{8-2}_{V}	2^{9-3}_{IV}	2^{10-4}_{IV}	2^{11-5}_{IV}	2^{12-6}_{IV}
128						2^{7}_{VI}	2^{8-1}_{VI}	2^{9-2}_{VI}	2^{10-3}_{V}	2^{11-4}_{V}	2^{12-5}_{IV}
256							2^{8}_{VII}	2^{9-1}_{VI}	2^{10-2}_{VI}	2^{11-3}_{VI}	2^{12-4}_{VI}
512								2^{9}_{VIII}	2^{10-1}_{VII}	2^{11-2}_{VII}	2^{12-3}_{VI}

Diagnostics/Figures of merit

- Model related:
  - Variation Inflation Factor/Leverage
  - Condition number (more about this later)
  - Residuals
  - Cook's Distance
  - Model stability
  - Percent contribution per variable (more informative than p-values)
- Model performance:
  - R^2
  - Adjusted R^2
  - Predicted R^2
  - Root mean square error
  - Adequate precision ("signal–to-noise", preferably > 4)

Plots and visualizations

- Plots of effects (normal, half-normal and pareto plots)
- Various plots of residuals
- Response surface
- Predicted vs. actual
- Plots for detecting outliers
- Response surface plots

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Other topics

- Transformation of Y
  - If the ratio of max/min of the response variable is > 10 one might consider a transformation
  - Should also use background knowledge to decide on which transformation might be applied (first principles and theory; physics, chemistry)
  - NB! Remember to transform back to the original unit for plotting predicted vs. actual and calculate figures of merit!
- Blocking
  - Can be used to correct for unwanted effects
    - Day
    - Operator
    - Raw material batch
  - Solution: Include “block” variable(s) in the design

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Examples of DoE in DAT4.zero

- Fersa:
  - The DOE is based on the experience of FERSA and IDEKO for identifying parameters and variables with a larger influence on the process
  - Objective: Setting conditions to cause burns for establishing the critical limits of parameters for various process operations
- Dentsply-Sirona (KIT)
  - Tool tumble and the radial feed were modified to examine relations between parameters of the hobbing process
  - Objective: Analyse gear quality and acoustic emission (some dentist patients react psychologically to the noise type and level)
- Benteler (Idletechs)
  - Moving the extrusion of an aluminium profile to in-house production (the famous Volvo Backplate)
  - DoE for optimizing the extruder settings
  - Objective: Reduce faults and obtain stable dimensions prior to machining (MSPC)

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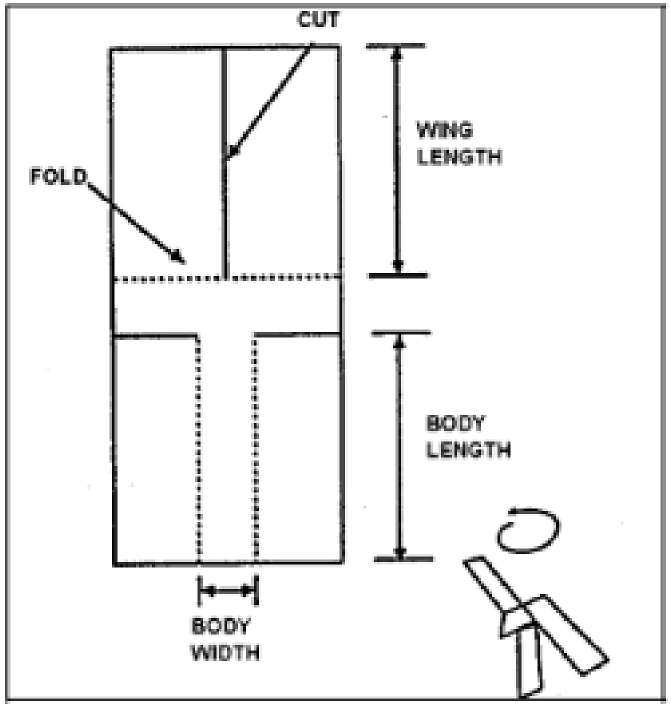
Case study: Paper helicopters - I

A case study by George Box with the purpose of teaching DoE

Part I: Screening

Factors:

	Name	Units	Type	Low	High
A [Categoric]	Paper Type		Categoric	Regular	Bond
B [Numeric]	Wing Length	Inches	Numeric	3	4.75
C [Numeric]	Body Length	Inches	Numeric	3	4.75
D [Numeric]	Body Width	Inches	Numeric	1.25	2
E [Categoric]	Fold		Categoric	No	Yes
F [Categoric]	Taped Body		Categoric	No	Yes
G [Categoric]	Paper Clip		Categoric	No	Yes
H [Categoric]	Taped Wing		Categoric	No	Yes



Response:

Flight time

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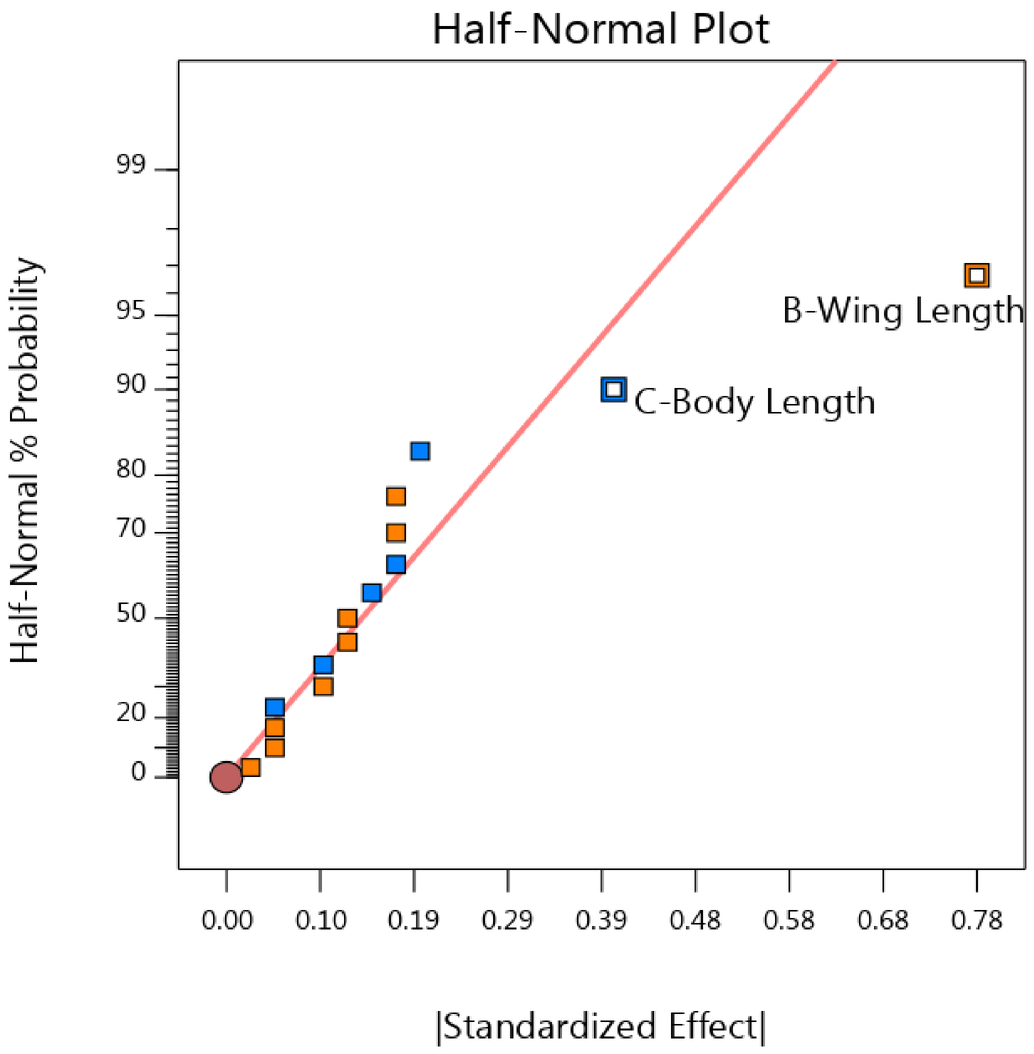
Helicopter - Half-Normal plot



