Lecture 9

Orthogonal design and analysis

An example in weighing

- Four objects with true weights μ_1, μ_2, μ_3, μ_4
- Error variance is σ^2 in one measurement
- If we have 4 measurements for the i^{th} object, i.e., y_{i1}, y_{i2}, y_{i3}, y_{i4}, we know

$$\mathrm{y}_{ij} \sim N(\mu_i, \sigma^2),\ j = 1, 2, 3, 4, \text{iid}$$

$$\hat{\mu}_i = \overline{\mathrm{y}}_{i\cdot} \sim N(\mu_i, \tfrac{1}{4}\sigma^2)$$

- Say, we want to achieve the same precision for the 4 objects, how many measurements we need to make? 16 or ?

An example in weighing

- Four indicators x_1, x_2, x_3, x_4
  - 0: not weighted
  - -1: in the left
  - 1: in the right
- Y: weight of stacks
  - positive if on the left side
  - negative if on the right side

$$y_i = x_1\mu_1 + x_2\mu_2 + x_3\mu_3 + x_4\mu_4 + \varepsilon_i$$

$$\varepsilon_i \sim N(0, \sigma^2), \text{iid}$$

Y	X_1	X_2	X_3	X_4
20.2	1	1	1	1
8	1	-1	1	-1
9.7	1	1	-1	-1
1.9	1	-1	-1	1

An example in weighing

$$y_1 = \mu_1 + \mu_2 + \mu_3 + \mu_4 + \varepsilon_1$$
$$y_2 = \mu_1 - \mu_2 + \mu_3 - \mu_4 + \varepsilon_2$$
$$y_3 = \mu_1 + \mu_2 - \mu_3 - \mu_4 + \varepsilon_3$$
$$y_4 = \mu_1 - \mu_2 - \mu_3 + \mu_4 + \varepsilon_4$$

Y	X_1	X_2	X_3	X_4
20.2	1	1	1	1
8	1	-1	1	-1
9.7	1	1	-1	-1
1.9	1	-1	-1	1

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{bmatrix}$$

The linear model of the example

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \end{bmatrix} \quad \mathbf{e} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{bmatrix}$$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e} \qquad LSE:\ \hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

Solution of the example

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix} \qquad (\mathbf{X}^T\mathbf{X})^{-1} = \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{bmatrix}$$

$$\hat{\beta} = \begin{bmatrix} \hat{\mu}_1 \\ \hat{\mu}_2 \\ \hat{\mu}_3 \\ \hat{\mu}_4 \end{bmatrix} = \begin{bmatrix} \frac{1}{4}y_1 + \frac{1}{4}y_2 + \frac{1}{4}y_3 + \frac{1}{4}y_4 \\ \frac{1}{4}y_1 - \frac{1}{4}y_2 + \frac{1}{4}y_3 - \frac{1}{4}y_4 \\ \frac{1}{4}y_1 + \frac{1}{4}y_2 - \frac{1}{4}y_3 - \frac{1}{4}y_4 \\ \frac{1}{4}y_1 - \frac{1}{4}y_2 - \frac{1}{4}y_3 + \frac{1}{4}y_4 \end{bmatrix} = \begin{bmatrix} 9.95 \\ 5 \\ 4.15 \\ 1.1 \end{bmatrix}$$

