Fractional Factorial Designs

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10-variable 2-level Factorial Experiments

- 2^{10}=1024 tests:

1	Mean response
C_1^{10}=10	Main effects
C_2^{10}=45	Two-factor interaction effects
C_3^{10}=120	Three-factor interaction effects
C_4^{10}=210	Four-factor interaction effects
C_5^{10}=252	Five-factor interaction effects
C_6^{10}=210	Six-factor interaction effects
C_7^{10}=120	Seven-factor interaction effects
C_8^{10}=45	Eight-factor interaction effects
C_9^{10}=10	Night-factor interaction effects
C_{10}^{10}=1	Ten-factor interaction effects
1024	**Number of tests**

2^3 Factorial Design

- Effect calculation matrix:

Test	Avg.	1	2	3	12	13	23	123
1	+	−	−	−	+	+	+	−
2	+	+	−	−	−	−	+	+
3	+	−	+	−	−	+	−	+
4	+	+	+	−	+	−	−	−
5	+	−	−	+	+	−	−	+
6	+	+	−	+	−	+	−	−
7	+	−	+	+	−	−	+	−
8	+	+	+	+	+	+	+	+

- All 8 columns are mutually **orthogonal, i.e., statistically uncorrelated (correlation=0)**
- 8 effects can be independently estimated:
  - **average, 1, 2, 3, 12, 13, 23, 123**

2-level 4-variable Experiment Using 2^3 Factorial Design

- To keep all main effects orthogonal: assign the 4th variable to the 3-factor interaction in 2^3 design matrix

Test	1	2	3	123=4
1	−	−	−	−
2	+	−	−	+
3	−	+	−	+
4	+	+	−	−
5	−	−	+	+
6	+	−	+	−
7	−	+	+	−
8	+	+	+	+

2^{4-1} Fractional Design

- Effect calculation matrix:

Test	1	2	3	4	12	13	14	23	24	34	123	124	134	234	1234
1	−	−	−	−	+	+	+	+	+	+	−	−	−	−	+
2	+	−	−	+	−	−	+	+	−	−	+	−	−	+	+
3	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+
4	+	+	−	−	+	−	−	−	−	+	−	−	+	+	+
5	−	−	+	+	+	−	−	−	−	+	+	+	−	−	+
6	+	−	+	−	−	+	−	−	+	−	−	+	−	+	+
7	−	+	+	−	−	−	+	+	−	−	−	+	+	−	+
8	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

- Confused or confounded effects:
  - 4 and 123; 3 and ?; 2 and ?; 1 and ?
  - 23 and 14; 13 and ?; 12 and ?
  - 1234 and ?

8 Effects Estimated from 2^3 Tests

- 8 effects estimated from the original 2^3 design:

l_0: mean+(1234)/2 l_{12}: 12+34
l_1: 1+234 l_{13}: 13+24
l_2: 2+134 l_{23}: 23+14
l_3: 3+124 l_{123}: 123+4

- Assuming three- and four-factor interactions can be neglected:

l_0: mean l_{12}: 12+34
l_1: 1 l_{13}: 13+24
l_2: 2 l_{23}: 23+14
l_3: 3 l_{123}: 4

Another Example: 2^{5-2} Design

- Base design: 2^3 factorial design

Test	Avg. I	1	2	3	**12=4**	**13=5**	23	123
1	+	−	−	−	+	+	+	−
2	+	+	−	−	−	−	+	+
3	+	−	+	−	−	+	−	+
4	+	+	+	−	+	−	−	−
5	+	−	−	+	+	−	−	+
6	+	+	−	+	−	+	−	−
7	+	−	+	+	−	−	+	−
8	+	+	+	+	+	+	+	+

- Assign 4 and 5th variables to 12 and 13 interaction effects – **How to figure out the confounding effects?**

Design Generators

4	=	12
+		+
−		−
−		−
+		+
+	=	+
−		−
−		−
+		+

4	×	4	=	I
+		+		+
−		−		+
−		−		+
+		+		+
+	×	+	=	+
−		−		+
−		−		+
+		+		+

- 2^{5-2}: 4=12 and 5=13 $\Rightarrow$ 4×4=12 ×4 and 5 ×5=13 ×5
- **Design generators**: I=124 and I=135

Defining Relation

- Design generators: I=124 and I=135
  $\Rightarrow$ **products of any combinations of generators will produce I**
- 2^{5-2} example:
  $124 \times 135 = I \Rightarrow (1)(1)2345 = I \Rightarrow 2345 = I$
- **2^{5-2} Defining Relation:**

$$\boxed{I=124=135=2345}$$

Complete Confounding Pattern

- Effects of base design 2^3: 1, 2, 3, 12, 13, 23, 123
- l_1: (1)I=(1)124=(1)135=(1)2345 $\Rightarrow$
  1=24=35=12345
  l_2: (2)I=(2)124=(2)135=(2)2345 $\Rightarrow$
  2=14=1235=345
  l_3: ?
  l_{12}: 12=4=235=1345
  l_{13}: ?
  l_{23}: ?
  l_{123}:?

Procedure for Design Characterization

- Step 1: Defining the Base Design
- Step 2: Introduction of Additional Variables
- Step 3: Obtaining the Defining Relation
- Step 4: Complete Confounding Structure

Step 1 :Defining the Base Design

- Base design: 2^3 factorial design

Test	I	1	2	3	12	13	23	123	y
1	+	−	−	−	+	+	+	−	y_1
2	+	+	−	−	−	−	+	+	y_2
3	+	−	+	−	−	+	−	+	y_3
4	+	+	+	−	+	−	−	−	y_4
5	+	−	−	+	+	−	−	+	y_5
6	+	+	−	+	−	+	−	−	y_6
7	+	−	+	+	−	−	+	−	y_7
8	+	+	+	+	+	+	+	+	y_8
Divisor	8	4	4	4	4	4	4	4	

Step 2: Introduction of Additional Variables

- 4=12; 5=13; 6=23

Test	1	2	3	4	5	6
1	−	−	−	+	+	+
2	+	−	−	−	−	+
3	−	+	−	−	+	−
4	+	+	−	+	−	−
5	−	−	+	+	−	−
6	+	−	+	−	+	−
7	−	+	+	−	−	+
8	+	+	+	+	+	+

The eight tests may now be conducted in accordance with these test recipes.