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Helicopter - ANOVA table and fit statistics

ANOVA for selected factorial model

Response 1: Flight time

Source	Sum of Squares	df	Mean Square	F-value	p-value
Model	3.04	2	1.52	23.13	< 0.0001
B-Wing Length	2.40	1	2.40	36.53	< 0.0001
C-Body Length	0.6400	1	0.6400	9.73	0.0081
Residual	0.8550	13	0.0658		
Cor Total	3.90	15			

Fit Statistics

Std. Dev.	0.2565		**R^2**	0.7806
Mean	2.74		**Adjusted R^2**	0.7469
C.V. %	9.37		**Predicted R^2**	0.6677
			Adeq Precision	10.5810

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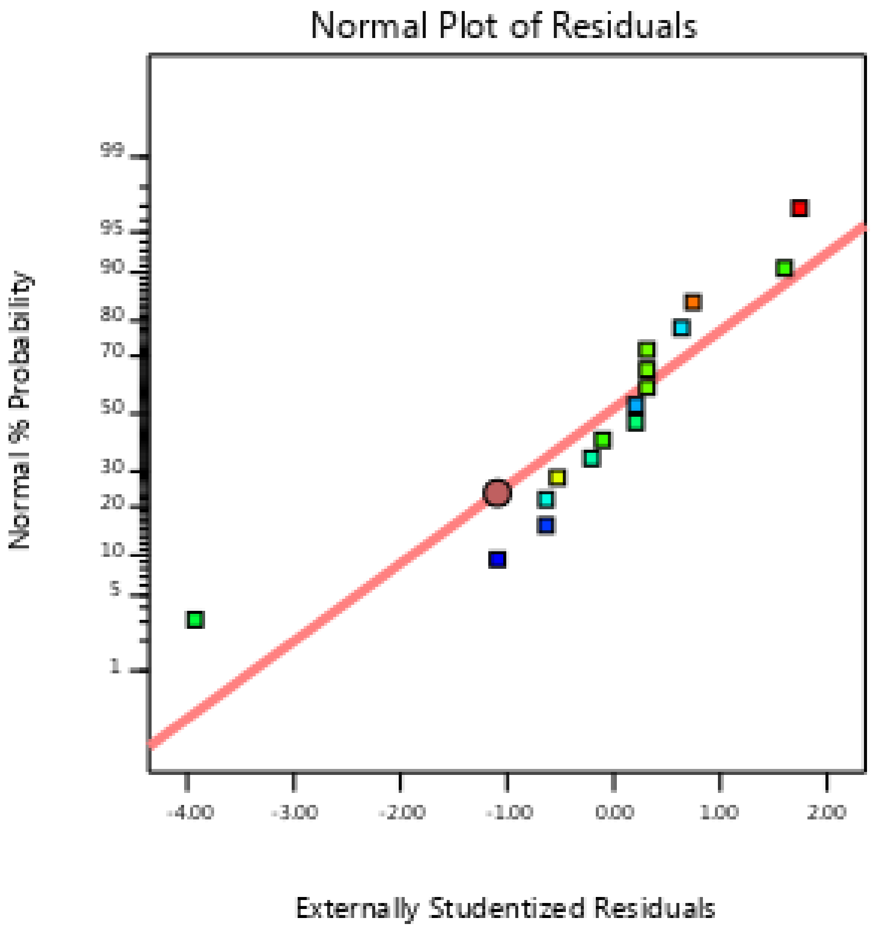
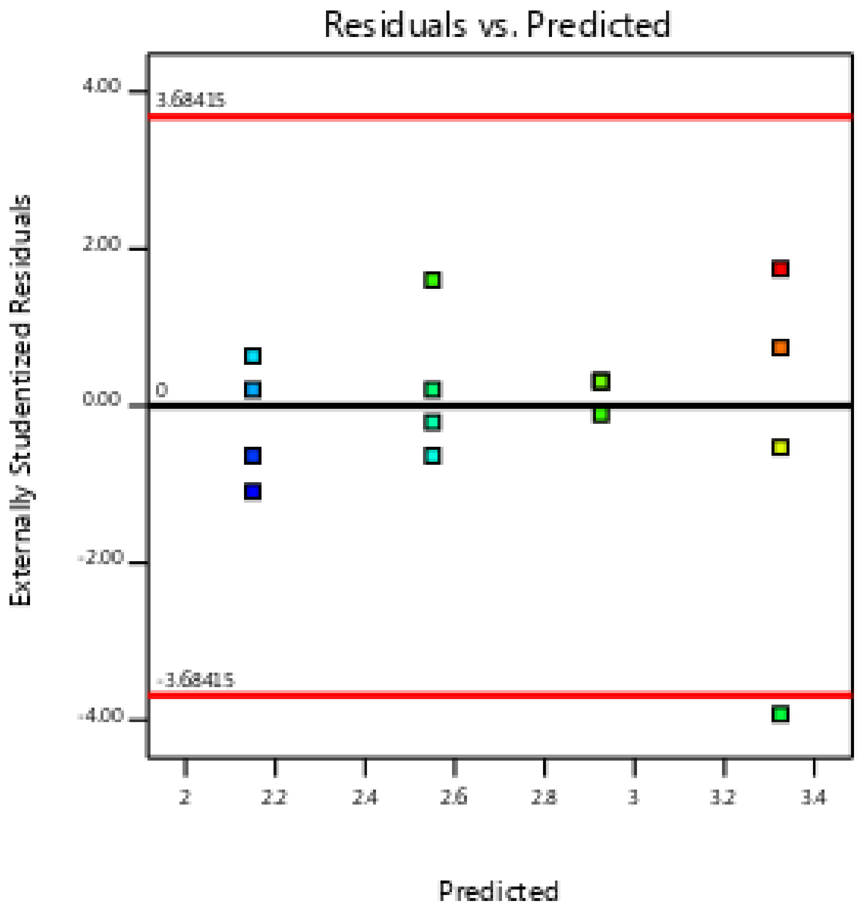
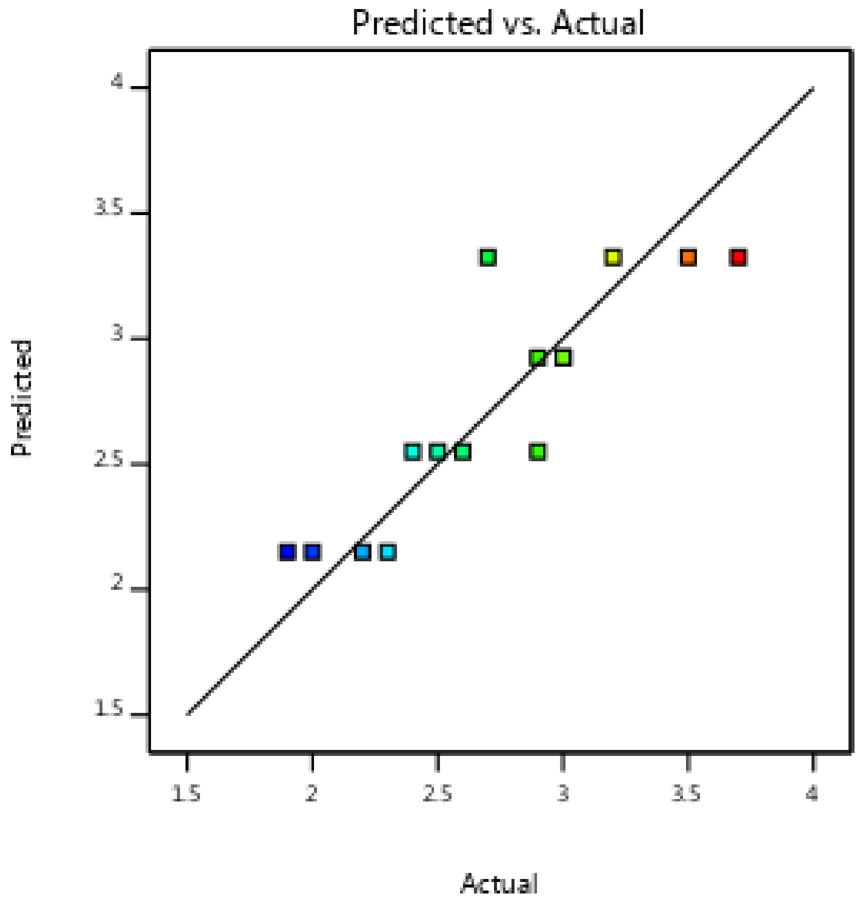
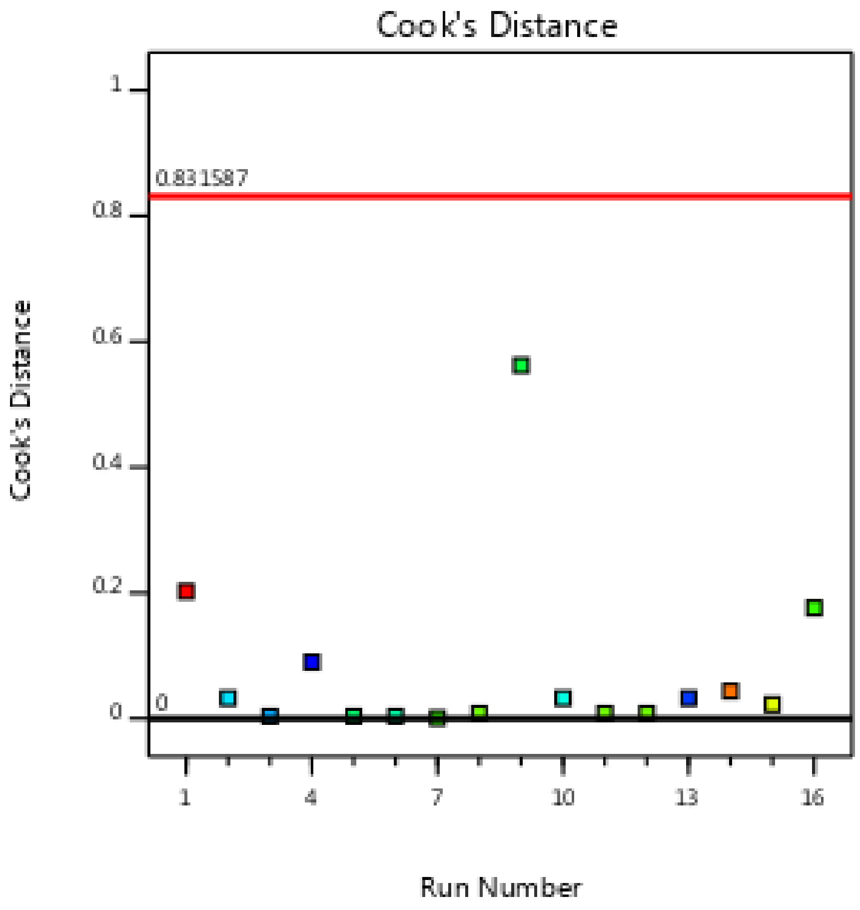
Helicopter - Diagnostics - 1