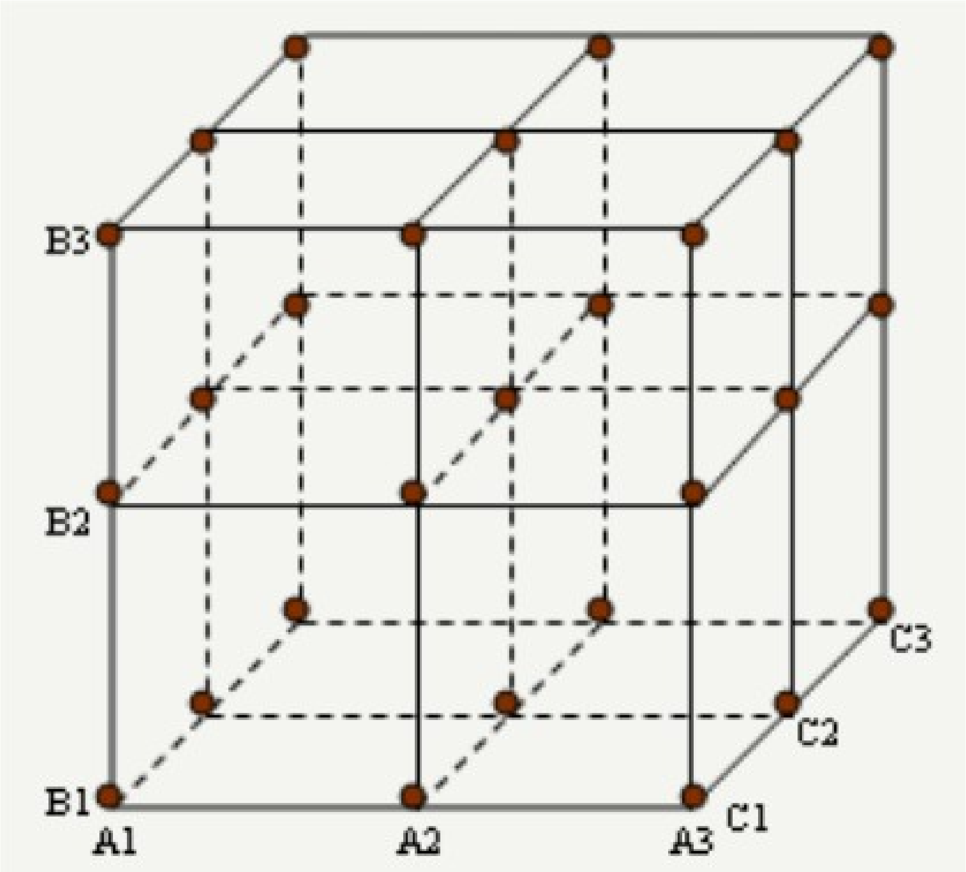
$$\hat{\mu}_i \sim N(\mu_i, \tfrac{1}{4}\sigma^2), i = 1, 2, 3, 4 \text{ and are independent}$$

Full factorial design

- Consider all possible combinations of the factors. For example, three factors with 3 levels:

A1B1C1	A2B1C1	A3B1C1
A1B1C2	A2B1C2	A3B1C2
A1B1C3	A2B1C3	A3B1C3
A1B2C1	A2B2C1	A3B2C1
A1B2C2	A2B2C2	A3B2C2
A1B2C3	A2B2C3	A3B2C3
A1B1C1	A2B1C1	A3B1C1
A1B1C2	A2B1C2	A3B1C2
A1B1C3	A2B1C3	A3B1C3

Full factorial design



- The number of full trials is 3^3=27.

