

Examination 12-10-25

Problem 1

Single - factor experiment

Data and calculated mean values and effects:

Dosage (g)	Observations				$y_{i\bullet}$	$\bar{y}_{i\bullet}$	$\tau = \bar{y}_{i\bullet} - \bar{y}_{\bullet\bullet}$
20	24	28	37	30	119	29.75	-7.333
30	37	44	31	35	147	36.75	-0.333
40	42	47	52	38	179	44.75	7.667

A = dosage level

y = bioactivity

a = 3

n = 4

N = a · n

 $\bar{y}_{\bullet\bullet} = 37.083$

A.

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Fixed effects model:

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij} \quad \begin{cases} i = 1, 2, \dots, a \\ j = 1, 2, \dots, m \end{cases}$$

$$N = a \cdot m$$

Sum of squares:

$$SS_T = \sum_{i=1}^a \sum_{j=1}^m (y_{ij} - \bar{y}_{..})^2 = \sum \sum y_{ij}^2 - \frac{y_{..}^2}{N}$$

$$SS_A = m \cdot \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2 = \frac{1}{m} \sum y_{i.}^2 - \frac{y_{..}^2}{N}$$

$$SS_E = SS_T - SS_A$$

$$\text{df: } N-a \quad N-1 \quad a-1$$

Mean squares:

$$MS_A = \frac{SS_A}{a-1}$$

$$MS_E = \frac{SS_E}{N-a}$$

Expected values:

$$E(MS_A) = \sigma^2 + \frac{m \sum \tau_i^2}{a-1}$$

$$E(MS_E) = \sigma^2$$

Hypothesis:

$$H_0: \tau_1 = \tau_2 = \dots = \tau_a = 0$$

$$H_a: \tau_i \neq 0 \text{ for at least one } i$$

$$\text{Test variable: } F_{\text{obs}} = MS_A / MS_E$$

B. The significance of the difference between the pair of means,

$$|\bar{y}_{i0} - \bar{y}_{j0}|, \quad i \neq j$$

is examined with the LSD-method

$$LSD = t(1 - \alpha/2, N - a) \cdot \sqrt{s^2(1/m + 1/m)}$$

Significance: $|\bar{y}_{i0} - \bar{y}_{j0}| > LSD$

c. Residual analysis.

$$e_{ij} = y_{ij} - \hat{y}_{ij}, \quad i = 1, \dots, 3$$

$$\hat{y}_{ij} = \hat{\mu} + \hat{\tau}_i$$

$$j = 1, \dots, 4$$

$$\hat{\mu} = \bar{y}_{..}, \quad \hat{\tau}_i = \bar{y}_{i0} - \bar{y}_{..}$$

$$\hat{y}_{ij} = \bar{y}_{..} + \bar{y}_{i0} - \bar{y}_{..} = \bar{y}_{i0}$$

$$e_{ij} = y_{ij} - \bar{y}_{i0}$$

Calculations and conclusions:

see pages 4-7

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Problem 1

A: ANOVA

Source	SS	df	MS	Fobs	sign	p
Dosage	450.67	2	225.33	7.0356	*	0.014
Residual	288.25	9	32.028			
Totcorr	738.92	11				