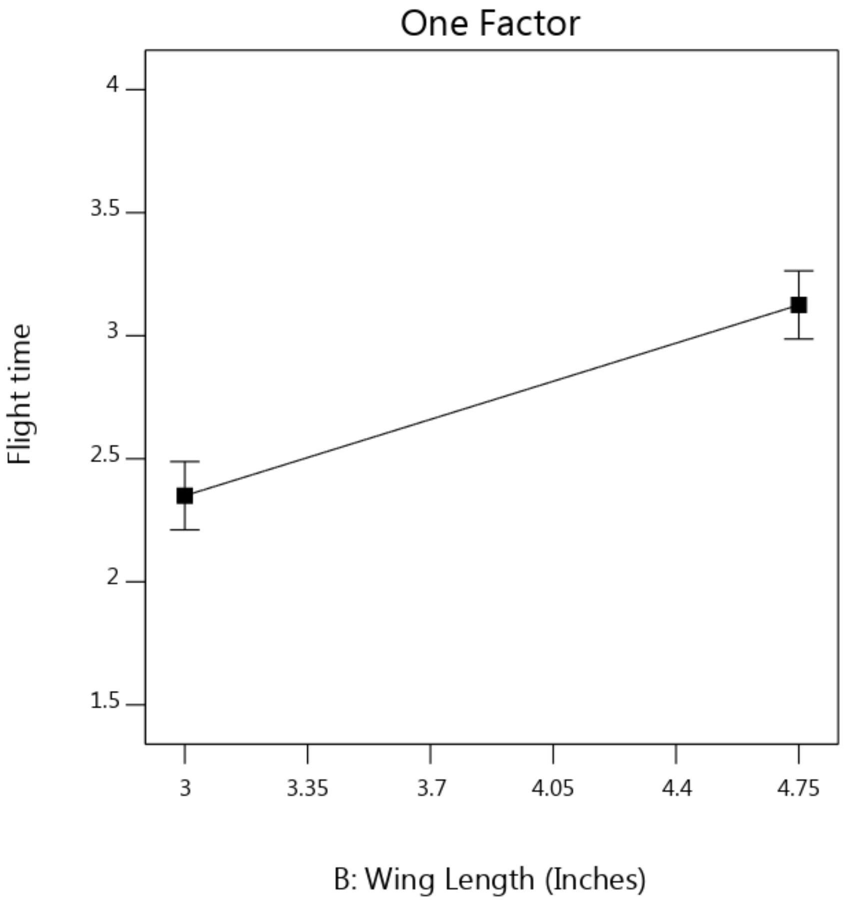


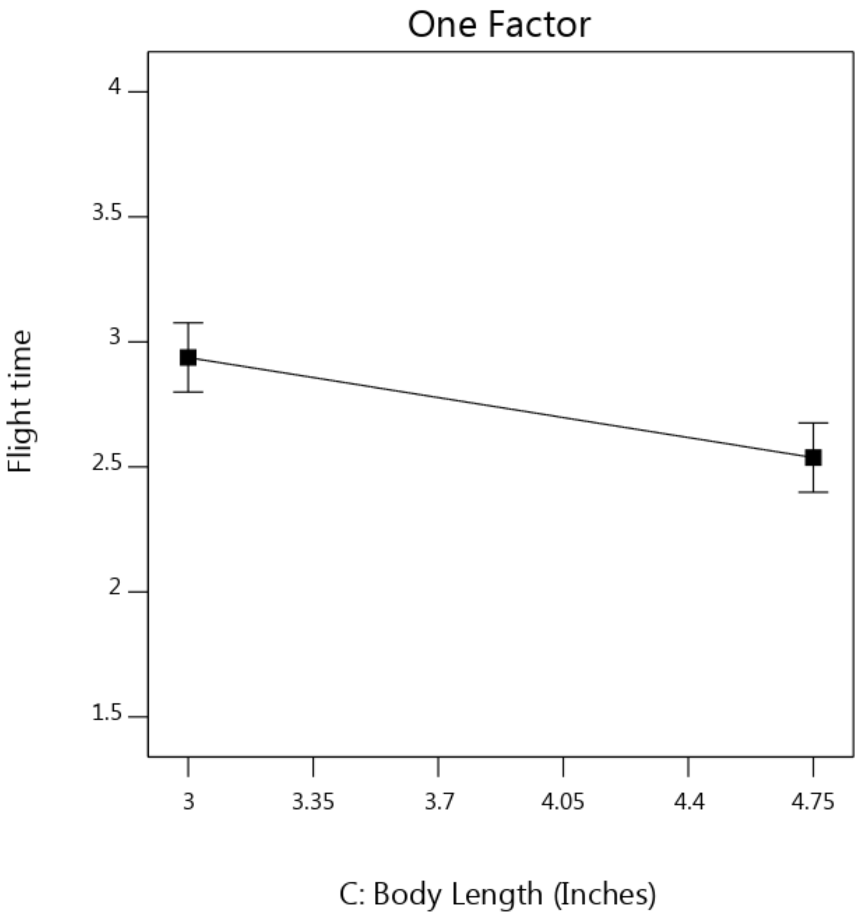
Helicopter - Diagnostics - 2





Helicopter - Effects





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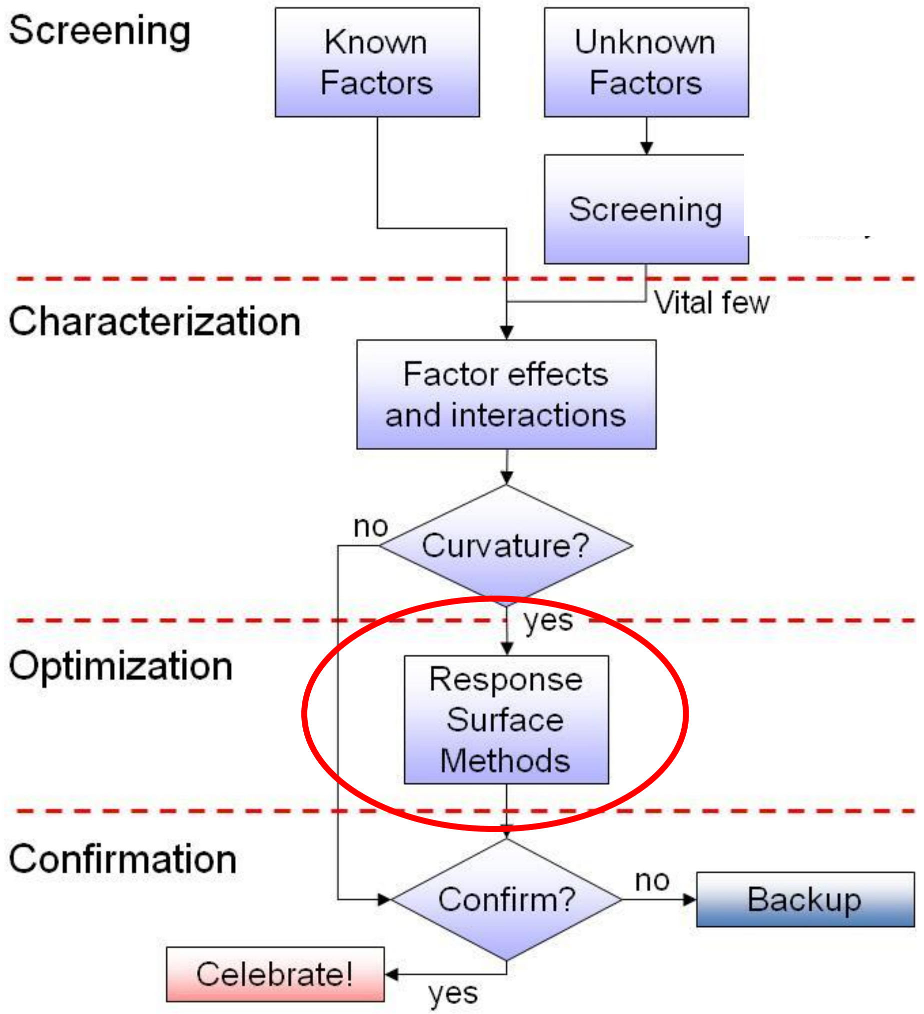
Strategy of Experimentation