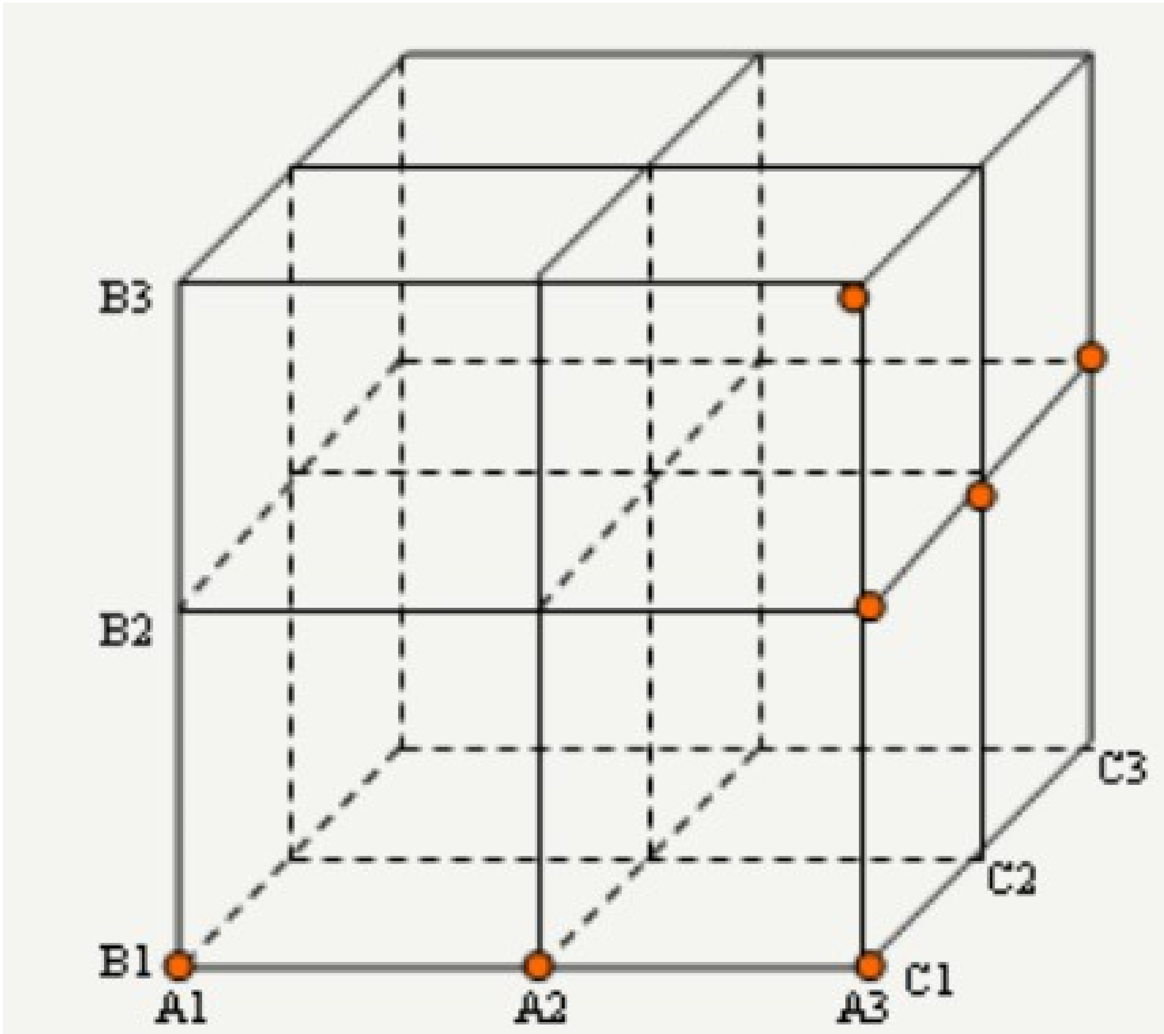
Full factorial design

- Advantage:
  - It analyzes the relationship between factors and levels in detail.
- Disadvantage:
  - The number of combinations is large.
  - The error could not be calculated without replications.
  - The importance of factors could not be found out.

Simple comparison

- Change only one factor in a trial.
- For example:
  - 1. Fix B and C in level B1 and C1, then find that A3 is the best.
  - 2. Fix A in A3, C in C1, then find that B2 is the best.
  - 3. Fix A in A3, B in C2, then find that C2 is the best.
  - So the best one is A3B2C2.

Simple comparison



Simple comparison

- Advantage:
  - The number of trials is small.
- Disadvantage:
  - The trials are not typical.
  - Only consider part of levels of factors. It may not reflect the actual conditions of factors.
  - The importance of factors could not be found out. The error could not be calculated without replications. So it is hard to analyze the precision of the best condition.
  - Hard to use statistical methods for analysis.