The dosage level has significant effect on bioactivity

B: Comparisons between the pairs of means with the LSD method

$$\text{dosage } 20-30: \quad \text{abs}(y_{1m}-y_{2m}) = 7$$

$$20-40: \quad \text{abs}(y_{1m}-y_{3m}) = 15$$

$$30-40: \quad \text{abs}(y_{2m}-y_{3m}) = 8$$

$$\text{LSD} = t(0.975, N-a) * \text{sqrt}(MSE * (1/n+1/n)) = 9.05$$

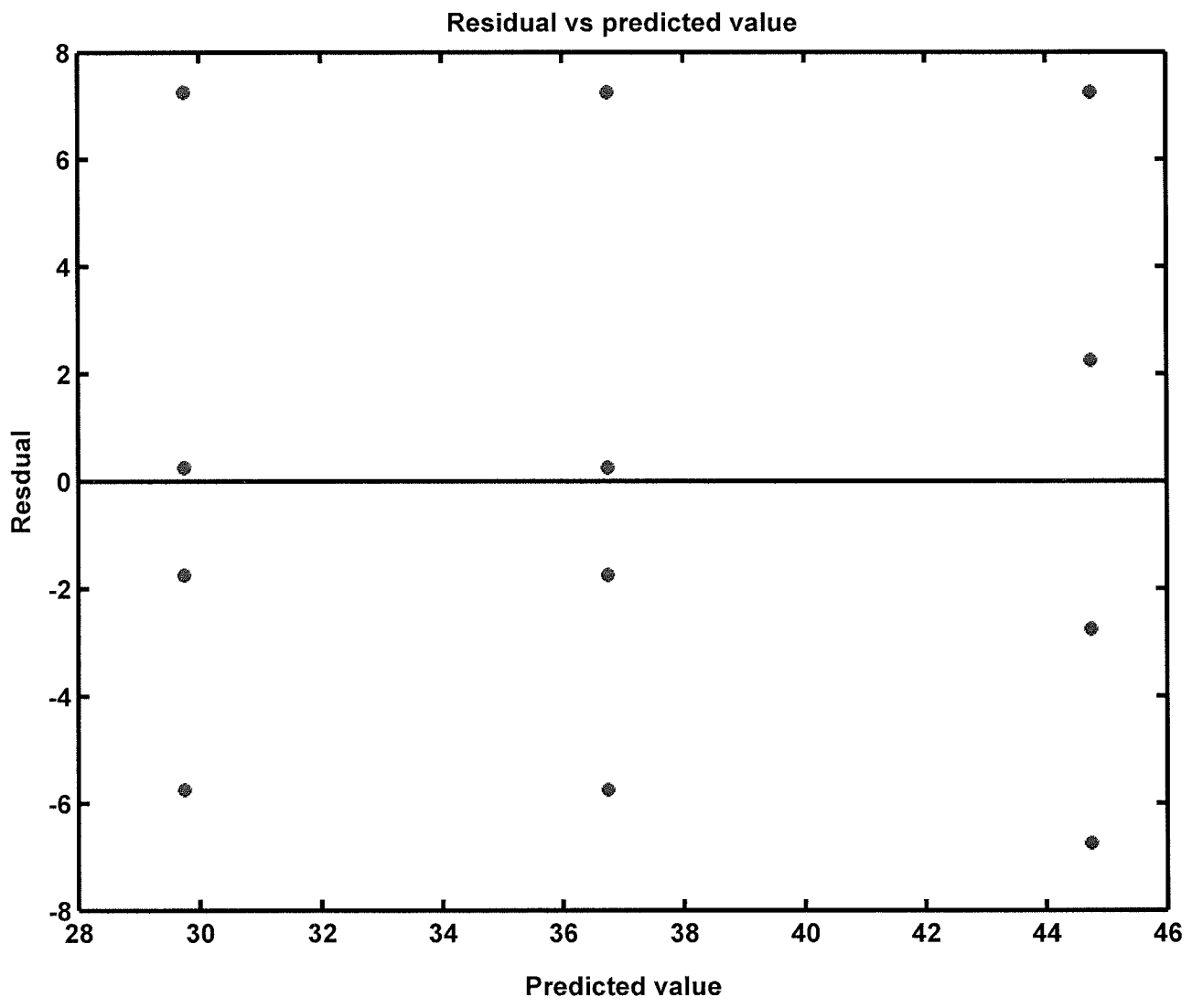
There is a difference in the mean between the 20g and 40g dosages.