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Response Surface Methodology

Subject Matter Knowledge
(Plus Factorial Screening)

↓

Vital Few Factors

↓

Process → Measured Response(s)

↓

Model fitting

↓

Polynomial Model

↓

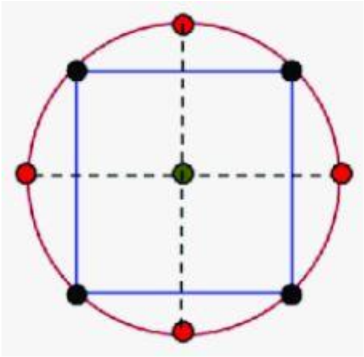
Response Surface

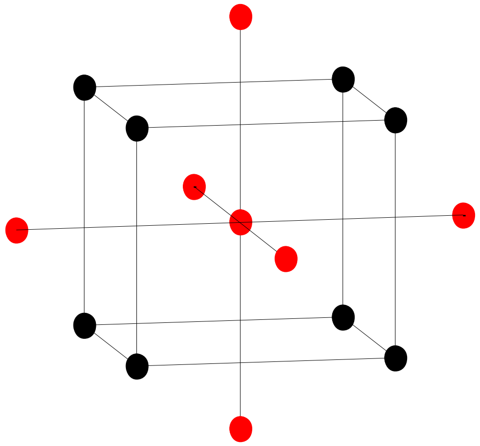
Optimisation Designs

- Objective
  - Model the variations of the responses with accuracy, so as to know the precise shape of the response surface and (optionally) find optimum values
- Problem formulation
  - Include main effects
  - Include interactions (two- and/or three-variable)
  - Include squared and/or cubic terms
- Designs
  - Central composite design
  - Box Behnken design

Central Composite Designs

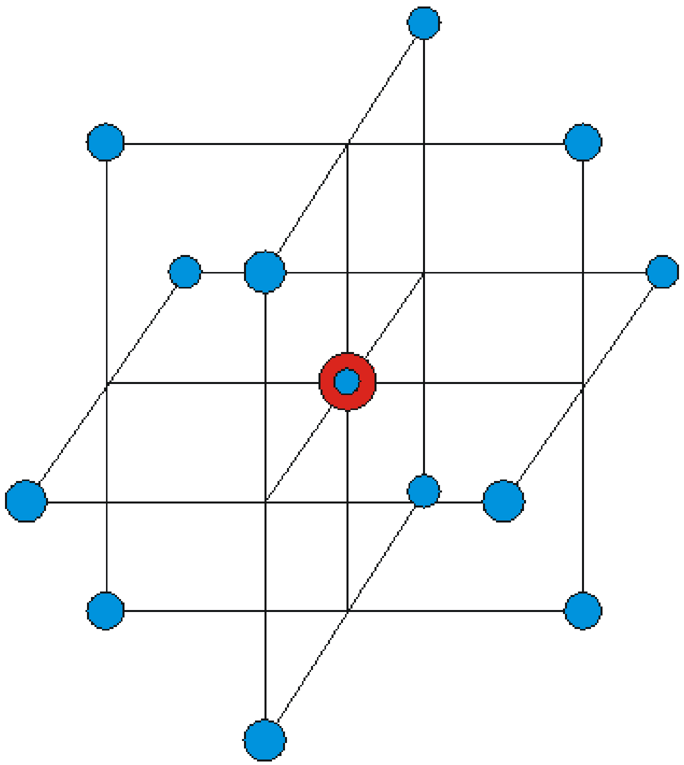
- Objective
  - Model a response surface
  - 5 levels for each variable
- Advantage
  - Can be built as an extension of a full factorial
  - Additional points (red) are called *star points*





Box-Behnken Design

- Each factor has only three levels. Use when region of interest and region of operability nearly the same.
- Good design properties, little collinearity, rotatable or nearly rotatable, some have orthogonal blocks, insensitive to outliers and missing data.
- Does not predict well as CCD at the corners of the design space.



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Polynomial Approximations

Factorial designs fit a factorial model:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$$

Most response surface designs fit a full quadratic model:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$$

Shape parameters *(pictures on following slides)*:

- Intercept – a horizontal plane.
- Linear terms – slopes (gradients) of the plane.
- Two-Factor interactions – twists in the plane.
- Squared terms – symmetric curvature.
- Cubic terms – asymmetry (inflection).

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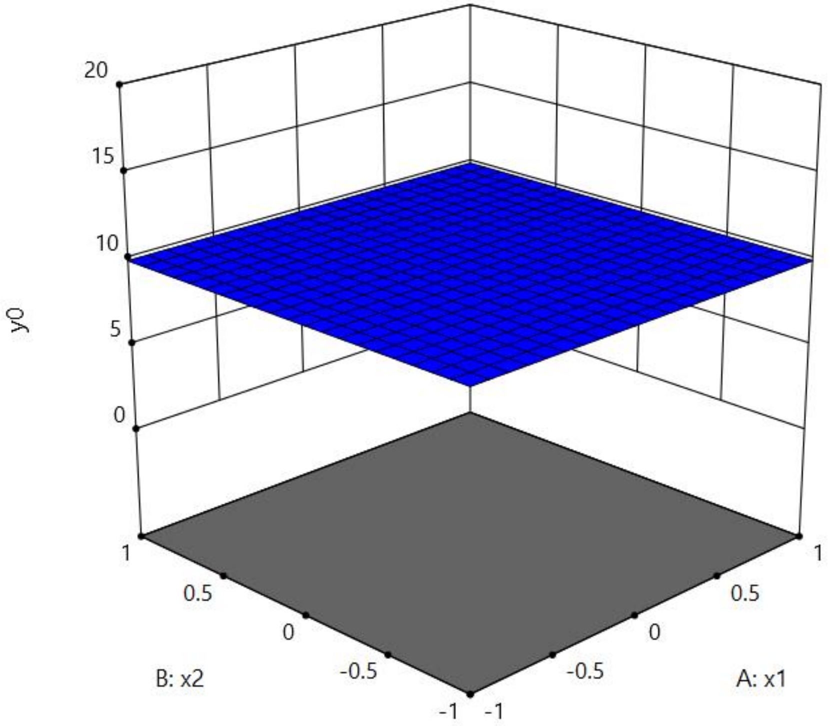
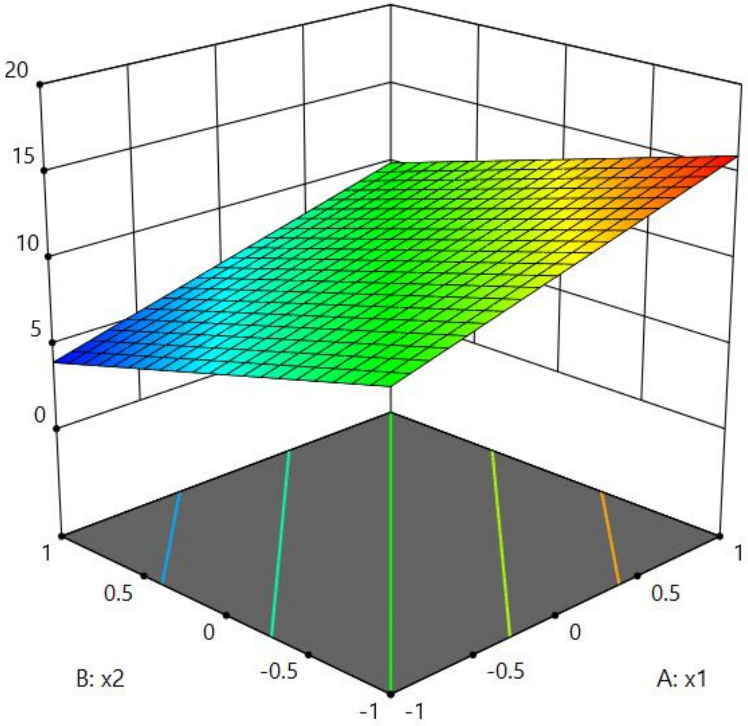
Polynomial Models - 1