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Step 3: Obtaining Defining Relation

- I=124, I=135, I=236
- Two-at-a-time combination:
  (124)(135)=2345
  (124)(236)=1346
  (135)(236)=1256
- Three-at-a-time combination:
  (124)(135)(236)=456
- **Defining Relation:**
  I=124=135=236=2345=1346=1256=456

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Step 4: Complete Confounding Structure

- l_1: (1)I=(1)124=(1)135=(1)236=(1)2345=(1)1346=(1)1256=(1)456
  Look at main and two-factor interaction effects ⇒ 1=24=35
- Relevant confounding structure:
  l_0: mean
  l_1: 1 + 24 + 35
  l_2: 2 + 14 + 36
  l_3: 3 + 15 + 26
  l_{12}: 12 + 4 + 56
  l_{13}: 13 +5 + 46
  l_{23}: 23 + 6 + 45
  l_{123}: 34 + 25 + 16

Resolution of Two-level Fractional Factorial Design

The ***Resolution*** is the length of the s**hortest** term in the **defining relation**

Example: I=124=135=2345 → Resolution III
I=1235=2346=1456 → Resolution IV

- **Resolution III**: some main effects are confounded with 2-factor interactions
- **Resolution IV**: some main effects are confounded with 3-factor interactions while some 2-factor interactions are confounded with other 2-factor interactions
- **Resolution V**: some main effects are confounded with 4-factor interactions and some 2-factor interactions are confounded with 3-factor interactions

$L_8(2^7)$ Orthogonal Array

Test	A 1	B 2	C 3	D 4	E 5	F 6	G 7	Result
	Factor							
1	1	1	1	1	1	1	1	y_1
2	1	1	1	2	2	2	2	y_2
3	1	2	2	1	1	2	2	y_3
4	1	2	2	2	2	1	1	y_4
5	2	1	2	1	2	1	2	y_5
6	2	1	2	2	1	2	1	y_6
7	2	2	1	1	2	2	1	y_7
8	2	2	1	2	1	1	2	y_8

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2_{III}^{7-4} Fractional Factorial Design

Test	1	2	3	−12 4	−13 5	−23 6	+123 7
1	−	−	−	−	−	−	−
2	+	−	−	+	+	−	+
3	−	+	−	+	−	+	+
4	+	+	−	−	+	+	−
5	−	−	+	−	+	+	+
6	+	−	+	+	−	+	−
7	−	+	+	+	+	−	−
8	+	+	+	−	−	−	+
	D (4)	B (2)	A (1)	F (6)	E (5)	C (3)	G (7)

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2^{8-4} Fractional Factorial Design

Test	1	2	3	4	234 5	−14 6	123 7	−1234 8
1	−	−	−	−	−	−	−	−
2	+	−	−	−	−	+	+	+
3	−	+	−	−	+	−	+	+
4	+	+	−	−	+	+	−	−
5	−	−	+	−	+	−	+	+
6	+	−	+	−	+	+	−	−
7	−	+	+	−	−	−	−	−
8	+	+	+	−	−	+	+	+
9	−	−	−	+	+	+	−	+
10	+	−	−	+	+	−	+	−
11	−	+	−	+	−	+	+	−
12	+	+	−	+	−	−	−	+
13	−	−	+	+	−	+	+	−
14	+	−	+	+	−	−	−	+
15	−	+	+	+	+	+	−	+
16	+	+	+	+	+	−	+	−
	C	*B*	*A*	*F*	*E*	*H*	*G*	*D*

[Variable "names" given by Taguchi and Wu in the $L_{16}(2^{15})$ orthogonal array]

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Sequential and Iterative Experiments

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Variables Under Study Together with Their Low and High Settings

Variable	Ingredient	Level (weight %) Low (−)	High (+)
1	Soybean emulsion: 9.3% soybean solids	1.67	5.00
2	Vegetable fat: hydrogenated coconut oil	10.00	20.00
3	Carbohydrates: corn syrup solids	0.00	5.00
4	Emulsifiers: mono- and diglycerides	0.17	0.50
5	Primary stabilizer: hydroxypropyl methyl cellulose	0.00	0.50
6	Secondary stabilizer: microcrystalline cellulose	0.00	0.25
7	Salt: sodium chloride	0.00	0.10

* Amount of sucrose kept constant at 7%; water added to balance to 100%.

Performance measure: whipability (100% overrun)

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Base Design Calculation Matrix

Test	*I*	1	2	3	12	13	23	123
1	+	−	−	−	+	+	+	−
2	+	+	−	−	−	−	+	+
3	+	−	+	−	−	+	−	+
4	+	+	+	−	+	−	−	−
5	+	−	−	+	+	−	−	+
6	+	+	−	+	−	+	−	−
7	+	−	+	+	−	−	+	−
8	+	+	+	+	+	+	+	+

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Design (Recipe) Matrix

Test	1	2	3	4	5	6	7	Overrun (%)
1	−	−	−	+	+	+	−	115
2	+	−	−	−	−	+	+	81
3	−	+	−	−	+	−	+	110
4	+	+	−	+	−	−	−	69
5	−	−	+	+	−	−	+	174
6	+	−	+	−	+	−	−	99
7	−	+	+	−	−	+	−	80
8	+	+	+	+	+	+	+	63