Orthogonal design

Orthogonal design

- An experimental design is orthogonal if each factor can be evaluated independently of all the other factors.
- In a two level factorial design, this is achieved by matching each level of each factor with an equal number of each level of the other factors.
- An extension of the Latin Design

Orthogonal tables

- An experimental design is orthogonal if each factor can be evaluated independently of all the other factors.
- In a two level factorial design, this is achieved by matching each level of each factor with an equal number of each level of the other factors.
- An extension of the Latin Design

Common tables $L_a(b^c)$

- **L: orthogonal; a: no. rows (or trials); b: no. levels of each factor; c: no. columns (or max number of factors). b^c = number of all combinations. Ratio a/b^c is the minimum proportion of trials in orthogonal design.**
- For tables has the relationship: $c=(a-1)/(b-1)$
  - For example: $L_4(2^3)$ (a=4, c=3, b=2), $L_8(2^7)$ (a=8, c=7, b=2), $L_{16}(2^{15})$, $L_{32}(2^{31})$ and so on.
  - They can be used for considering interaction between factors, if the factor number < c.
- Some tables may not satisfy $c=(a-1)/(b-1)$
  - For example: $L_{18}(3^7)$, $L_{36}(3^{13})$ and so on

The simplest one: $L_4(2^3)$

- For example, in the left table '+1' level of Factor A (runs 2 and 4) is matched with one instance of Factor B at '-1' and one at '+1'. If any two columns are compared, the same thing will be found for both factor levels.
- **$L_4(2^3)$ was given in the right table.**

Treatment	A	B
1	-1	-1
2	+1	-1
3	-1	+1
4	+1	+1

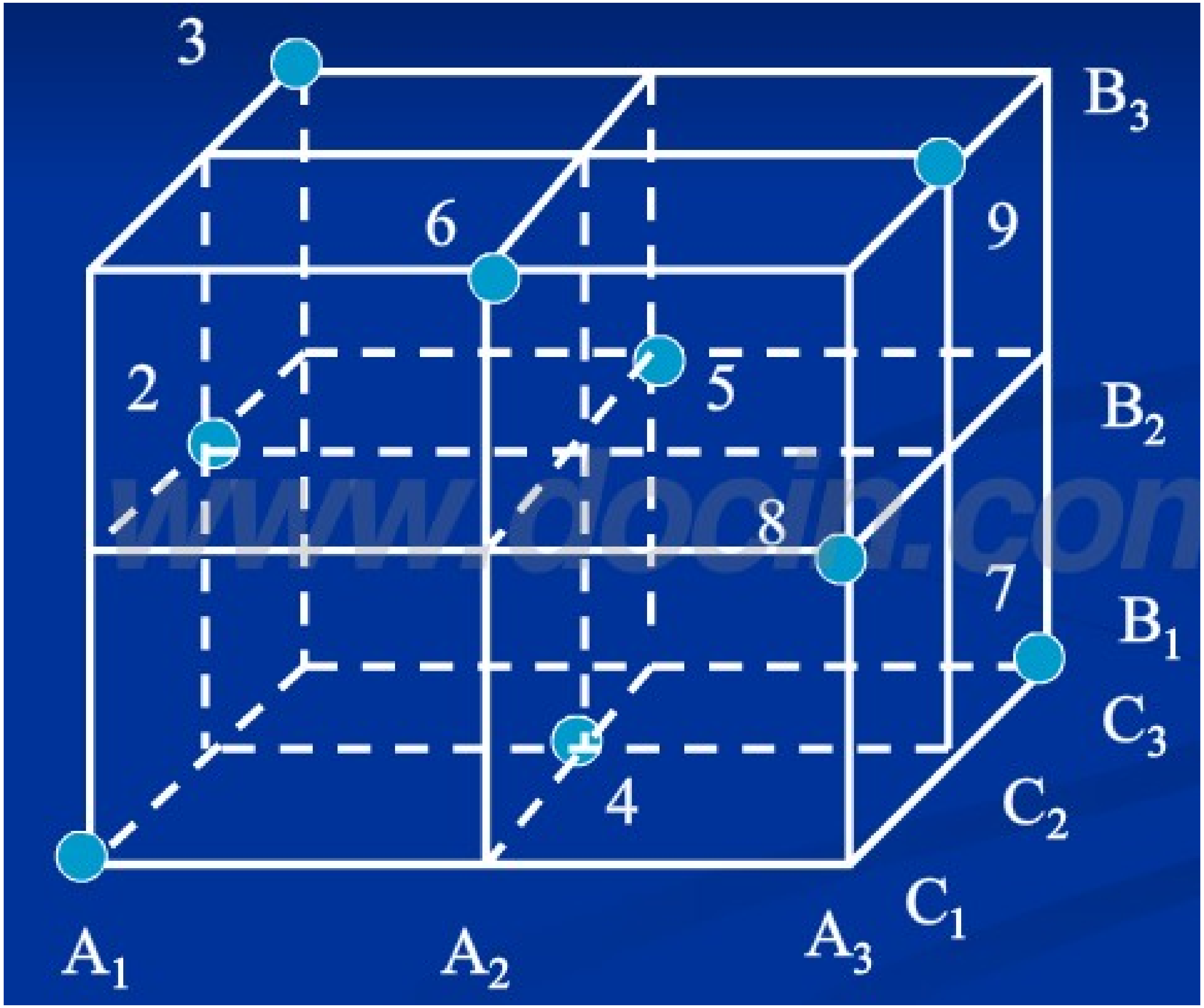
Trial	1	2	3
1	1	1	1
2	1	2	2
3	2	1	2
4	2	2	1