Shape Parameters

Intercept
a horizontal plane
y=10



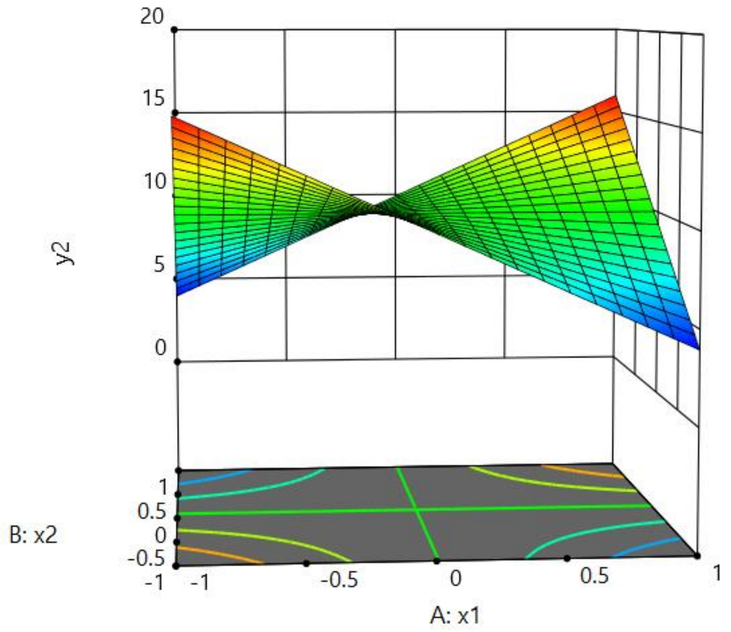
Linear terms
slopes (gradients) of the plane
y=10+3A-3B