4=12 5=13 6=23 7=123

I=124=135=236=1237=2345=1346=347=1256

=257=167=456=1457=2467=3567=1234567

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Effect Estimates for the 2_{III}^{7-4} Fractional Factorial Design for Overrun(%)

l_0 = 98.875 and estimates mean

l_1 = −41.750 and estimates 1 + 24 + 35 + 67

l_2 = −36.750 and estimates 2 + 14 + 36 + 57

l_3 = 10.250 and estimates 3 + 15 + 26 + 47

l_{12} = 12.750 and estimates 12 + 4 + 37 + 56

l_{13} = −4.250 and estimates 13 + 5 + 27 + 46

l_{23} = −28.250 and estimates 23 + 6 + 17 + 45

l_{123} = 16.250 and estimates 34 + 25 + 16 + 7

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QQ Plot of Effects Based on Tests 1 to 8

E1= -41.75

E2= -36.75

E6= -28.25

E5= -4.25

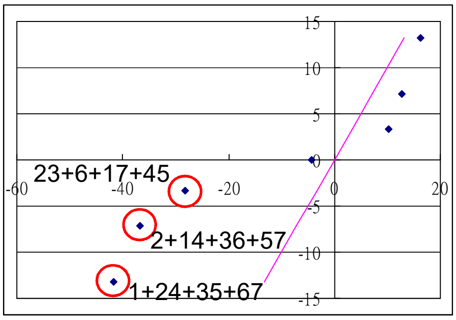
E3= 10.25

E4= 12.75

E7= 16.25

4 smallest effects to estimate S.D.

S.D.= 9.009255



E_i~N(0, 9,01)

Design Matrix for the Mirror Image Design

Test	1	2	3	4	5	6	7	Overrun (%)
9	+	+	+	−	−	−	+	84
10	−	+	+	+	+	−	−	69
11	+	−	+	+	−	+	−	56
12	−	−	+	−	+	+	+	161
13	+	+	−	−	+	+	−	56
14	−	+	−	+	−	+	+	40
15	+	−	−	+	+	−	+	92
16	−	−	−	−	−	−	−	208

4=–12 5=–13 6=–23 7=123

I=–124=–135=–236=1237=2345=1346=–347

=1256=–257=–167=–456=1457=2467=3567

=–1234567

Comparison of Original and Mirror Image Tests

Original Eight Tests			Mirror Image Design Additional Eight Tests		
l_0	= 98.875	and estimates mean	l'_0	= 95.750	and estimates mean
l_1	= −41.750	and estimates 1 + 24 + 35 + 67	l'_1	= −47.500	and estimates 1 − 24 − 35 − 67
l_2	= −36.750	and estimates 2 + 14 + 36 + 57	l'_2	= −67.000	and estimates 2 − 14 − 36 − 57
l_3	= 10.250	and estimates 3 + 15 + 26 + 47	l'_3	= − 6.500	and estimates 3 − 15 − 26 − 47
l_{12}	= 12.750	and estimates 12 + 4 + 37 + 56	l'_{12}	= 63.000	and estimates 12 − 4 + 37 + 56
l_{13}	= − 4.250	and estimates 13 + 5 + 27 + 46	l'_{13}	= 2.500	and estimates 13 − 5 + 27 + 46
l_{23}	= −28.250	and estimates 23 + 6 + 17 + 45	l'_{23}	= 35.000	and estimates 23 − 6 + 17 + 45
l_{123}	= 16.250	and estimates 34 + 25 + 16 + 7	l'_{123}	= − 3.000	and estimates −34 − 25 − 16 + 7

$$\frac{l_1 + l_1'}{2} = (\tfrac{1}{2})[(-41.75) + (-47.5)]$$

estimates $(\tfrac{1}{2})[(1+24+35+67)+(1-24-35-67)]$

$\Rightarrow -44.625$ estimates 1.

$$\frac{l_1 - l_1'}{2} = (\tfrac{1}{2})[(-41.75) - (-47.5)]$$

estimates $(\tfrac{1}{2})[(1+24+35+67)-(1-24-35-67)]$

$\Rightarrow 2.875$ estimates $24+35+67$.

$$\frac{l_0 + l_0'}{2} = 97.313 \text{ estimates } I + (\tfrac{1}{2})(1237+2345+1346+1256+1457+2467+3567)$$

$$Error = l_0 - l_0' = 98.875 - 95.750 = 3.125$$

Results of the Combined Designs

Estimate of 1	=	−44.625
Estimate of 2	=	−51.875
Estimate of 3	=	1.875
Estimate of 12 + 37 + 56	=	37.875
Estimate of 13 + 27 + 46	=	−0.875
Estimate of 23 + 45 + 17	=	3.375
Estimate of 7	=	6.625
Estimate of error	=	3.125
Estimate of 24 + 35 + 67	=	2.875
Estimate of 14 + 36 + 57	=	15.125
Estimate of 15 + 26 + 47	=	8.375
Estimate of 4	=	−25.125
Estimate of 5	=	−3.375
Estimate of 6	=	−31.625
Estimate of 34 + 25 + 16	=	9.625

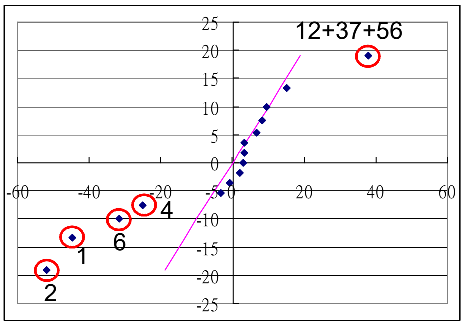
The result is exactly the same as 2_{IV}^{7-3} design with I=1237 I=2345 I=1346 generators

QQ Plot of Effect Estimates Based on Tests 1 to 16

2=	-51.875
1=	-44.625
6=	-31.625
4=	-25.125
5=	-3.375
13+27+46=	-0.875
3=	1.875
24+35+67=	2.875
error=	3.125
23+45+17=	3.375
7=	6.625
15+26+47=	8.375
34+25+16=	9.625
14+36+57=	15.125
12+37+56=	37.875

11 smallest effects to estimate S.D. 10.3406

E_i~N(0, 10.34)