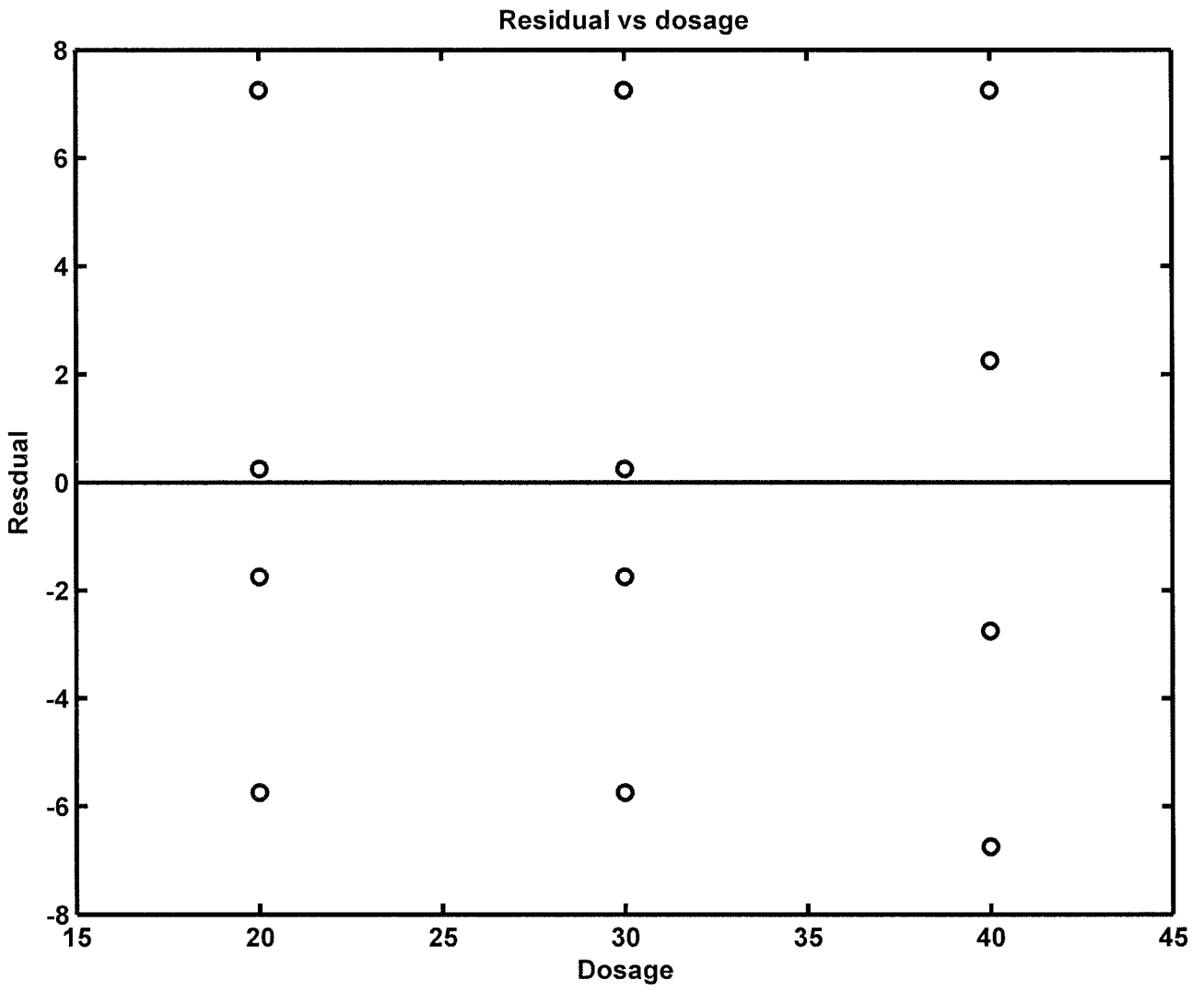
C: Residuals

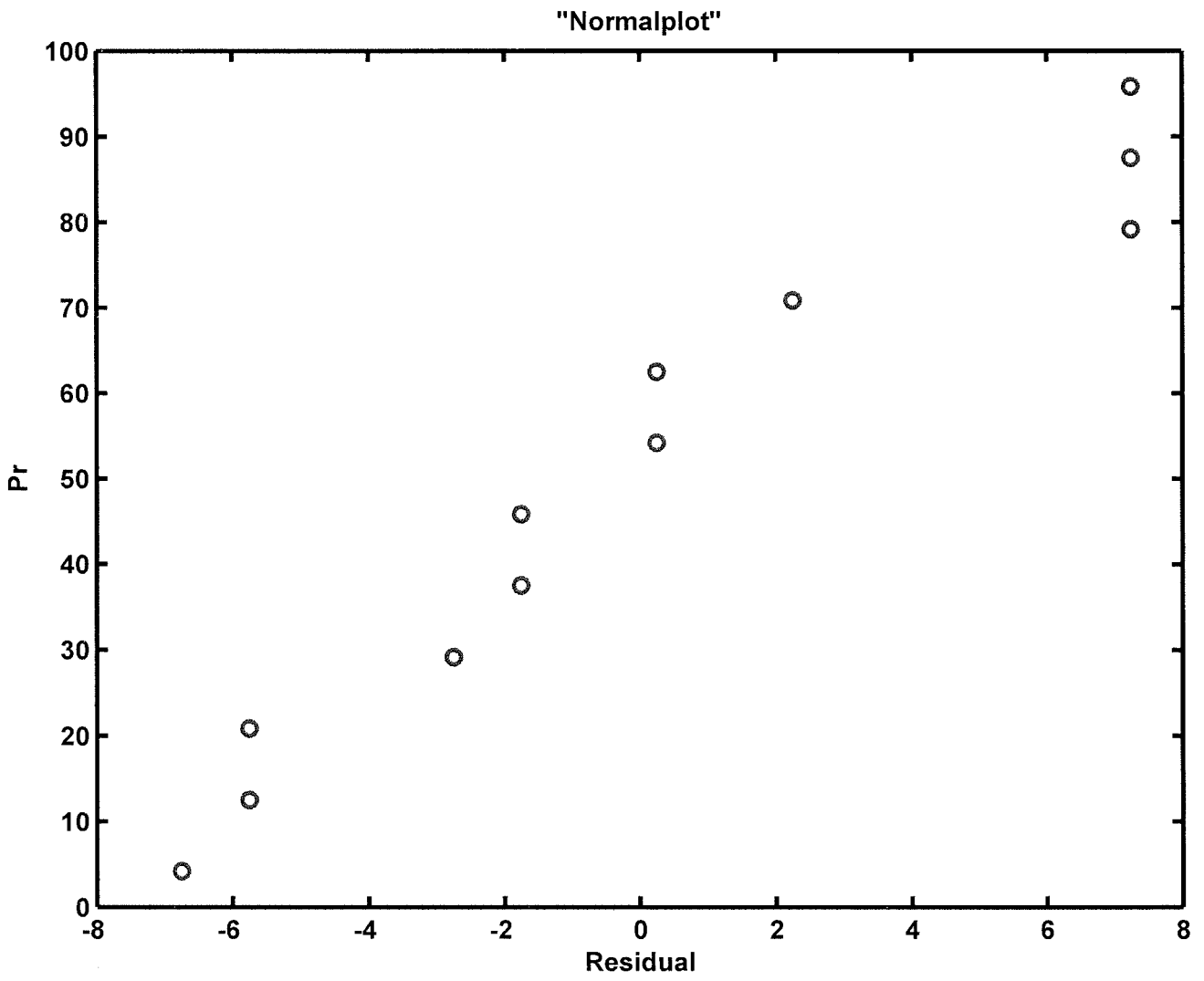
-5.75	-1.75	7.25	0.25
0.25	7.25	-5.75	-1.75
-2.75	2.25	7.25	-6.75

