

Illustration with Adapted Epi-Layer Growth Experiment

1. In Table 4 (LNp.5-11),

• $\text{median}|\hat{\theta}_i| = 0.078$, ← median of 15 $|\hat{\theta}_i|$'s

closer
to
zero

• $s_0 = 1.5 \times 0.078 = 0.117$.

• trimming constant $2.5s_0 = 2.5 \times 0.117 = 0.292$,

which eliminates 0.490 (D) and 0.345 (CD). → 2 out of 15 effects

• $\text{median}_{\{|\hat{\theta}_i| < 2.5s_0\}}|\hat{\theta}_i| = 0.058$ ← median of 13 smaller $|\hat{\theta}_i|$'s

• $PSE = 1.5 \times 0.058 = 0.087$ ← cf. $s.e.(\hat{\theta}_i)$

The corresponding $|t_{PSE}|$ values appear in Table 6 (LNp.5-28).

2. Choose $\alpha = 0.01$.

larger

• $\text{IER}_{0.01} = 3.63$ for $I = 15$. By comparing with the $|t_{PSE}|$ values, D and CD are significant at 0.01 level.

• $\text{EER}_{0.01} = 6.45$ (for $I = 15$). No effect is detected as significant.

- Analysis of the $|t_{PSE}|$ values for $\ln s^2$ (Table 6, LNp.5-28) detects no significant effect (details on textbook, p.182), thus confirming the half-normal plot analysis in Figure 4.10 of section 4.8 (textbook, p.179).

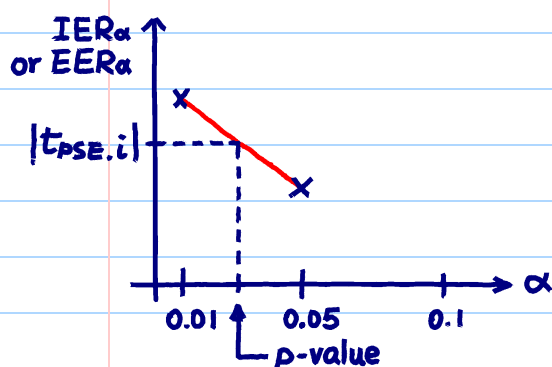


$|t_{PSE}|$ Values for Adapted Epi-Layer Growth Experiment

Table 6: $|t_{PSE}|$ Values, Adapted Epitaxial Layer Growth Experiment

Effect	\bar{y}	$\ln s^2$
A	0.90	0.25
B	1.99	1.87
C	0.90	1.78
D	✓ 5.63	0.89
AB	0.09	0.71
AC	1.07	0.41
AD	0.57	0.46
BC	0.67	1.27
BD	0.34	0.16
CD	✓ 3.97	1.35
ABC	1.13	0.51
ABD	0.29	0.67
ACD	0.34	0.00
BCD	1.26	0.05
ABCD	0.23	1.63

unreplicated



$$y_x \sim N(\mu_x, \sigma_x^2)$$

$$E(y_x)$$

$$\hat{\mu}_x \approx \hat{\beta}_0 + \hat{\beta}_D \chi_D + \hat{\beta}_{CD} \chi_{CD}$$

$$\Rightarrow \sigma_x^2 \approx \text{a constant}$$

$$\text{Var}(y_x)$$

- p -values of effects can be obtained from packages or by interpolating the critical values in the tables in appendix H (textbook, p.701). (See textbook, p.182 for illustration).

❖ Reading: textbook, 4.9

Nominal-the-Best Problem ← Recall objective in LNp.5-1

- There is a nominal or target value t ($=14.5$ in the case) based on engineering design requirements.
- Define a quantitative loss due to deviation of y_x from t .

Quadratic loss: $L(y_x, t) = \frac{1}{2} \cdot (y_x - t)^2$. $-E(y_x) + E(y_x)$

$\arg \min_x \rightarrow E(L(y_x, t)) = \frac{1}{2} \cdot \text{Var}(y_x) + \frac{1}{2} \cdot [E(y_x) - t]^2$.