Alternative Experimental Strategies

- Example 2^{7-4} design:
  I=124 I=135 I=236 I=1237
- A family of fractional factorial designs:
  I= ±124 I= ±135 I= ±236 I= ±1237
- If only main effects of variable 1 and its all related two-factor interaction are important:
  "only the variable 1 column in the original design is multiplied by –1"
  I=–124 I=–135 I=236 I=–1237

Principal Fraction Design Matrix

Test	1	2	3	4	5	6	7	Overrun (%)
1	−	−	−	+	+	+	−	115
2	+	−	−	−	−	+	+	81
3	−	+	−	−	+	−	+	110
4	+	+	−	+	−	−	−	69
5	−	−	+	+	−	−	+	174
6	+	−	+	−	+	−	−	99
7	−	+	+	−	−	+	−	80
8	+	+	+	+	+	+	+	63

Generators: $I = 124$, $I = 135$, $I = 236$, $I = 1237$

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Alternative Fraction Design Matrix to Clarify Main Effect of Variable 1 and Its All Two-factor Interactions

Test	1	2	3	4	5	6	7	Overrun (%)
17	+	−	−	+	+	+	−	66
18	−	−	−	−	−	+	+	171
19	+	+	−	−	+	−	+	147
20	−	+	−	+	−	−	−	122
21	+	−	+	+	−	−	+	51
22	−	−	+	−	+	−	−	148
23	+	+	+	−	−	+	−	49
24	−	+	+	+	+	+	+	14

Generators: $I = -124$, $I = -135$, $I = 236$, $I = -1237$

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Comparison of Test Results

Principal Fraction Design Tests 1–8			Alternative Fraction Design Tests 17–24		
l_0	=	98.875 estimates mean)	l''_0	=	96.000 estimates mean)
l_1	=	−41.750 estimates 1 + 24 + 35 + 67	l''_1	=	−35.500 estimates 1 − 24 − 35 − 67
l_2	=	−36.750 estimates 2 + 14 + 36 + 57	l''_2	=	−26.000 estimates 2 − 14 + 36 + 57
l_3	=	10.250 estimates 3 + 15 + 26 + 47	l''_3	=	−61.000 estimates 3 − 15 + 26 + 47
l_{12}	=	12.750 estimates 12 + 4 + 37 + 56	l''_{12}	=	−65.500 estimates 12 − 4 − 37 − 56
l_{13}	=	−4.250 estimates 13 + 5 + 27 + 46	l''_{13}	=	4.500 estimates 13 − 5 − 27 − 46
l_{23}	=	−28.250 estimates 23 + 6 + 17 + 45	l''_{23}	=	−42.000 estimates 23 + 6 − 17 + 45
l_{123}	=	16.250 estimates 34 + 25 + 16 + 7	l''_{123}	=	0.500 estimates − 34 − 25 + 16 − 7

$$\frac{l_1 + l_1''}{2} = -38.625 \text{ estimates } 1.$$

$$\frac{l_{12} + l_{12}''}{2} = 39.125 \text{ estimates } 12.$$

$$\frac{l_{13} + l_{13}''}{2} = 0.125 \text{ estimates } 13.$$

$$\frac{l_{123} + l_{123}''}{2} = 8.375 \text{ estimates } 16.$$

$$\frac{l_2 - l_2''}{2} = -5.375 \text{ estimates } 14.$$

$$\frac{l_3 - l_3''}{2} = 35.625 \text{ estimates } 15.$$

$$\frac{l_{23} - l_{23}''}{2} = 6.875 \text{ estimates } 17.$$

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2_{III}^{7-4} Family of Fractional Factorials

Fraction	Generators				Combined with Principal Fraction Gives Estimates of:*
Principal	$I = +124$	$I = +135$	$I = +236$	$I = +1237$	—
A_1	$I = -124$	$I = +135$	$I = +236$	$I = +1237$	4, 14, 24, 34, 45, 46, 47
A_2	$I = +124$	$I = -135$	$I = +236$	$I = +1237$	5, 15, 25, 35, 45, 56, 57
A_3	$I = -124$	$I = -135$	$I = +236$	$I = +1237$	
A_4	$I = +124$	$I = +135$	$I = -236$	$I = +1237$	6, 16, 26, 36, 46, 56, 67
A_5	$I = -124$	$I = +135$	$I = -236$	$I = +1237$	
A_6	$I = +124$	$I = -135$	$I = -236$	$I = +1237$	
A_7	$I = -124$	$I = -135$	$I = -236$	$I = +1237$	All main effects
A_8	$I = +124$	$I = +135$	$I = +236$	$I = -1237$	7, 17, 27, 37, 47, 57, 67
A_9	$I = -124$	$I = +135$	$I = +236$	$I = -1237$	
A_{10}	$I = +124$	$I = -135$	$I = +236$	$I = -1237$	
A_{11}	$I = -124$	$I = -135$	$I = +236$	$I = -1237$	1, 12, 13, 14, 15, 16, 17
A_{12}	$I = +124$	$I = +135$	$I = -236$	$I = -1237$	
A_{13}	$I = -124$	$I = +135$	$I = -236$	$I = -1237$	2, 12, 23, 24, 25, 26, 27
A_{14}	$I = +124$	$I = -135$	$I = -236$	$I = -1237$	3, 13, 23, 34, 35, 36, 37
A_{15}	$I = -124$	$I = -135$	$I = -236$	$I = -1237$	

* Assuming that third- and higher-order interactions are negligible.