The residuals are plotted vs predicted value, and dosage, and also as a "normal plot".

There is nothing too unusual about the residual plots.







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Problem 2

Factors: solution (row)
days (column)

Response (y): bacteria growth

$$\text{Model: } y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}$$

τ_i = row effect (solution) $i=1, 2, \dots, a$
 $a=3$

β_j = column effect (days), $j=1, 2, \dots, b$
 $b=4$

μ = overall mean

ε_{ij} = random error NID $(0, \sigma^2)$

Experimental data, mean values
and effects, see page 3

Sum of squares:

$$SS_T = \sum \sum (y_{ij} - \bar{y}_{..})^2 = \sum \sum y_{ij}^2 - y_{..}^2 / N$$

$$SS_T = 1862.3$$

$$SS(\text{solution}) = b \cdot \sum (\bar{y}_{i.} - \bar{y}_{..})^2 = \frac{1}{b} \sum y_{i.}^2 - y_{..}^2 / N$$

$$SS(\text{solution}) = 703.5$$

$$SS(\text{days}) = a \cdot \sum (\bar{y}_{.j} - \bar{y}_{..})^2 = \frac{1}{a} \sum y_{.j}^2 - y_{..}^2 / N$$

$$SS(\text{days}) = 1862.3$$

$$SSE = SS_T - SS(\text{rotations}) - SS(\text{days})^{2/4}$$

$$SSE = 51.83$$

ANOVA - table and comments,
see page 4.

Examination 12_10_25 Problem 2

Randomized block design

Data and calculated mean values and parameters

Solution	Days				$y_{i\bullet}$	$\bar{y}_{i\bullet}$	$\tau = \bar{y}_{i\bullet} - \bar{y}_{\bullet\bullet}$
	1	2	3	4			
I	13	22	18	39	92	23	4.25
II	16	24	17	44	101	25.25	6.5
III	5	4	1	22	32	8	-10.75
$y_{\bullet j}$	34	50	36	105			
$\bar{y}_{\bullet j}$	11.33	16.67	12	35			
$\beta_j = \bar{y}_{\bullet j} - \bar{y}_{\bullet\bullet}$	-7.42	-2.08	-6.75	16.25			

A = solution B = days

a = 3 b = 4 $\bar{y}_{\bullet\bullet} = 18.75$

Model parameters : $\mu = 18.75$ $\tau = [4.25 \ 6.5 \ -10.75]$ $\beta = [-7.42 \ -2.08 \ -6.75 \ 16.25]$

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Problem 2

A: ANOVA

Source	SS	df	MS	Fobs	sign
Solution	703.5	2	351.75	40.72	*
Day	1106.9	3	368.97	42.71	*
Residual	51.83	6	8.64		
Totcorr	1862.3	11			

$$F_{\text{statsolution}} = F(1-\alpha, a-1, (a-1) * (b-1)) = 5.14$$

$$F_{\text{statday}} = F(1-\alpha, b-1, (a-1) * (b-1)) = 4.75$$

Solutions and days have a significant effect on retarding bacteria growth.