↑ variance ↑ bias²

- Two-step procedure for nominal-the-best problem:

- Select levels of some factors to minimize $\text{Var}(y_x)$.
- Select the level of a factor not in (i) to move $E(y_x)$ closer to t .

- A factor in step (ii) is an adjustment factor if it has a significant effect on $E(y_x)$ but not on $\text{Var}(y_x)$.
 - Procedure is effective only if an adjustment factor can be found.
- This is often done on engineering ground.

- Examples of adjustment factors: deposition time in surface film deposition process, mold size in tile fabrication, location and spacing of markings on the dial of a weighing scale.

a factor whose effects appears in $\hat{\beta}_1$, but not $\hat{\beta}_2$

If an adjustment factor does not exist, some trade-off between (i) and (ii) is required.

❖ Reading: textbook, 4.10

Why Take $\ln s^2$? → as a response of linear model

- It maps s^2 over $(0, \infty)$ to $\ln s^2$ over $(-\infty, \infty)$.

Regression and ANOVA assume the responses are nearly normal, i.e. over $(-\infty, \infty)$.

- Better for variance prediction.

- Suppose $z_x = \ln s_x^2$.
- \hat{z}_x = predicted value of $\ln \sigma_x^2$
- $e^{\hat{z}_x}$ = predicted value of σ_x^2 , always nonnegative.

response ← approximate linear structure

$$\begin{array}{l} S^2 \in (0, \infty) \\ \ln(S^2) \in (-\infty, \infty) \end{array} \quad \left| \quad X\beta + \varepsilon \in (-\infty, \infty) \right.$$

- Most physical laws have a multiplicative component.

Log converts multiplicity into additivity.

- Variance stabilizing property: next slide.

error part of y :

$$\varepsilon = \varepsilon_1 \times \cdots \times \varepsilon_k$$

Assume independence and zero means:

$$\text{Var}(\varepsilon) = \text{Var}(\varepsilon_1) \times \cdots \times \text{Var}(\varepsilon_k) \leftarrow \text{c.f.}$$

produce "constant" error variance in the model:

$$\ln S_x^2 = X\beta + \varepsilon$$

$$\ln(\text{Var}(\varepsilon)) = \sum_{i=1}^k \ln(\text{Var}(\varepsilon_i))$$

may get a better approximation by linear structure $X\beta$ and follow normal.

$\ln s^2$ as a Variance Stabilizing Transformation

- Assume $y_{\underline{x},j} \stackrel{i.i.d.}{\sim} N(\mu_{\underline{x}}, \sigma_{\underline{x}}^2)$, $j = 1, \dots, n_{\underline{x}}$. Then,

$$(n_{\underline{x}} - 1)s_{\underline{x}}^2 = \sum_{j=1}^{n_{\underline{x}}} (y_{\underline{x},j} - \bar{y}_{\underline{x}})^2 \sim \sigma_{\underline{x}}^2 \chi_{n_{\underline{x}}-1}^2,$$

and a random variable

$$\left. \begin{array}{l} E(\ln S_{\underline{x}}^2) = ? \\ \text{Var}(\ln S_{\underline{x}}^2) = ? \end{array} \right\} \leftarrow \ln s_{\underline{x}}^2 = \ln \sigma_{\underline{x}}^2 + \ln \left(\chi_{n_{\underline{x}}-1}^2 / (n_{\underline{x}} - 1) \right) \quad \text{a random variable } \sim \chi_{n_{\underline{x}}-1}^2 \quad \text{--- } W_{\underline{x}} \quad (3)$$

- $W_{\underline{x}}$: a random variable, h : a smooth function, by δ -method,

$$E(h(W_{\underline{x}})) \approx h(E(W_{\underline{x}})) \quad \text{and} \quad \text{Var}(h(W_{\underline{x}})) \approx [h'(E(W_{\underline{x}}))]^2 \text{Var}(W_{\underline{x}}) \quad (4)$$

- Suppose $W_{\underline{x}} \sim \chi_{v_{\underline{x}}}^2 / v_{\underline{x}}$. Then, $E(W_{\underline{x}}) = 1$ and $\text{Var}(W_{\underline{x}}) = 2/v_{\underline{x}}$.