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Principal Fraction Combined with Fraction A_3

$(l_0 + l_0^*)/2$	estimates mean
$(l_1 + l_1^*)/2$	estimates 1 + 67
$(l_2 + l_2^*)/2$	estimates 2 + 36
$(l_3 + l_3^*)/2$	estimates 3 + 26
$(l_{12} + l_{12}^*)/2$	estimates 12 + 37
$(l_{13} + l_{13}^*)/2$	estimates 13 + 27
$(l_{23} + l_{23}^*)/2$	estimates 23 + 6 + 17 + 45
$(l_{123} + l_{123}^*)/2$	estimates 16 + 7
$l_0 - l_0^*$	estimates error
$(l_1 - l_1^*)/2$	estimates 24 + 35
$(l_2 - l_2^*)/2$	estimates 14 + 57
$(l_3 - l_3^*)/2$	estimates 15 + 47
$(l_{12} - l_{12}^*)/2$	estimates 4 + 56
$(l_{13} - l_{13}^*)/2$	estimates 5 + 46
$(l_{23} - l_{23}^*)/2$	estimates error
$(l_{123} - l_{123}^*)/2$	estimates 34 + 25

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Experimental Designs for 2^{nd} Order Model

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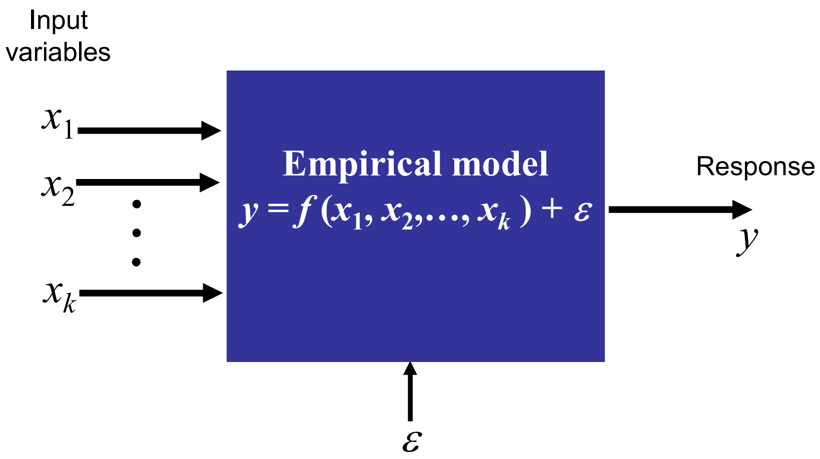
Input-Output System and Empirical Model



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2^{nd}-order Regression Model

If the response is well modeled by a linear function of the independent variables, then the approximating function is the first-order model (linear):

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + \varepsilon$$

This model can be obtained from a 2^k or 2^{k-p} design.

If there is curvature in the system, then a polynomial of higher degree must be used, such as the second-order model:

$$Y = \beta_0 + \Sigma\beta_i x_i + \Sigma\beta_{ii} x^2_i + \Sigma\Sigma\beta_{ij} x_i x_j + \varepsilon \Rightarrow \boxed{\hat{y} = b_0 + bx + x^T Bx}$$

This model has linear + interaction + quadratic terms and can be estimated by regression analysis.

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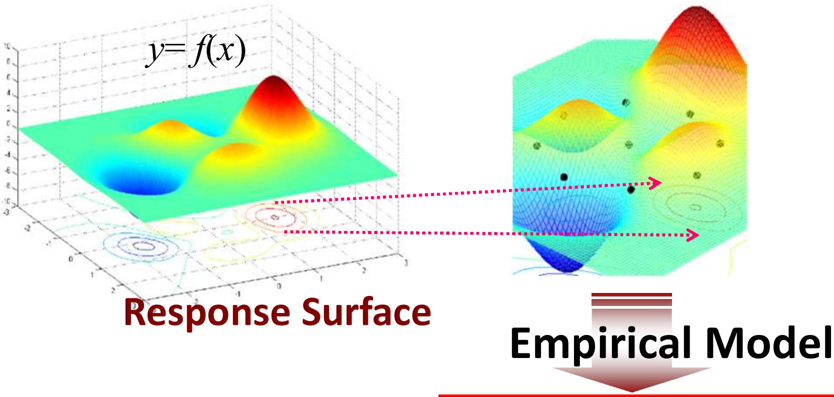
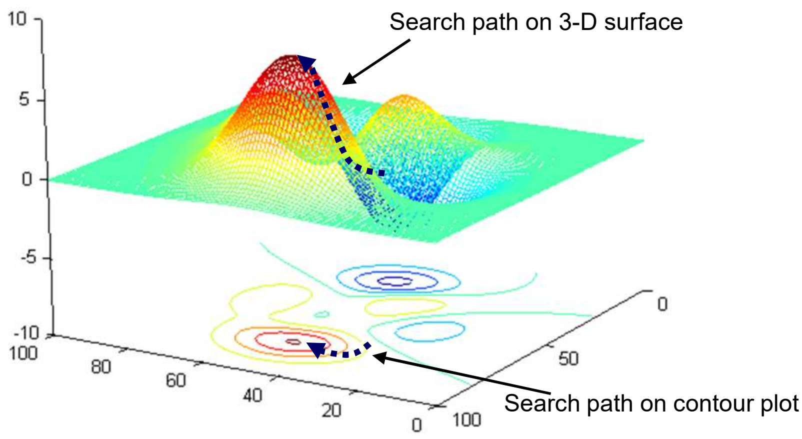
Quadratic Empirical Model



$$\hat{y} = b_0 + bx + x^T Bx$$

Searching for the Optimum



Response Surface Method (RSM)

- RSM is a collection of mathematical and statistical techniques that are useful for modeling and analysis in applications where a response of interest is influenced by several variables and **the objective is to optimize the response**.

- Optimize → maximize, minimize, or getting to a target.

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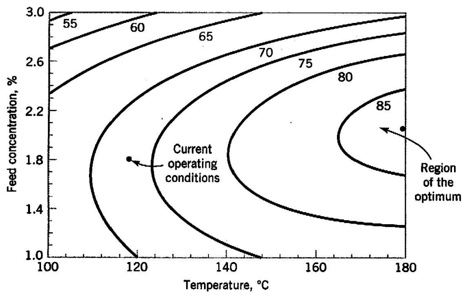
Sequential Nature of RSM

- **When far** from the optimum: **little curvature** (slight slope only) ⇒ **first-order model**
- Objective: to lead the experimenter rapidly and efficiently to the general vicinity of the optimum.