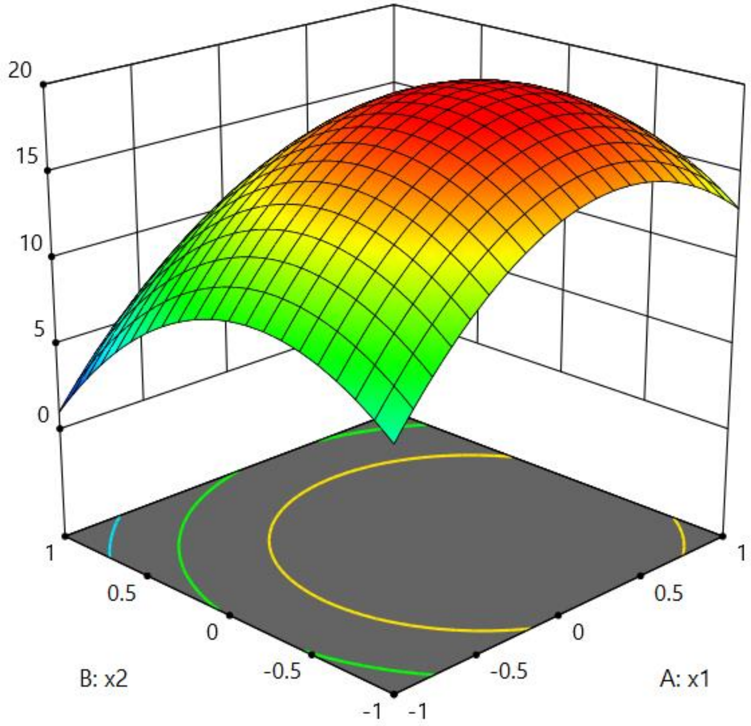
Polynomial Models - 2

Shape Parameters

Two-Factor interactions
twists in the plane
$y=10+6AB$



Squared terms
symmetric curvature
$y=19+3A-3B-6A^2-6B^2$



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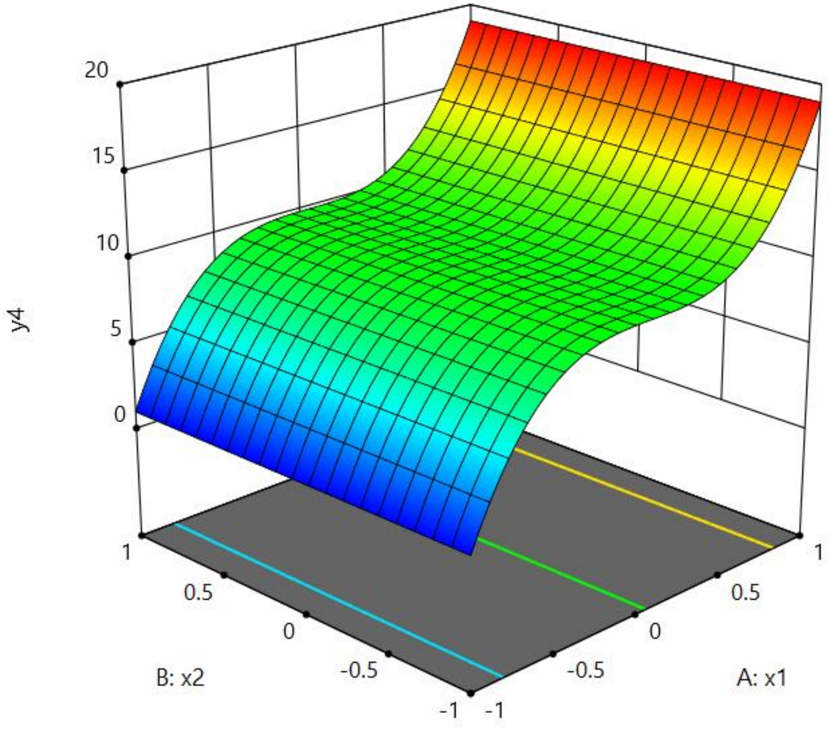
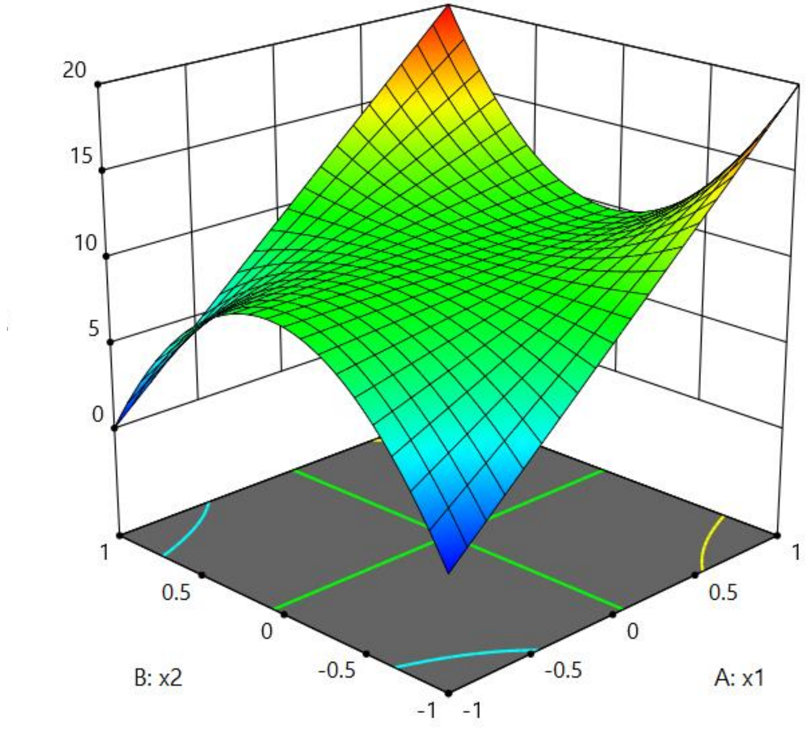
Polynomial Models - 3

Shape Parameters

Cubic terms asymmetry (inflection) $Y= 10+5A^3$



Cubic terms asymmetry (inflection) $Y=10+10AB^2$



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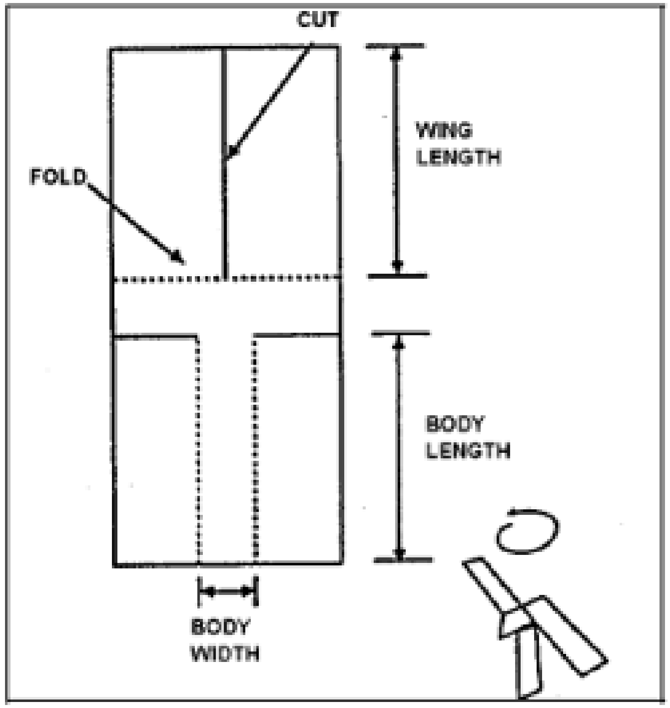
Case study: Paper helicopters - II

A case study by George Box with the purpose of teaching DoE

Part II: Response surface model – Central Composite Design

Design and results:

Std	Run	Factor 1 A:Body length	Factor 2 B:Wing length	Response 1 Flight time
2	1	70	109.2	2.9
4	2	70	128.4	3.2
11	3	60	118.8	3.6
8	4	60	132.376	3.4
3	5	50	128.4	3.3
1	6	50	109.2	3.1
6	7	74.1421	118.8	3.4
9	8	60	118.8	3.7
10	9	60	118.8	3.6
7	10	60	105.224	3.5
5	11	45.8579	118.8	3.3



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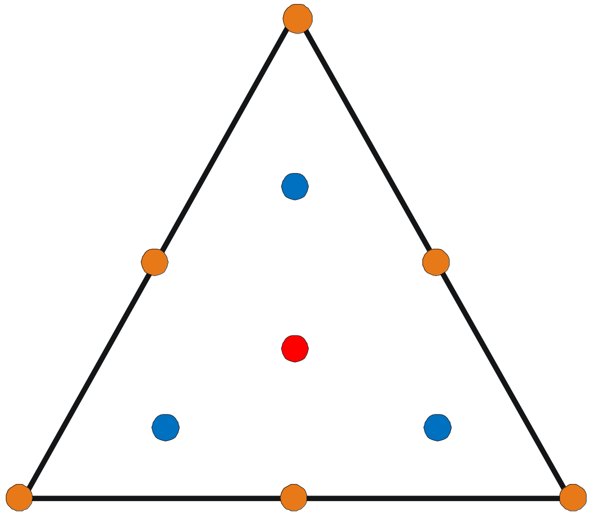
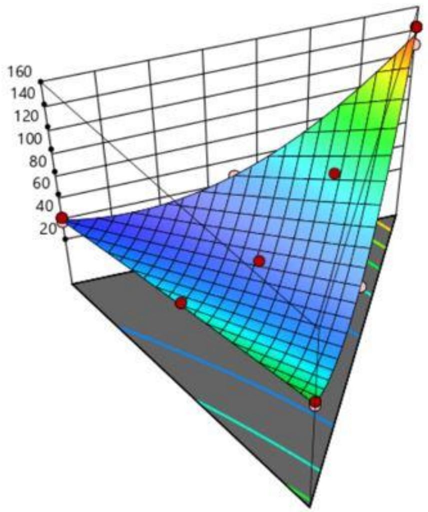
Designs with constraints

- Optimal designs
  - Example: Baking a cake: with long time and high temperature the cake is burned
- Mixture designs
  - Example 2: Fruit punch: The sum of ingredients is 100% (Orange juice, tequila and grenadine syrup)





Example of a constrained situation - I

- Cooked Meat
- Design variables: Marinating Time, Steaming Time, Frying Time
- Responses: Sensory measurements
- Full Factorial solution
- 8 experiments combining the low and high levels of the variables