- Take $h = \ln$. Applying (4) to $W_{\underline{x}} (\sim \chi_{v_{\underline{x}}}^2 / v_{\underline{x}})$ leads to

In LM,
 $Z_{\underline{x}} \sim N(\mu_{\underline{x}}, \sigma_{\underline{x}}^2)$

$$E(\ln(W_{\underline{x}})) \approx \ln(E(W_{\underline{x}})) = \ln(1) = 0, \rightarrow E(\ln S_{\underline{x}}^2) \approx \ln \sigma_{\underline{x}}^2$$

$$\text{Var}(\ln(W_{\underline{x}})) \approx [h'(1)]^2 (2/v_{\underline{x}}) = 2/v_{\underline{x}}. \rightarrow \text{Var}(\ln S_{\underline{x}}^2) \approx 2/v_{\underline{x}}$$

In (3), $v_{\underline{x}} = n_{\underline{x}} - 1$, we have $\ln s_{\underline{x}}^2 \sim N(\ln \sigma_{\underline{x}}^2, 2(n_{\underline{x}} - 1)^{-1})$.

The variance of $\ln s_{\underline{x}}^2$, i.e., $2(n_{\underline{x}} - 1)^{-1}$, is nearly constant for $n_{\underline{x}} - 1 \geq 9$.

a constant if we have same # of replicates for each run.

$\sigma_{\underline{x}}^2$ only appears in the mean structure of $\ln(S_{\underline{x}}^2)$

❖ Reading: textbook, 4.11 (exercise) Compare the result with $E(S_{\underline{x}}^2)$ and $\text{Var}(S_{\underline{x}}^2)$

Epi-layer Growth Experiment Revisited

- Original data from Shoemaker, Tsui and Wu (1991) ★ Conceptual model:

$$Z_{\underline{x}} \sim \beta_0 + \beta_A \chi_A + \dots$$

$$+ \beta_{AB} \chi_A \chi_B + \dots$$

$$+ \beta_{ABC} \chi_A \chi_B \chi_C + \dots$$

$$+ \beta_{ABCD} \chi_A \chi_B \chi_C \chi_D$$

$$+ \epsilon \quad \leftarrow \text{constant variance}$$

① Use $Z_{\underline{x}} = \bar{y}_{\underline{x}}$ to build a mean model

(Q: Why not use $Z_{\underline{x}} = y_{\underline{x}}$ to build a mean model?

Ans. $\text{Var}(y_{\underline{x}})$ not regarded constant over \underline{x})

(Q: Why $\bar{y}_{\underline{x}}$ better than $y_{\underline{x}}$?

$$\text{Ans. } 0 < \text{Var}(y_{\underline{x}}) = \sigma_{\underline{x}}^2 \\ 0 < \text{Var}(\bar{y}_{\underline{x}}) = \sigma_{\underline{x}}^2/6)$$

Table 2
(LNp 5-2)

2⁴ design

Table 7: Design Matrix and Thickness Data, Original Epitaxial Layer Growth Experiment