- **Once approaching** the region of the optimum: a more elaborate model, i.e., **second-order model** may be required for locating the optimum.

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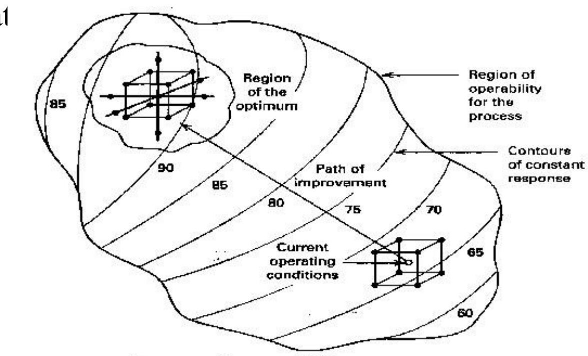
Objective of RSM

- The eventual objective of RSM: to **determine the optimum operating conditions** for the system or to **determine a region of the factor space in which operating specifications are satisfied**.
- The "**hill climbing**" procedures of RSM guarantee convergence only to a local optimum only.

Experimental Designs for RSM

- **When far from optimum:** a simple $\mathbf{2^k}$ **(or** $\mathbf{2^{k-l}}$ **fractional) factorial experiment to fit a first-order model** to find the climbing direction.
- **When near to the peak:** a more **elaborate design with at least 3 factor levels (e.g. a Central Composite Design, CCD)** is required to fit a **second-order model** for capturing the curvature and locat



The sequential nature of RSM.

Method of Steepest Ascent

- The **method of steepest ascent** is a procedure for moving sequentially along the path of steepest ascent (PSA), that is, in the direction of the maximum increase in the response. If minimization is desired, then we are talking about the **method of steepest descent**.
- For a first-order model, the contours of the response surface is a series of parallel lines. The direction of steepest ascent is the direction in which the response ***y*** increases most rapidly. This direction is normal (perpendicular) to the fitted response surface contours.

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First-order response and PSA

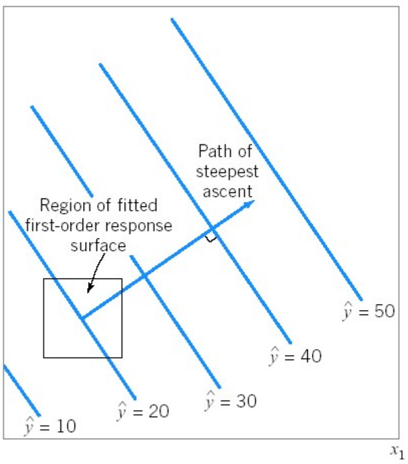

Figure 13-3 First-order response surface and path of steepest ascent.

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Path of Steepest Ascent (PSA)

- The PSA is usually the line through the center of the region of interest and normal to the fitted surface contours.
  - **PSA direction**: the **regression coefficient** ($b_1, b_2, \ldots, b_i, \ldots, b_k$) is the **normal vector** of the **linear** response surface:

    $\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_k x_k$
  - **Step size**: not too far from the experimental region and depending on the experimenter's knowledge of the process or other practical considerations.

EXAMPLE 12-8

An article in *Solid State Technology* ("Orthogonal Design for Process Optimization and Its Application in Plasma Etching," May 1987, pp. 127–132) describes the application of factorial designs in developing a nitride etch process on a single-wafer plasma etcher. The process uses C_2F_6 as the reactant gas. It is possible to vary the gas flow, the power applied to the cathode, the pressure in the reactor chamber, and the spacing between the anode and the cathode (gap). Several response variables would usually be of interest in this process, but in this example we will concentrate on etch rate for silicon nitride.

We will use a single replicate of a 2^4 design to investigate this process. Since it is unlikely that the three-factor and four-factor interactions are significant, we will tentatively plan to combine them as an estimate of error. The factor levels used in the design are shown here:

Design Factor Level	Gap *A* (cm)	Pressure *B* (m Torr)	C_2F_6 Flow *C* (SCCM)	Power *D* (W)
Low (−)	0.80	450	125	275
High (+)	1.20	550	200	325

Table 12-15 The 2^4 Design for the Plasma Etch Experiment

Run	A (Gap)	B (Pressure)	C (C_2F_6 flow)	D (Power)	Etch Rate (Å/min)
1	−1	−1	−1	−1	550
2	1	−1	−1	−1	669
3	−1	1	−1	−1	604
4	1	1	−1	−1	650
5	−1	−1	1	−1	633
6	1	−1	1	−1	642
7	−1	1	1	−1	601
8	1	1	1	−1	635
9	−1	−1	−1	1	1037
10	1	−1	−1	1	749
11	−1	1	−1	1	1052
12	1	1	−1	1	868
13	−1	−1	1	1	1075
14	1	−1	1	1	860
15	−1	1	1	1	1063
16	1	1	1	1	729

EXAMPLE 13-1

In Example 12-8, we described an experiment on a plasma etching process in which four factors were investigated to study their effect on the etch rate in a semiconductor water-etching application. We found that two of the four factors, the gap (x_1) and the power (x_4), significantly affected etch rate. Recall from that example that if we fit a model using only these main effects we obtain

$$\hat{y} = 776.0625 - 50.8125x_1 + 153.0625x_4$$

as a prediction equation for the etch rate.

Figure 13-4 shows the contour plot from this model, over the original region of experimentation—that is, for gaps between 0.8 and 1.2 cm and power between 275 and 325 W. Note that within the original region of experimentation, the maximum etch rate that can be obtained is approximately 980 Å/m. The engineers would like to run this process at an etch rate of 1100–1150 Å/m. Therefore, it is necessary to move away from the original region of experimentation to increase the etch rate.