Orthogonal design $L_8(2^7)$

Trial	1	2	3	4	5	6	7
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	1	1
4	1	2	2	2	2	1	2
5	2	1	2	1	2	1	2
6	2	1	2	2	1	2	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

- When the factor number < 7, some columns can be used for studying interactions.

The example of 3 levels



Orthogonal design $L_9(3^4)$

(use the first three columns if there are 3 factors, if interaction is ignored; Otherwise, Column 3 is reserved for interaction between A and B, factor will take column 4)

Trial No.	Column (Factor)			
	1 (A)	2 (B)	3 (C)	4 (D)
1	1 (A1)	1 (B1)	1 (C1)	1 (D1)
2	1 (A1)	2 (B2)	2 (C2)	2 (D2)
3	1 (A1)	3 (B3)	3 (C3)	3 (D3)
4	2 (A2)	1 (B1)	2 (C2)	3 (D3)
5	2 (A2)	2 (B2)	3 (C3)	1 (D1)
6	2 (A2)	3 (B3)	1 (C1)	2 (D2)
7	3 (A3)	1 (B1)	3 (C3)	2 (D2)
8	3 (A3)	2 (B2)	1 (C1)	3 (D3)
9	3 (A3)	3 (B3)	2 (C2)	1 (D1)

Orthogonal table ($L_9(3^4)$)

Trial	Factor			
	1	2	3	4
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

- **"L" stands for orthogonal;**
- **"9" is the number of conditions in the experiment;**
- **"3" the number of levels for each factor;**
- **"4" is the maximum number of factors.**

Property I of Orthogonal design

- Each number (or factor level) appears same number of times in each column (or factor).
  - In $L_4(2^3)$, there are 2 numbers in each column, i.e. 1 and 2. Each number appears two times.
  - In $L_8(2^7)$, there are 2 numbers in each column, i.e. 1 and 2. Each number appears three times.
  - In $L_9(3^4)$, there are 3 numbers in each column, i.e. 1, 2, and 3. Each number appears three times.

Property II of Orthogonal design

- Consider any two columns, each pair of levels appears the same number of times.
  - In $L_4(2^3)$, pairs of numbers (1, 1), (1, 2), (2, 1), and (2, 2). Each pair appears once.
  - In $L_8(2^7)$, pairs of numbers (1, 1), (1, 2), (2, 1), and (2, 2). Each pair appears twice.
  - In $L_9(3^4)$, one pair may be (1, 1), (1, 2), (1, 3), (2, 1), (2, 2), (2, 3), (3, 1), (3, 2), or (3, 3). Each pair appears once and only once.

Advantages of orthogonal design

- Advantages
  - The trials are typical.
  - No need for replications when calculating errors.
  - The importance of factors could be found out.
  - We could use statistical methods for analysis.
- Disadvantages
  - The best condition may not be in the trials.

Why we need orthogonal design?

- For factorial design with k factors; the i^{th} factor has s_i levels, i=1, 2, …,k; dependent variable y. Consider the effect of the i^{th} factor and j^{th} level as

$$\mu_i' = \begin{pmatrix} \mu(i,1) \\ \mu(i,2) \\ \vdots \\ \mu(i,s_\mathrm{i}) \end{pmatrix}_{s_i \times 1} \qquad \sum_{j=1}^{s_i} \mu(i,j) = 0, i = 1, \cdots, k$$

- So $\mu_i' \mathbf{1}_{s_i} = 0, i = 1, \cdots, k$

Why we need orthogonal design?