Comparisons between the pairs of solution means with the LSD method

$$\text{solution I-II: } \text{abs}(y_{1m} - y_{2m}) = 2.25$$

$$\text{I-III: } \text{abs}(y_{1m} - y_{3m}) = 15$$

$$\text{II-III: } \text{abs}(y_{2m} - y_{3m}) = 17.25$$

$$\text{LSD} = t(0.975, (a-1) * (b-1)) * \sqrt{\text{MSE} * 2/b} = 5.09$$

The LSD procedure indicates that solution III is significantly different from the other two.

Problem 3

$$\text{Model: } y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \\ + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 + \varepsilon$$

A. Model fitting

$$\underline{b} = (\underline{X}^T \underline{X})^{-1} \cdot \underline{X}^T \underline{y}$$

\underline{X} = calculation matrix

\underline{y} = response vector

Significance:

I. t-test. $t_{\text{obj}} > t_{\text{stat}}$

$$t_{\text{obj}} = \frac{b_j}{\text{se}(b_j)}$$

$$t_{\text{stat}} = t(0.975, N-p)$$

II. F-test $F_{\text{obj}} > F_{\text{stat}}$

$$F_{\text{obj}} = \frac{SS(b_j) / 1}{SS_E / (N-p)}$$

$$F_{\text{stat}} = F(0.95, 1, N-p)$$

$$t_{\text{obj}}^2 = F_{\text{obj}} \quad t_{\text{stat}}^2 = F_{\text{stat}}$$

B. Lack of fit,

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$$SSE = SS_{PE} + SS_{LOF}$$

Replicates in the center point give SS_{PE} :

$$SS_{PE} = \sum_{i=1}^{m_c} (y_{ci} - \bar{y}_c)^2$$

m_c = number of replicates.

$$df_{PE} = m_c - 1$$

$$SS_{LOF} = SSE - SS_{PE}$$

$$df_{LOF} = N - p - (m_c - 1)$$

Test:

$$F_{LOF} = \frac{SS_{LOF} / (N - p - m_c + 1)}{SS_{PE} / (m_c - 1)}$$

$$F_{stat} = F(0.95, N - p - m_c + 1, m_c - 1)$$

No lack of fit if $F_{LOF} < F_{stat}$

C: Model with pure quadratic terms. ^{3/6}

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \epsilon$$

With the given data only the sum of the parameters for the pure quadratic terms can be estimated

$$b_{11} + b_{22} + b_{33} = b_{\text{quad}} = \bar{y}_f - \bar{y}_c$$

\bar{y}_f = mean value of the responses in the factorial points

n_f = number of factorial points

\bar{y}_c = mean value of responses in the center point.

$$SS_{\text{purequad}} = \frac{n_f \cdot n_c (\bar{y}_f - \bar{y}_c)^2}{n_f + n_c}$$

with $df = 1$

$$F_{\text{obs}} = \frac{SS_{\text{purequad}} / 1}{SS_E / (N - P)}$$

$$F_{\text{stat}} = F(0.95, 1, N - P)$$

Significance if $F_{\text{obs}} > F_{\text{stat}}$.

Summary of all calculations, (A, B, C) with conclusions; see pages 5 and 6

D. Fitting a second-order model. ^{4/6}

Complementary addition of 2^k axial points to a 2^k -design to form a central composite design (CCD)

Add here 2×3 axial points to the 2^3 -design at a distance α from the design center.

The design is made rotatable by setting $\alpha = (n_f)^{1/4} = 8^{1/4} = 1.68$.

To get a low and almost constant prediction variance for the CCD the best choice is

$\alpha = \sqrt{3} = 1.73$, which gives a spherical CCD.

The axial points are added as:

x_1	x_2	x_3
$-\alpha$	0	0
α	0	0
0	$-\alpha$	0
0	α	0
0	0	$-\alpha$
0	0	α

Calculation matrix and observations

		x0	x1	x2	x3	x1x2	x1x3	x2x3
exp	obs	M	A	B	C	AB	AC	BC
(1)	10	1	-1	-1	-1	1	1	1
a	12	1	1	-1	-1	-1	-1	1
b	4	1	-1	1	-1	-1	1	-1
ab	4	1	1	1	-1	1	-1	-1
c	9	1	-1	-1	1	1	-1	-1
ac	10	1	1	-1	1	-1	1	-1
bc	5	1	-1	1	1	-1	-1	1
abc	4	1	1	1	1	1	1	1
center	6	1	0	0	0	0	0	0
center	7	1	0	0	0	0	0	0
center	8	1	0	0	0	0	0	0
center	7	1	0	0	0	0	0	0