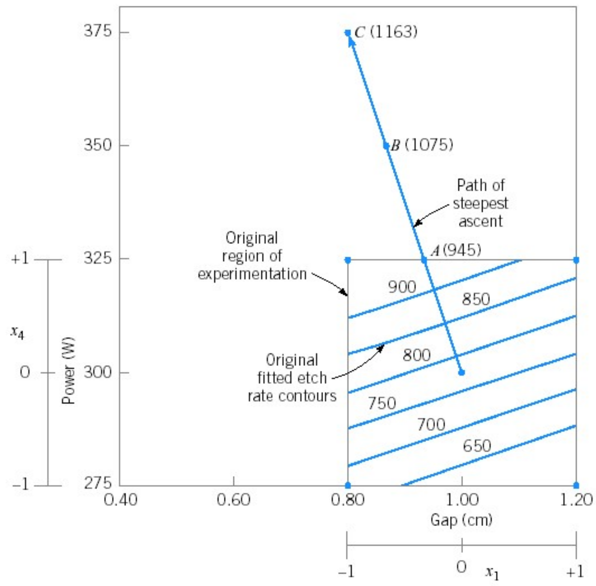

Figure 13-4 Steepest ascent experiment for Example 13-1.

- Experiments are then conducted along the PSA until no further increase in the response is observed.

- Then a new first-order model may be fitted, a new direction of steepest ascent determined, and further experiments conducted in that direction until the experimenter feels that the process is near the optimum (peak of hill is within grasp!).

Steps in RSM

- Fit linear model/planar models using two-level factorials
- From results, determine PSA (Descent)
- Move along path until no improvement occurs
- Repeat steps 1 and 2 until near optimal (change of direction is possible)
- **Fit quadratic model near optimal in order to determine curvature and find peak. This phase is often called "method of local exploration"**
- Run confirmatory tests

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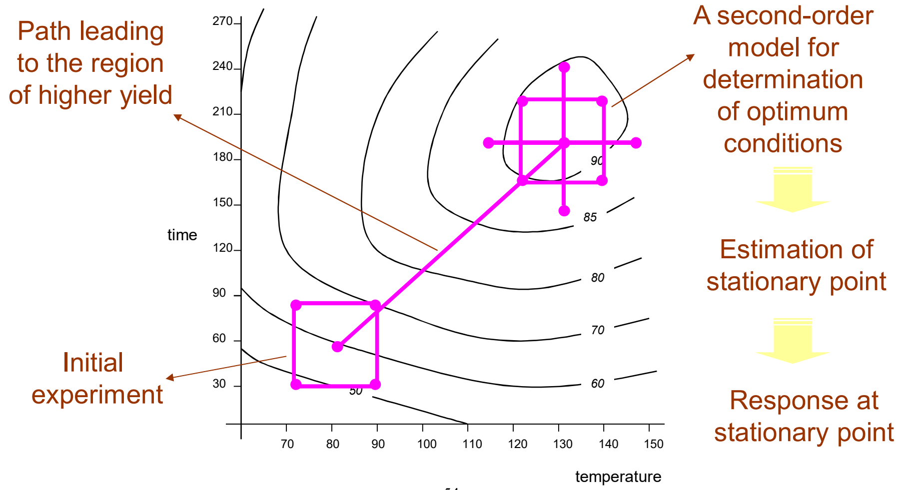
Response Surface Methodology



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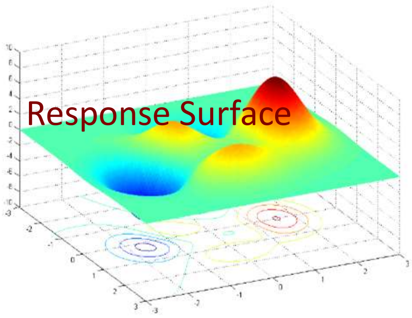
- With well-behaved functions with a single peak or valley, the above procedure works very well. It becomes more difficult to use RSM or any other optimization routine when the surface has many peaks, ridges, and valleys.

Response surface with many peaks and valleys



Designs for fitting 2nd order models

- Two very useful and popular experimental designs that allow a 2^{nd} order model to be fit are the:
  - **Central Composite Design (CCD)**
  - **Box-Behnken Design (BBD)**
- Both designs are built up from simple factorial or fractional factorial designs.

The Central Composite Design (CCD)

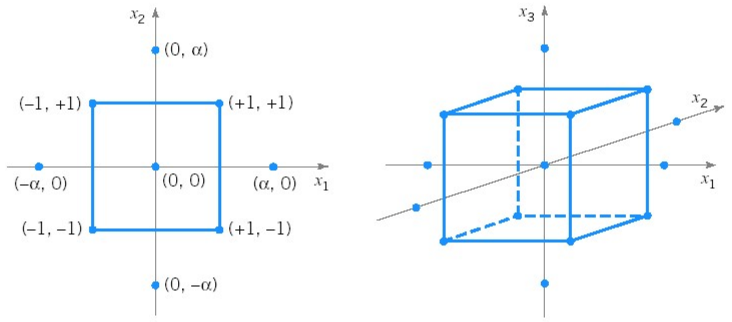


Figure 13-9 Central composite designs for $k = 2$ and $k = 3$.