- Consider *n* trials. When the effects are additive, for the t^{th} trial, assume the i^{th} factor is in the $a_{ti}{}^{th}$ level,

$$E(y_{(a)}) = \mu_0 + \mu(1, a_{t1}) + \cdots + \mu(k, a_{tk}), t = 1, \cdots, n$$

- Introduce

$$x_{tj}^{(i)} = \begin{cases} 1, & a_{ti} = j \\ 0, & a_{ti} \neq j \end{cases}, 1 \leq j \leq s_i, i = 1, \cdots, k, t = 1, \cdots, n$$

- Which shows the level the i^{th} factor is in for the t^{th} trial.

Defining the orthogonal tables

- How could we arrange 1 to 9 in a 3×3 square so that the sum of each row and the sum of each column are equal?

4	9	2
3	5	7
8	1	6

The design matrix

- Define $$\underset{n\times s_i}{\mathbf{X}_i} = \left(\mathrm{x}_{\mathrm{tj}}^{(\mathrm{i})}\right), i = 1, \cdots, k$$
$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_1 & \mathbf{X}_2 & \cdots & \mathbf{X}_k \end{pmatrix}$$
- X is the design matrix of the n trials. Then
$$\mathbf{Y} = \begin{pmatrix} y_{(1)} \\ \vdots \\ y_{(n)} \end{pmatrix}, \quad \mathrm{E}(\mathbf{Y}) = \begin{pmatrix} \mathbf{1} & \mathbf{X} \end{pmatrix} \begin{pmatrix} \mu_0' \\ \mu_1' \\ \vdots \\ \mu_k' \end{pmatrix} \overset{\Delta}{=} \begin{pmatrix} \mathbf{1} & \mathbf{X} \end{pmatrix} \begin{pmatrix} \mu_0' \\ \mu' \end{pmatrix}$$
- Here $y_{(1)}, \cdots, y_{(n)}$ are not correlated and they have the same covariance matrix V. So it is a linear model.

The design matrix

- The properties of design matrix X:
- (1) all elements in X are 0 or 1.
- (2) $X_i 1_{s_i} = 1_n, i = 1, \cdots, k$, each factor will appear in exactly 1 level.
- (3)

$$X_i' 1_n = \begin{pmatrix} r_{i1} \\ \vdots \\ r_{is_i} \end{pmatrix}, i = 1, \cdots, k$$

- where r_{ij} is the number of replications for each level of factors. $0 \le r_{ij} \le n$

The design matrix

- (4) $X_i'X_{j=}(\lambda_{\alpha\beta}^{(i,j)})_n, i, j = 1, \cdots, k; \lambda_{\alpha\beta}^{(i,j)}$ is the number that the (*j*1)th level of *i*th factor and the (*j2)*th level of the *j*th factor occurs together in the *n* trials.

$$\Lambda_{\text{ii}} = \begin{pmatrix} \text{r}_{i1} & & & \text{O} \\ & \text{r}_{i2} & & \\ & & \ddots & \\ \text{O} & & & \text{r}_{is_i} \end{pmatrix}, i = 1, \cdots, k$$

Restriction

$$\begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 1'_{s_1} & 0 & \cdots & 0 \\ 0 & 0 & 1'_{s_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1'_{s_k} \end{pmatrix} \begin{pmatrix} \mu'_0 \\ \mu'_1 \\ \mu'_2 \\ \vdots \\ \mu'_k \end{pmatrix} = 0, i = 1, \cdots, k$$

- So define

$$A = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & \mathbf{1}'_{s_1} & 0 & \cdots & 0 \\ 0 & 0 & \mathbf{1}'_{s_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{1}'_{s_k} \end{pmatrix}, \text{then } A^+ = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{s_1}\mathbf{1} & 0 & \cdots & 0 \\ 0 & 0 & \frac{1}{s_2}\mathbf{1} & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{s_k}\mathbf{1} \end{pmatrix}$$