A: ANOVA

Source	Param	SS	df	MS	Fobs	sign
Model		77.5	6	12.92	29.81	*
b0	7.167	616.3	1	616.3	1422.3	*
b1	0.25	0.5	1	0.5	1.154	
b2	-3	72	1	72	166.2	*
b3	-0.25	0.5	1	0.5	1.154	
b1b2	-0.5	2	1	2	4.615	
b1b3	-0.25	0.5	1	0.5	1.154	
b2b3	0.5	2	1	2	4.615	
Residual		2.167	5	0.4333		
Stotcorr		79.67	11			

$F_{statmod} = F(0.95, p-1, N-p) = 4.95$

$F_{statparam} = F(0.95, 1, N-p) = 6.61$

$R^2 = 0.9728$

$R^2_{adj} = 0.9402$

B: Lack of fit

$$SSPE = 2 \quad SSLOF = 0.1667 \quad FLOF = 0.125$$

$$FstatLOF = F(0.95, N-p-nc+1, nc-1) = 9.55 \quad \text{No lack of fit}$$

C: Pure quadratic terms

$$ycm = 7 \quad yfm = 7.25 \quad nc = 4 \quad nf = 8$$

$$bquad=0.25 \quad SSquad = 0.167 \quad Fquad = 0.385$$

$$Fstatquad = F(0.95, 1, N-p) = 6.61 \quad \text{No significance}$$

Problem 4

A. A simplex is a regular sided figure.

Here with 3 variables the design must be a regular tetrahedron.

Proof: Equal distances between the vertices.

Coordinates for the vertices:

$$z_1 = [0 \quad \sqrt{2} \quad -1] \quad z_3 = [0 \quad -\sqrt{2} \quad -1]$$

$$z_2 = [-\sqrt{2} \quad 0 \quad 1] \quad z_4 = [\sqrt{2} \quad 0 \quad 1]$$

Distances between two vertices:

$$d_{ij} = \|z_i - z_j\|, \quad i=1,2,3, \quad j=2,3,4 \\ i \neq j$$

$$d_{ij} = 2\sqrt{2} \quad \text{for all } i, j$$

Alternative:

Equal distances from centre point to vertices.

$$d_{ic} = \|z_i\|, \quad i=1,2,\dots,4$$

$$d_{ic} = \sqrt{3} \quad \text{for all } i;$$

B. Fitting first order model. 2/5

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

$$\underline{X} = \begin{bmatrix} 1 & 6 & \sqrt{2} & -1 \\ 1 & -\sqrt{2} & 0 & 1 \\ 1 & 0 & -\sqrt{2} & -1 \\ 1 & \sqrt{2} & 0 & 1 \end{bmatrix} \quad \underline{y} = \begin{bmatrix} 18.5 \\ 19.8 \\ 17.4 \\ 22.5 \end{bmatrix}$$

$$\underline{b} = (\underline{X}^T \underline{X})^{-1} \underline{X}^T \underline{y}$$

$$\underline{b} = \begin{bmatrix} 19.55 \\ 0.9546 \\ 0.3889 \\ 1.6 \end{bmatrix}$$

c. Path of steepest ascent

Path of steepest ascent = the gradient direction.

$$\underline{g} = \underline{\nabla} y = \left[\frac{\partial y}{\partial x_1} \quad \frac{\partial y}{\partial x_2} \quad \frac{\partial y}{\partial x_3} \right]^T = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

The steps along the path are proportional to the parameters b

$$\underline{\Delta x} = \text{stepfactor} \cdot k \cdot \underline{g}$$

$$\underline{x}_{\text{new}} = \underline{x}_0 + \underline{\Delta x}$$

$$x_3 = \text{konstant} = 1$$

$$x_0 = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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$$\underline{g} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 0.9546 \\ 0.3889 \end{bmatrix}$$

$$h = 1 / \max[\text{abs}(g)] = 1 / \text{abs}(g_1) = \frac{1}{0.9546}$$

$$\underline{\Delta x} = \text{stepfactor} \cdot \begin{bmatrix} 1 \\ 0.4074 \end{bmatrix}$$

$$\underline{x}_{\text{new}} = \underline{x}_0 + \text{stepfactor} \cdot \begin{bmatrix} 1 \\ 0.4074 \end{bmatrix}$$

an overall step is taken to the final point.

$$x_{1\text{max}} = \sqrt{2} \quad \Rightarrow \quad \text{stepfactor} = \sqrt{2}$$

$$\underline{x}_{\text{final}} = \underline{x}_0 + \sqrt{2} \cdot \begin{bmatrix} 1 \\ 0.4074 \end{bmatrix} = \begin{bmatrix} 1.414 \\ 0.576 \end{bmatrix}$$

$$x_2 = 0.576$$

$$y_0 = 21.15$$

$$y_{\text{final}} = 22.72$$

Remarks

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(not included in the problem statement)

steps, which is taken in the gradient direction from the starting point $\underline{x}_0 = [0 \ 0 \ 1]^T$

at once result in poorer variables outside the simplex region.