Design				original response (6 replicates)						unreplicated		
A	B	C	D	Thickness (y)						\bar{y}	s^2	$\ln s^2$
-	-	-	+	14.812	14.774	14.772	14.794	14.860	14.914	14.821	0.003	-5.771
-	-	-	-	13.768	13.778	13.870	13.896	13.932	13.914	13.860	0.005	-5.311
-	-	+	+	14.722	14.736	14.774	14.778	14.682	14.850	14.757	0.003	-5.704
-	-	+	-	13.860	13.876	13.932	13.846	13.896	13.870	13.880	0.001	-6.984
-	+	-	+	14.886	14.810	14.868	14.876	14.958	14.932	14.888	0.003	-5.917
-	+	-	-	14.182	14.172	14.126	14.274	14.154	14.082	14.165	0.004	-5.485
-	+	+	+	14.758	14.784	15.054	15.058	14.938	14.936	14.921	0.016	-4.107
-	+	+	-	13.996	13.988	14.044	14.028	14.108	14.060	14.037	0.002	-6.237
+	-	-	+	15.272	14.656	14.258	14.718	15.198	15.490	14.932	0.215	-1.538
+	-	-	-	14.324	14.092	13.536	13.588	13.964	14.328	13.972	0.121	-2.116
+	-	+	+	13.918	14.044	14.926	14.962	14.504	14.136	14.415	0.206	-1.579
+	-	+	-	13.614	13.202	13.704	14.264	14.432	14.228	13.907	0.226	-1.487
+	+	-	+	14.648	14.350	14.682	15.034	15.384	15.170	14.878	0.147	-1.916
+	+	-	-	13.970	14.448	14.326	13.970	13.738	13.738	14.032	0.088	-2.430
+	+	+	+	14.184	14.402	15.544	15.424	15.036	14.470	14.843	0.327	-1.118
+	+	+	-	13.866	14.130	14.256	14.000	13.640	13.592	13.914	0.070	-2.653

② Use $Z_{\underline{x}} = \ln S_{\underline{x}}^2$ to build a variance model

Epi-layer Growth Experiment: Effect Estimates

Table 8: Factorial Effects, Original Epitaxial Layer Growth Experiment

$$\begin{aligned} & \hat{\beta}_i = \hat{\theta}_i \\ & \uparrow \\ & (X^T X)^{-1} X^T Z \\ & \uparrow \\ & 16I \end{aligned}$$

Effect	\bar{y}	$\ln s^2$
A	-0.055	3.834
B	0.142	0.078
C	-0.109	0.077
D	0.836	0.632
AB	-0.032	-0.428
AC	-0.074	0.214
AD	-0.025	0.002
BC	0.047	0.331
BD	0.010	0.305
CD	-0.037	0.582
ABC	0.060	-0.335
ABD	0.067	0.086
ACD	-0.056	-0.494
BCD	0.098	0.314
ABCD	0.036	0.109

Understand the meaning of these effect estimates, e.g.,

$ME(A) = -0.055$
 \parallel
 $\bar{Z}(A+) - \bar{Z}(A-)$

$INT(A.B) = -0.032$
 \parallel
 $ME(A|B+) - ME(A|B-)$

⋮



Epi-layer Growth Experiment: Half-Normal Plots

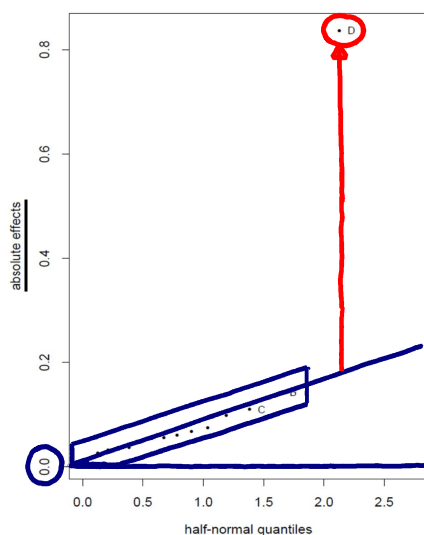


Figure 7 : Location effects (\bar{y}_X)