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Central Composite Design (CCD)

- Each factor varies over five levels
- Typically smaller than Box-Behnken designs
- Built upon two-level factorials or fractional factorials of Resolution V or greater
- Can be done in stages → factorial + centerpoints + axial points
- Rotatable

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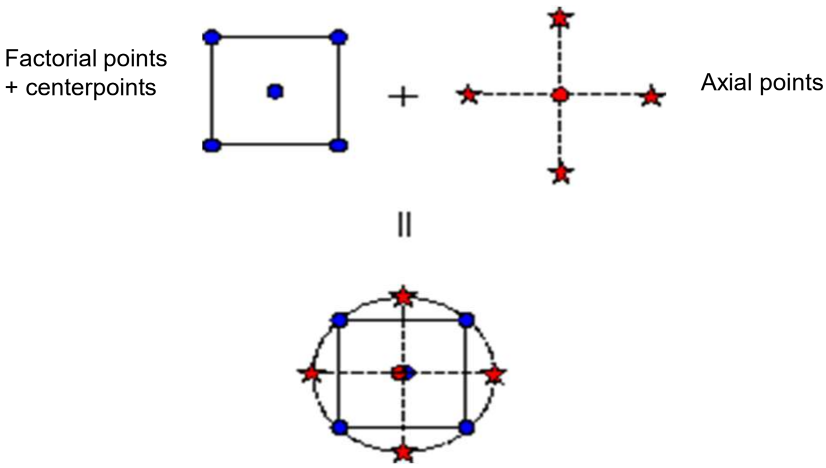
General Structure of CCD

- 2^k Factorial + 2k Star or axial points + n_c Centerpoints
- **The factorial part can be a fractional factorial as long as it is of Resolution V** or greater so that the 2 factor interaction terms are not aliased with other 2 factor interaction terms.
- The "star" or "axial" points in conjunction with the factorial and centerpoints allows the quadratic terms (β_{ii}) to be estimated.

Generation of a CCD



Axial points are points on the coordinate axes at distances "α" from the design center; that is, with coordinates: For 3 factors, we have 2k = 6 axial points like so:

(+α, 0, 0), (-α, 0, 0), (0, +α, 0), (0, -α, 0), (0, 0, +α), (0, 0, -α)

The "α" value is usually chosen so that the CCD is **rotatable**.

At least one point must be at the design center (0, 0, 0). Usually more than one to get an estimate of "pure error". See earlier 3-D figure.

If the "α" value is 1.0, then we have a face-centered CCD → Not rotatable but easier to work with.

A 3-Factor CCD with 1 centerpoint

A 3 factor CCD with n_c=1

Runs	x_1	x_2	x_3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1
9	-1.682	0	0
10	1.682	0	0
11	0	-1.682	0
12	0	1.682	0
13	0	0	-1.682
14	0	0	1.682
15	0	0	0

2^k Factorial Design

2k Axial Points

Center Points

Values of a for CCD to be rotatable

k=2	3	4	5	6	7
1.414	1.682	2.000	2.378	2.828	3.364

The α value is calculated as the 4^{th} root of 2^k.

For a rotatable design the variance of the predicted response is constant at all points that are equidistant from the center of the design

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Box-Behnken Designs (BBD)

- The Box-Behnken design is an independent quadratic design in that it does not contain an embedded factorial or fractional factorial design.
- In this design the treatment combinations are at the midpoints of edges of the process space and at the center.
- These designs are rotatable (or near rotatable) and require 3 levels of each factor.
- The designs have limited capability for orthogonal blocking compared to the central composite designs.

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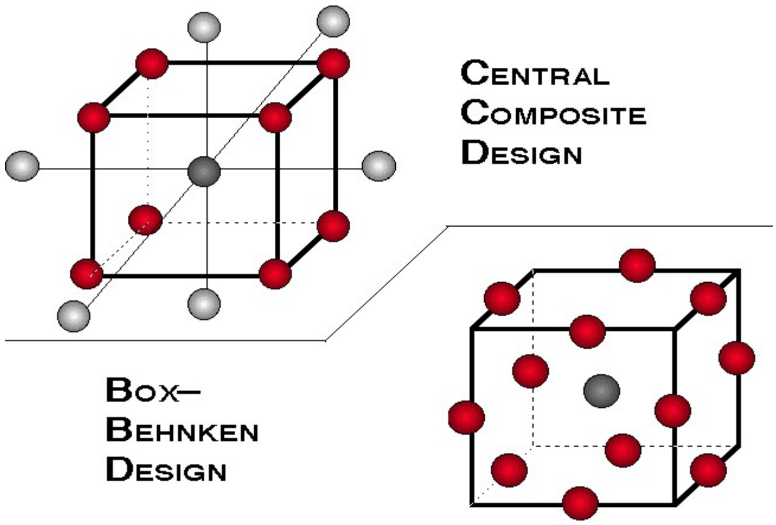
3-D views of CCD and BBD



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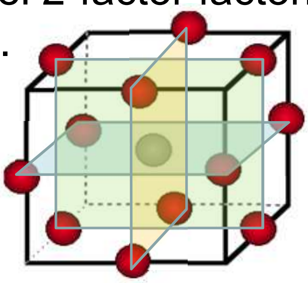
BBD - summary

- Each factor is varied over three levels (within low and high value)
- Alternative to central composite designs which requires 5 levels
- BBD not always rotatable
- Combinations of 2-level 2-factor factorial designs form the BBD.

  ($2^2 * C^k_2 + n_c$)



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A 3-Factor BBD with 1 centerpoint

A 3-factor BBD with n_c=1

Runs	x_1	x_2	x_3
1	-1	-1	0
2	-1	1	0
3	1	-1	0
4	1	1	0
5	-1	0	-1
6	-1	0	1
7	1	0	-1
8	1	0	1
9	0	-1	-1
10	0	-1	1
11	0	1	-1
12	0	1	1
13	0	0	0

2^2 Factorial Design

2^2 Factorial Design

2^2 Factorial Design

Center Points

Brief Comparison of CCD and BBD

With one centerpoint, for
k = 3, CCD requires 15 runs (2^3+2*3+1); BBD requires 13 runs (2^2*C^3_2+1=13)
k = 4, CCD requires 25 runs (2^4+2*4+1); BBD also requires 25 runs (2^2*C^4_2+1=25)
k = 5, CCD requires 43 runs (2^5+2*5+1); BBD requires 41 runs (2^2*C^5_2+1=41)

but, for CCD we can run a 2^{5-1} FFD with Resolution V. Hence we need only 27 runs (2^{5-1}+2*5+1).

In general CCD is preferred over BBD.