To avoid this, variable x_2 must be kept constant, $x_2 = 0$

$$\underline{x}_{\text{limit}} = [\sqrt{2} \ 0 \ 1]^T$$

$$f_{\text{limit}} = 22.5$$

The gradient and limit paths are shown in fig. 1 and 2.

Problem 4

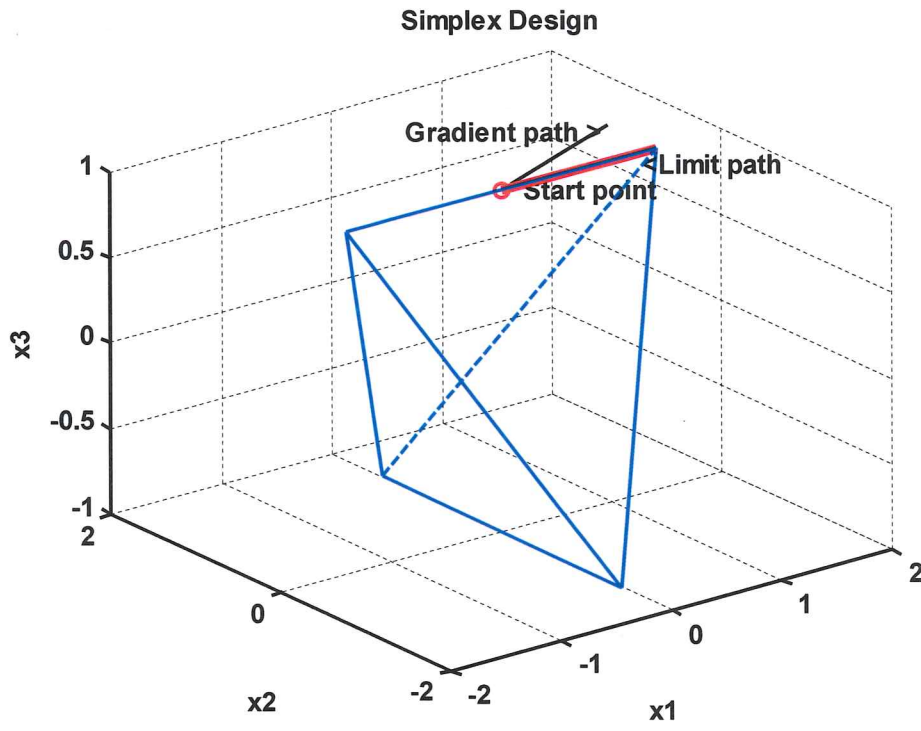


Fig.1 Regular tetrahedron

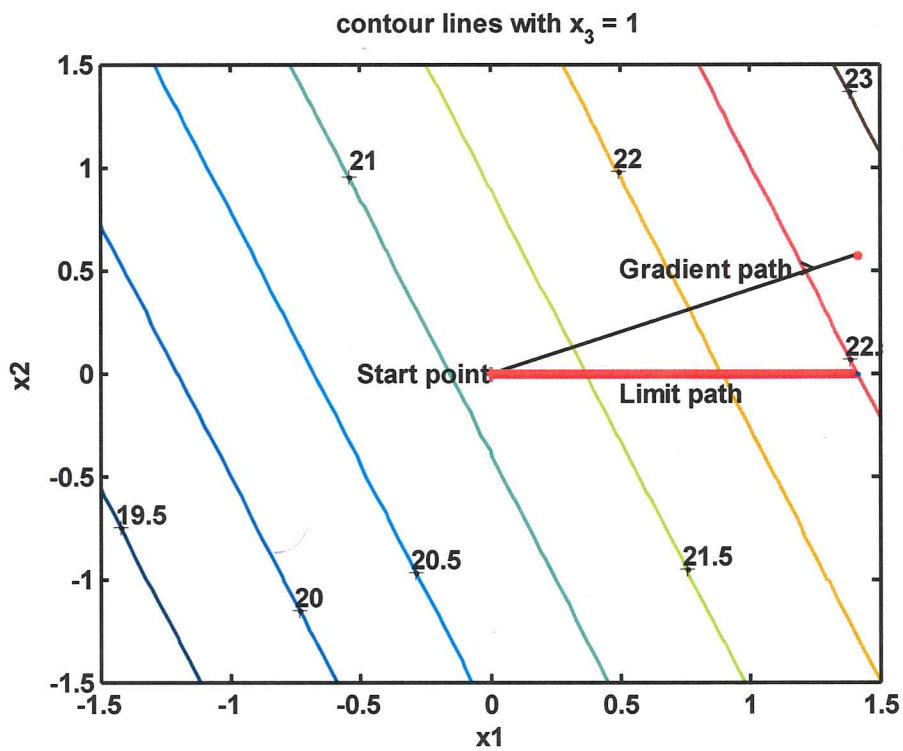


Fig.2 Contour plot

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Problem 5

A: Alias structure

2^{3-1} fractional factorial design.