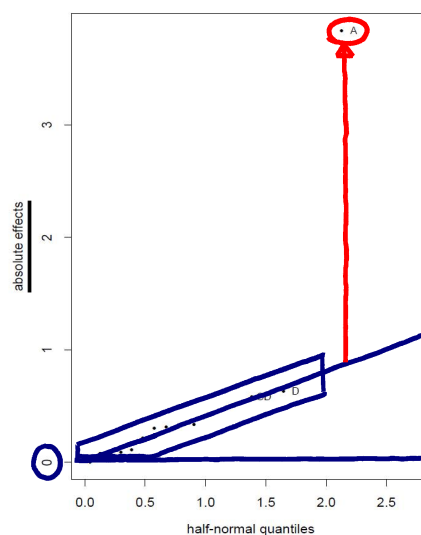


Figure 8 : Dispersion effects ($\ln s_X^2$)

(exercise) Perform Lenth's method to identify significant effects

Epi-layer Growth Experiment: Analysis and Optimization

- From the two plots, ME D is significant for $z = \bar{y}$ and ME A is significant for $z = \ln s^2$. Fitted models:

location model $\rightarrow \hat{y}_x = \hat{\beta}_0 + \hat{\beta}_D x_D = 14.389 + 0.418 x_D$

dispersion model $\rightarrow \ln \hat{s}_x^2 = \hat{\gamma}_0 + \hat{\gamma}_A x_A = -3.772 + 1.917 x_A$

- Factor D is an adjustment factor.

All the effects related to factors B and C do not appear in the fitted models.

- Two-step procedure:

- Choose A at $-$ level (continuous rotation) \leftarrow qualitative factor
- Choose $x_D = 0.266$ to satisfy $14.5 = 14.389 + 0.418 x_D$. (If $D = 30$ and 40 sec for $x_D = -1$ and $+1$, $x_D = 0.266$ corresponds to $35 + 0.266(5) = 36.33$ sec.) \leftarrow quantitative factor

- Predicted variance (Q: What if D is a qualitative factor?) \leftarrow cf.

$$\hat{\sigma}^2 = \exp[-3.772 + 1.917(-1)] = (0.058)^2 \approx 0.0034$$

This is too optimistic! Predicted values should be validated with a confirmation experiment.

(Note. s_x^2 estimates subplot error variance)

❖ Reading: textbook, 4.12

check LNp.5-3

Q: Do we have information about the whole-plot error variance?
Ans. Check Fig 7 in LNp.5-34

optimal setting

x_A	x_B	x_C	x_D
-1	?	?	0.266

2^k Designs in 2^q Blocks

k treatment factors, each 2 levels

Full factorial $\Rightarrow 2^k$ treatments (\Rightarrow need 2^k EUs)

- Example: Arranging a 2^3 design in 2 blocks (of size 4).

Use the 123 column in Table 9 (LNp.5-37) to define the blocking scheme:

block I if 123 = $-$, and block II if 123 = $+$.

- The block effect estimate $\bar{y}(II) - \bar{y}(I)$ is identical to the estimate of the 123 interaction $\bar{y}(123 = +) - \bar{y}(123 = -)$.

The block effect b and the interaction 123 are called

confounded. Notationally,

① In design matrix, column $b = (\text{column 1}) * (\text{column 2}) * (\text{column 3})$

② In model matrix, block effect column = 123 interaction column

③ $B_b + B_{123}$ is jointly estimated

aliased (Ch5)

$$b = 123$$

sacrificing

- By giving up the ability to estimate 123, this blocking scheme increases the precision in the estimates of main effects and 2fi's by arranging 8 runs in two homogeneous blocks.

a good choice?