Sample	Marinating	Steaming	Frying
1	6	5	5
2	18	5	5
3	6	15	5
4	18	15	5
5	6	5	15
6	18	5	15
7	6	15	15
8	18	15	15

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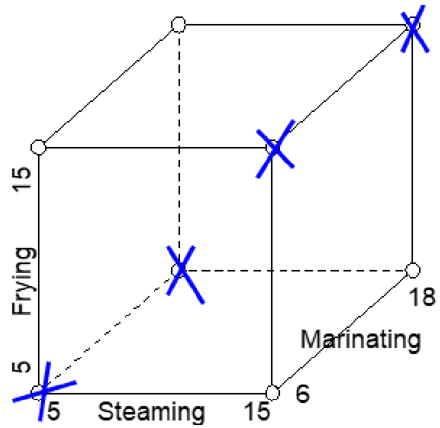
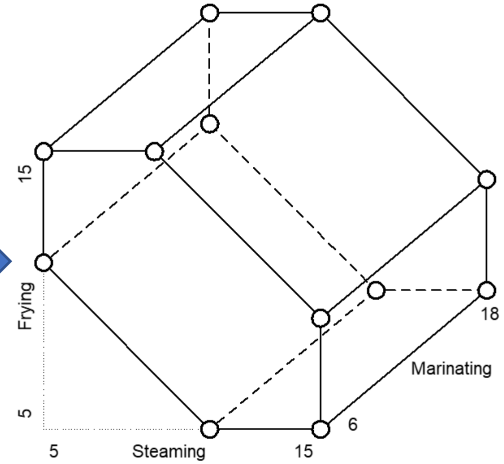
Example of a constrained situation - II

- Cooked Meat
- Extreme combinations are forbidden
- Steaming + Frying < 16 : raw meat
  Steaming + Frying > 24 : overcooked
- Full Factorial does not apply
- 4 out of 8 cube samples are excluded
- The remaining 4 are not enough to explore the region of interest
- Must find other combinations of the factors





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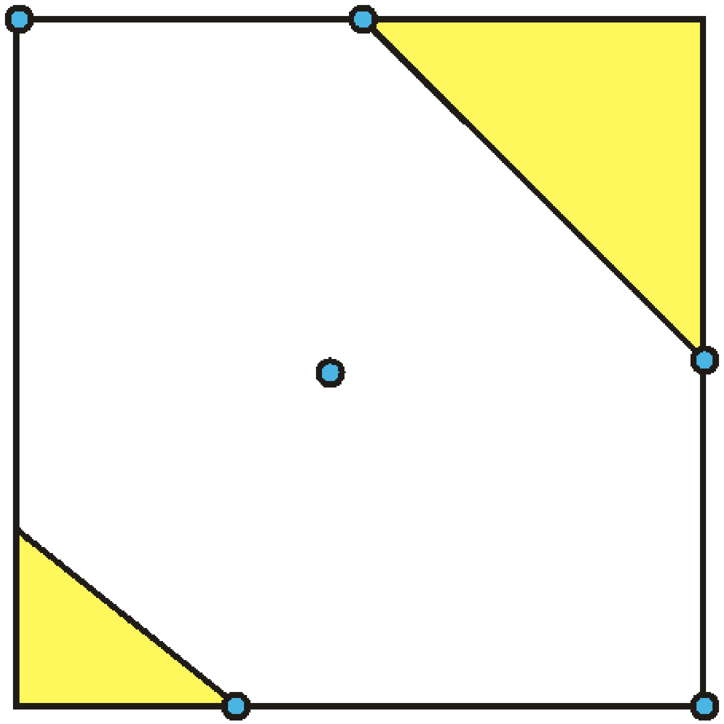
Response Surface Designs - Optimal Design

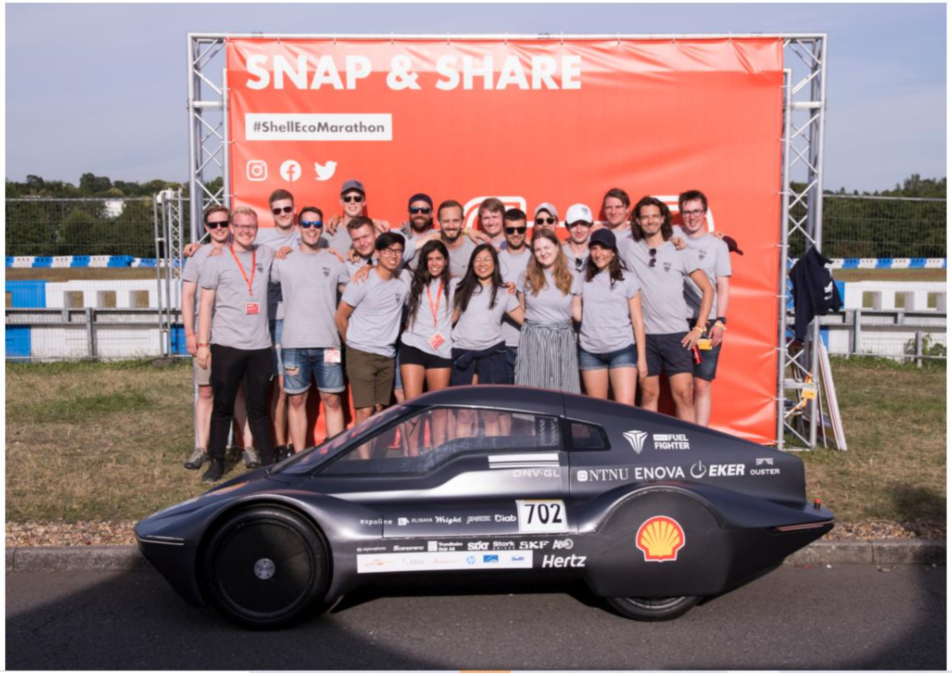
- Chooses runs based on minimizing the error of the model coefficients
- The optimal points are augmented with additional runs to provide estimates of lack of fit and pure error
- You must choose a model (quadratic is default) and this determines the number of runs necessary
- Primary use is for constrained design spaces
- Two of many options:
    - D-optimal (maximize the determinant)
    - I-optimal (gives a better coverage inside the design space)



External

Hands-on demo – Fuel fighter

- Problem: What influences the vertical acceleration on the front and rear of the car when driving over speed bumps and how to find the optimal settings given a maximum value for the acceleration?
- Design factors: Height of bump, center of gravity, weight and speed



Summary

- DoE is the best way of generating meaningful experiments that will provide the maximum information with the minimal experimental effort
- Designed experiments can be performed sequentially, i.e., more information can be added if need be, to an existing design
- Many factors can be analyzed in a small number of experiments to screen out important factors
- When a small number of factors have been isolated, the design can be extended to become an optimization design
- DoE is also an important tool for metamodelling for optimizing first principle and simulation based systems

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