C is confounded with AB, $C = AB$

Generator: ABC

Defining relation for the reduced plan:

$$I = ABC \quad ; \quad \text{resolution: III}$$

Alias:

$$[A] \rightarrow A + BC$$

$$[B] \rightarrow B + AC$$

$$[C] \rightarrow C + AB$$

B and C tests:

ANOVA - table and conclusions,
see page 3

D. Final model in terms of coded factors:

$$y = b_0 + b_1 X_A + b_2 X_B + b_3 X_C$$

$$y = 778.88 - 51.88 X_A - 73.13 X_B + 140.63 X_3$$

Coding:

$$X_A = \frac{A - 1.00}{0.20}$$

$$A: 0.80 - 1.20$$

$$X_A = 5A - 5$$

$$x_B = \frac{B - 162.5}{37.5}$$

$$B: 125 - 200$$

$$x_B = \frac{B}{37.5} - \frac{162.5}{37.5}$$

$$x_C = \frac{C - 262.5}{62.5}$$

$$C: 200 - 325$$

$$x_C = \frac{C}{62.5} - \frac{262.5}{62.5}$$

The expressions for x_A , x_B and x_C are inserted in the model equation above and give the etch rate in terms of the actual factors:

$$y = 764.51 - 259.38 A - 1.95 B + 2.25 C$$

Design for two replicates

exp	obs	M	A	B	C=AB
c	1037	1	-1	-1	1
a	669	1	1	-1	-1
b	633	1	-1	1	-1
abc	729	1	1	1	1
c	1052	1	-1	-1	1
a	650	1	1	-1	-1
b	601	1	-1	1	-1
abc	860	1	1	1	1

ANOVA

Source	Param	SS	df	MS	Fobs	sign
Model		222509.4	3	74169.79	31.61	*
A	-51.875	21528.13	1	21528.13	9.18	*
B	-73.125	42778.13	1	42778.13	18.23	*
C=AB	140.625	158203.1	1	158203.1	67.42	*
Residual		9385.5	4	2346.37		
Totcorr		231894.9	7			

intercept: $b_0 = 778.875$

$$SS_{Reg} = SS(A) + SS(B) + SS(C) = 222509.4 \quad df = 3$$

$$SSE = SST(\text{corr}) - SS_{Reg} = 9385.5 \quad SSE = SS_{PE}$$

parameter standard error: $se = 17.13$

$$F_{statmodel} = F(0.95, 3, 4) = 6.59$$

$$F_{statparam} = F(0.95, 1, 4) = 7.71$$

$$R^2 = 0.95953 \quad R^2_{adj} = 0.9291$$

Model in terms of coded variables: $y = b_0 + b_1x_A + b_2x_B + b_3x_C$

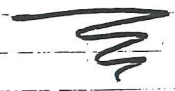
It is not unexpected that factor C is significant, since it is confounded with AB.

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6 E - ABD
E
ABD

ABDE = GENERATOR

Exp



A	B	C	D	ABD	Exp
-	-	-	-	-	(1)
+	-	-	-	+	ae
-	+	-	-	+	be
+	+	-	-	-	ab
-	-	+	-	-	c
+	-	+	-	+	ace
-	+	+	-	+	bce
+	+	+	-	-	abc
-	-	-	+	+	de
+	-	-	+	-	ad
-	+	-	+	-	bd
+	+	-	+	+	abde
-	-	+	+	+	cde
+	-	+	+	-	acd
-	+	+	+	-	bed
+	+	+	+	+	abcde

I = ABDE

- A - BDE
- B - ADE
- C - ABDEFC
- D - ABE
- E - ABD
- AB - DE
- AC - BCDE
- AD - BE
- AE - BD
- BC - ACDE
- CD = ABCE
- CE = ABCD
- DE - AB

DISADVANTAGE 2 ORDER ALIAS - 2 ORDER

RESOLUTION IV

FOLD OVER

BUT TECKE PA⁰
MINSTA THROUGH EFFECT

SEPARATE AB - DE } BUT TECKEN PA^{AD}
BD - AE } (E)

OR NEW 2⁵¹ CORRECT

GENERATOR ABCDE

SEPARATE 2 ORDER EFFECTS

CHALMERS OF COURSE

CALTECH

MIT

ETH

IMPERIAL

UCLA

⇒ WILL ALSO DO