- Why sacrificing 123?

ans: Effect hierarchy principle.

the block effect ① can reduce $\hat{\sigma}^2$ ③ is orthogonal to other treatment effects (their estimates not biased by block effect)

123 is the least important effect among all the 8 factorial effects.

one block factor, 2^q levels

block size 2^{k-q} (\because total 2^k EUs)

block size $2^{k-q} < 2^k$ treatments \Rightarrow incomplete blocking

★ conceptual model:

$$Z \sim \beta_0 + \text{block effects}$$

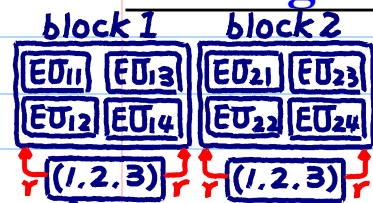
$\uparrow 2^q - 1$ parameters

+ all treatment effects + ϵ

$\uparrow 2^k - 1$ parameters

\Rightarrow no interaction btwn block & treatment factors

Arrangement of 2^3 Design in 2 Blocks



conceptual model: (Note, not interested in β_0)

$$Z = \beta_0 + \beta_b \chi_b + \beta_1 \chi_1 + \beta_2 \chi_2 + \beta_3 \chi_3 + \beta_{12} \chi_{12} + \beta_{13} \chi_{13} + \beta_{23} \chi_{23} + \beta_{123} \chi_{123} + \epsilon$$

block effect β_b

$$= \beta_0 + (\beta_b + \beta_{123}) \chi_b + \beta_1 \chi_1 + \beta_2 \chi_2 + \beta_3 \chi_3 + \beta_{12} \chi_{12} + \beta_{13} \chi_{13} + \beta_{23} \chi_{23} + \epsilon$$

Table 9: Arranging a 2^3 Design in Two Blocks of Size Four
(The 3 factors are denoted by 1, 2, and 3)

Run	T	1	2	3	12	13	23	123	Block
1	+	-	-	-	+	+	+	-	I
2	+	-	-	+	+	-	-	+	II
3	+	-	+	-	-	+	+	+	II
4	+	-	+	+	-	-	+	-	I
5	+	+	-	-	-	-	+	+	II
6	+	+	-	+	-	+	-	-	I
7	+	+	+	-	+	-	-	-	I
8	+	+	+	+	+	+	+	+	II

In the model matrix, the 8 d.f. are used to estimate

β_0 (intercept),
 $\beta_1, \beta_2, \beta_3$,
 $\beta_{12}, \beta_{13}, \beta_{23}$.

$\beta_b + \beta_{123}$

↑ a joint effect

model matrix (all treatment effects)

design matrix of treatment factors

combine

whole design matrix

design matrix of block factor

of possible choices:
 $\binom{8}{4} = \frac{8!}{4!4!}$

↑ Why might not be good choices?
Ans. It would be better to have orthogonality.

of possible columns: 7
⇒ guarantee orthogonality

A 2^3 Design in 4 Blocks

↑ 8 treatments

each with 2 levels

- Similarly we can use $b_1 = 12$ and $b_2 = 13$ to define two independent blocking variables.

The 4 blocks I, II, III and IV are defined by

$b_1 = \pm$ and $b_2 = \pm$:

$\beta_{b_1} \quad \beta_{b_2} \quad \beta_{b_1 b_2}$

pseudo block factors

	b_1	
b_2	\pm	\pm
\pm	I	III
\pm	II	IV

block	b_1	b_2	$b_1 b_2$
I	-	-	+
II	-	+	-
III	+	-	-
IV	+	+	+

This is not an interaction effect. It represents a block main effect.

A group structure in Algebra, with 2 generators b_1, b_2

a block factor with 4 levels needs 3 d.f. for its block effects.

Q: Why not sacrifice 123?

$\{I, b_1, b_2, b_1 b_2\}$

identity element	1 ×	23
Intercept	2 ×	13
	3 ×	12
	12	3 ×
	13	2 ×
	23	1 ×

- A 2^3 design in 4 blocks is given in Table 10

(LNp.5-39). Confounding relationships:

$b_1 = 12, b_2 = 13, b_1 b_2 = 12 \times 13 = 23. = 1^2 23$

Thus 12, 13 and 23 are confounded with block effects and thus sacrificed.