Restriction

$$P_A^* = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & I - \frac{1}{s_1} J & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & I - \frac{1}{s_k} J \end{pmatrix}$$

- Where J is the matrix that all elements equal 1

$$X_i 1_{s_i} = 1_n \Rightarrow \left(I - \frac{1}{s_i} J \right) X_i' = X_i' - \frac{1}{s_i} 1 1' X_i' = X_i' - \frac{1}{s_i} 1 1_n'$$

- Define $C = \begin{pmatrix} 1 & X_1 & \cdots & X_k \end{pmatrix}$

Restriction

$$CP_A^* = \begin{pmatrix}1 & X_1 & \cdots & X_k\end{pmatrix}\begin{pmatrix}1 & 0 & \cdots & 0 \\ 0 & I - \frac{1}{s_1}J & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & I - \frac{1}{s_k}J\end{pmatrix}$$

$$= \begin{pmatrix}1 & X_1 - \frac{1}{s_1}\mathbf{1}_n\mathbf{1}'_{s_1} & \cdots & X_k - \frac{1}{s_k}\mathbf{1}_n\mathbf{1}'_{s_k}\end{pmatrix}$$

- It is obvious that $rk\, CP_A^* = rk\, C$

Theorem

- If $rk\,CP_A^* = rk\,C$, then the model

$$\begin{cases} E(Y) = C\Theta, \text{and } A\Theta = O \\ \text{The rows of } Y \text{ are correlated,} \\ \text{and they have the same covariance matrix } V > 0 \end{cases}$$

- Where $\hat{\Theta} = (C'C)^- C'Y$. For any estimable parameter $\rho = trG'\Theta$, the Markov estimation is $\hat{\rho} = trG'\hat{\Theta}$, and the error matrix is still $L_{yy}(C)$.

Sum of squares

- Here $rk\, CP_A^* = rk\, C$, so from the theorem we know $L_{xx}\hat{\mu}' = L_{xy}$, and the error matrix is still $L_{yy}(1\ X)$

$$L_{yy}\begin{pmatrix}\mathbf{1} & X\end{pmatrix} = L_{yy} - L_{yx}L_{xx}^{-}L_{xy} = L_{yy} - L_{yx}\hat{\mu}'$$

$$= L_{yy} - \hat{\mu}'L_{xy} = L_{yy} - \hat{\mu}L_{xx}\hat{\mu}'$$

$$L_{xx} = X'(\mathrm{I} - \frac{1}{n}\mathrm{J})\mathrm{X} = \begin{pmatrix}\mathrm{X}_1' \\ \vdots \\ \mathrm{X}_\mathrm{k}'\end{pmatrix}(\mathrm{I} - \frac{1}{n}\mathrm{J})\begin{pmatrix}X_1 & \cdots & X_k\end{pmatrix}$$

$$= \begin{pmatrix}X_i' & (\mathrm{I} - \frac{1}{n}\mathrm{J})\, X_j\end{pmatrix}$$

Sum of squares

- Denote $L_{ij} = X_i'(I - \frac{1}{n} J)X_j$

- Then $L_{yy} = L_{yy}(\mathbf{1} \quad X) + \sum_{i,j=1}^{k} \hat{\mu}_i L_{ij} \hat{\mu}_j'$

- L_{yy} is the total sum of squares; $L_{yy}(\mathbf{1} \quad X)$ is SS of the errors; $\sum_{i,j=1}^{k} \hat{\mu}_i L_{ij} \hat{\mu}_j'$ is SS of the effects.
- Can SS of the effects be divided into each factor? i.e., when will

$$\sum_{i,j=1}^{k} \hat{\mu}_i L_{ij} \hat{\mu}_j' = \sum_{i=1}^{k} \hat{\mu}_i L_{ii} \hat{\mu}_i'$$

