Chemometrics

MA4605

Week 11. Lecture 20. Factorial designs

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- In a given experiment the reaction rate will depend on factors such as: temperature,pH, ionic strength, chemical composition of the buffer solution, enzyme concentration.
- The early stages of experimentation usually involve the investigation of a large number of potential factors to discover the vital few factors.
- We must determine which factors, and which interactions between them are important in affecting the response.

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- The two levels are known as: **low** and **high**.

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- We will consider in detail 2^3 designs

- The 2^3 design is a two level factorial experiment design with three factors **A** , **B** and **C**.
- This design tests
  - three main effects A,B and C;
  - three two-factor interaction effects AB,BC and AC ;
  - one three-factor interaction effect ABC.
- A plus sign (+) denotes that the factor is at the high level and a minus sign (-) that it is at low level.

Notation

Combination	A	B	C	Response
1	-	-	-	y_1
a	+	-	-	y_2
b	-	+	-	y_3
c	-	-	+	y_4
ab	-	+	+	y_5
ac	+	-	+	y_6
bc	+	+	-	y_7
abc	+	+	+	y_8

The presence of a letter indicates that the specified factor is at its high level(+) and the absence of a letter indicates that the specified factor is at its low (-) level.
(1) is used to indicate that all factors are at their lowest (-) values.

Example.

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For the curing temperature, the high level is set at 150 deg C while the low level is set at 100 deg C.
For the curing time, the high level is set at 90 minutes, while the low level is set at 30 minutes.
The output response monitored is process yield. Assume further that the data were gathered by performing just a single replicate (n=1) per combination treatment.

Run	Combination	Mix Ratio (a)	Temp(b)	Time(c)	Response
1	(1)	45% (-)	100C (-)	30m (-)	8
2	a	55% (+)	100C (-)	30m (-)	9
3	b	45% (-)	150C (+)	30m (-)	34
4	ab	55% (+)	150C (+)	30m (-)	52
5	c	45% (-)	100C (-)	90m (+)	16
6	ac	55% (+)	100C (-)	90m (+)	22
7	bc	45% (-)	150C (+)	90m (+)	45
8	abc	55% (+)	150C (+)	90m (+)	56

Effect-the average of observations when the factor is **high** minus the average when it is **low**.
Effect of A: (9+52+22+56-(8+34+16+45))/4 = 9

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4	ab	55% (+)	150C (+)	30m (-)	52
5	c	45% (-)	100C (-)	90m (+)	16
6	ac	55% (+)	100C (-)	90m (+)	22
7	bc	45% (-)	150C (+)	90m (+)	45
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Effect-the average of observations when the factor is **high** minus the average when it is **low**.
Effect of A: (9+52+22+56-(8+34+16+45))/4 = 9
Effect of B: (34+52+45+56-(8+9+16+22))/4 = 33

Run	Combination	Mix Ratio (a)	Temp(b)	Time(c)	Response
1	(1)	45% (-)	100C (-)	30m (-)	8
2	a	55% (+)	100C (-)	30m (-)	9
3	b	45% (-)	150C (+)	30m (-)	34
4	ab	55% (+)	150C (+)	30m (-)	52
5	c	45% (-)	100C (-)	90m (+)	16
6	ac	55% (+)	100C (-)	90m (+)	22
7	bc	45% (-)	150C (+)	90m (+)	45
8	abc	55% (+)	150C (+)	90m (+)	56

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Effect of A: (9+52+22+56-(8+34+16+45))/4 = 9
Effect of B: (34+52+45+56-(8+9+16+22))/4 = 33
Effect of C: (16+22+45+56-(8+9+34+52))/4 = 9

The following calculations for the main and interaction effects of these 3 factors are obtained:

A = 1/(4n) x [-(1)+a-b+ab-c+ac-bc+abc] =

[-8+9-34+52-16+22-45+56] = 1/4 x 36 = 9

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B = 1/4 x [-8-9+34+52-16-22+45+56] = 1/4 x 132 = 33

AB = 1/4 x [+8-9-34+52+16-22-45+56] = 1/4 x 22 = 5.5

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AB = 1/4 x [+8-9-34+52+16-22-45+56] = 1/4 x 22 = 5.5

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AC = 1/4 x [+8-9+34-52-16+22-45+56] = 1/4 x -2 = -0.5

BC = 1/4 x [+8+9-34-52-16-22+45+56] = 1/4 x -6 = -1.5

ABC = 1/4 x [-8+9+34-52+16-22-45+56] = 1/4 x -12 = -3

Interpret factor effects

- Based on these calculations, the main effect of temperature (B=33) has the greatest influence on the process yield, although the main effects of mixture ratio (A=9) and time (C=9) are also significant.

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- Based on these calculations, the main effect of temperature (B=33) has the greatest influence on the process yield, although the main effects of mixture ratio (A=9) and time (C=9) are also significant.
- The interaction between mixture ratio and temperature also produces a positive effect on yield (AB=5.5), but the rest of the factorial interactions affect the yield in the negative direction (although to much lower degrees).