Note. In model matrix, for every columns χ_i 's, we have $\chi_i^2 = I$

Arranging a 2^3 Design in 4 Blocks

Table 10: Arranging a 2^3 Design in Four Blocks of Size Two

(exercise)

- conceptual model = ?
- model matrix with block & treatment effects = ?
- 8 df. are used to estimate what ?

Run									block
	<u>I</u>	<u>1</u>	<u>2</u>	<u>3</u>	<u>12</u>	<u>13</u>	<u>23</u>	<u>123</u>	
1	+	+	+	+	+	+	+	+	IV
2	+	-	-	+	+	-	-	+	III
3	+	-	+	-	-	+	-	+	II
4	+	-	+	+	-	-	+	-	I
5	+	+	-	-	-	-	+	+	I
6	+	+	-	+	-	+	-	-	II
7	+	+	+	-	+	-	-	-	III
8	+	+	+	+	+	+	+	+	IV

of possible choices:
(2 2 2 2)True model: $Z = X_1\beta_1 + X_2\beta_2 + \epsilon$
 $H_1X_2\beta_2$ $(I-H_1)X_2\beta_2$ Fitted model: $Z = X_1\beta_1 + \epsilon$
(X_2 : block effects)

(a) If

 $X_1 = \begin{bmatrix} 1 & 1 & 2 & 3 \\ 1 & 1 & 2 & 3 \\ 1 & 1 & 2 & 3 \\ 1 & 1 & 2 & 3 \end{bmatrix} \Rightarrow H_1X_2\beta_2 = 0$
But, β^2 is larger than it should be.

(b) If

 $X_1 = \begin{bmatrix} 1 & 1 & 2 & 3 & 12 & 13 & 23 & 123 \\ 1 & 1 & 2 & 3 & 12 & 13 & 23 & 123 \\ 1 & 1 & 2 & 3 & 12 & 13 & 23 & 123 \\ 1 & 1 & 2 & 3 & 12 & 13 & 23 & 123 \end{bmatrix}$ $\Rightarrow (I-H_1)X_2\beta_2 = 0$
But, $\hat{\beta}_{12}, \hat{\beta}_{13}, \hat{\beta}_{23}$ are biasedmodel matrix
(treatment effects)

whole design matrix

- $\{I, 12, 13, 23\}$ forms the block defining contrast subgroup for the 2^3 design in 4 blocks. For a more complicated example (2^5 design in 8 blocks), see textbook, p.196.

3 pseudo block factors b_1, b_2, b_3 \Rightarrow 7 block effects: $b_1, b_2, b_3, b_1b_2, b_1b_3, b_2b_3, b_1b_2b_3$

Minimum Aberration Blocking Scheme

Only consider block schemes of the form:
 $B = \{I, \underline{b_1}, \underline{b_2}, \underline{b_1b_2}\} \leftarrow$ a group

criterion

of treatment factors

- For any blocking scheme B and $1 \leq i \leq k$, let

also called a word of length i $g_i(B)$ = number of i -factor effects that are confounded with block effects.# of i -factor (treatment) effects that are sacrificed.

- Must require $g_1(B) = 0$ (because no main effect should be confounded with block effects).

- For any two blocking schemes B_1 and B_2 , let

 $r =$ smallest i such that $g_i(B_1) \neq g_i(B_2)$.

- If $g_r(B_1) < g_r(B_2)$, scheme B_1 is said to have less aberration than scheme B_2 .
- A blocking scheme B has minimum aberration (MA) if no other blocking schemes have less aberration than B .

MA criterion

 $(g_1(B), g_2(B), \dots, g_k(B))$ sequentially minimize

wordlength pattern (WLP) of block scheme

- The minimum aberration criterion is justified by the effect hierarchy principle.
- Minimum aberration blocking schemes are given in Table 4A.1 (textbook, p.207).
- Theory is developed under the assumption of no block \times treatment interactions.

❖ Reading: textbook, 4.15