Sum of squares

- It will be right if $L_{ij} = 0$
- Note that $L_{ij} = X_i'(I - \frac{1}{n}J)X_j$
- It is always impossible that $L_{ij} = \mathrm{O}$
- But $\hat{\mu}_i 1_{s_i} = 0, i = 1, \cdots, k$
- So if $L_{ij} = a\mathbf{11}'$, then $\hat{\mu}_i' L_{ij} \hat{\mu}_j' = a\hat{\mu}_i' \mathbf{11}' \hat{\mu}_j' = 0, i \neq j$

Theorem

- In factorial design, if the design matrix obeys: for $i \neq j, i, j = 1, 2, \cdots, k$

- Then $X_i'(I - \frac{1}{n} J) X_j = \lambda_{ij} \mathbf{1}\mathbf{1}'$

$$L_{yy} = L_{yy}(\mathbf{1} \quad X) + \sum_{i=1}^{k} \hat{\mu}_i L_{ii} \hat{\mu}_i'$$

Orthogonal design

- The orthogonal design satisfied

$$L_{yy} = L_{yy}(\mathbf{1} \quad X) + \sum_{i=1}^{k} \hat{\mu}_i L_{ii} \hat{\mu}_i'$$

- It has two properties:
- 1. $X_i 1_{s_i} = \frac{n}{s_i} 1_{s_i}, i = 1, \cdots, k$
- 2. $X_i' X_j = \frac{n}{s_i s_j} 11', i \neq j, i, j = 1, \cdots, k$

Orthogonal design

- In orthogonal design,

$$\hat{\mu}_i' L_{ij} \hat{\mu}_j' = 0, i \neq j, i, j = 1, \cdots, k$$

$$L_{ii} = X_i'(I - \frac{1}{n}\mathbf{1}\mathbf{1}')X_i = \frac{n}{s_i} I - \frac{1}{n} \cdot \frac{n^2}{s_i^2}\mathbf{1}\mathbf{1}'$$

$$= \frac{n}{s_i} I - \frac{n}{s_i^2} J$$

$$\hat{\mu}_i' L_{ii} \hat{\mu}_i' = \hat{\mu}_i \left(\frac{n}{s_i} I \right) \hat{\mu}_i' - \frac{n}{s_i^2} \hat{\mu}_i' \mathbf{1}\mathbf{1}' \hat{\mu}_i = \frac{n}{s_i} \hat{\mu}_i \hat{\mu}_i'$$

$$L_{yy} = L_{yy}(\mathbf{1} \quad X) + \sum_{i=1}^{k} \frac{n}{s_i} \hat{\mu}_i \hat{\mu}_i'$$

ANOVA of an orthogonal design

The linear model

- Here we consider a orthogonal design with 3 factors: A, B and C. And no interactions between factor effects.
- Define μ as the mean value; α_i, β_j and λ_k are effects of level A_i, B_j and C_k; y is the dependent variable.
- Model: $y_{ijk} = \mu + \alpha_i + \beta_j + \lambda_k + \varepsilon_{ijk}$
- $\sum \alpha_i = \sum \beta_j = \sum \lambda_k = 0$, $\varepsilon_{ijk} \sim N(0, \sigma^2)$ are independent

Hypothesis

- $H0_1$: $\alpha_1 = \alpha_2 = \alpha_3$
- $H0_2$: $\beta_1 = \beta_2 = \beta_3$
- $H0_3$: $\lambda_1 = \lambda_2 = \lambda_3$

ANOVA

- Similar to designs with two factors,

$$SS_T = \sum_{i=1}^{n} (\mathrm{y}_\mathrm{i} - \overline{\mathrm{y}})^2 = \sum_{i=1}^{n} \mathrm{y}_\mathrm{i}^{\ 2} - n\overline{\mathrm{y}}^2,\ f_T = n - 1$$

- Where *n* is the number of trials, i.e. the number of rows in the orthogonal table

$$SS_A = \sum_{i=1}^{a} r_\mathrm{i} (\overline{\mathrm{y}}_i - \overline{\mathrm{y}})^2 = \sum_{i=1}^{a} r_i \overline{\mathrm{y}}_i^{\ 2} - n\overline{\mathrm{y}}^2,\ f_A = r_i - 1$$

- *a* is the number of levels of A; r_i is the number of trials in the *i*th level. $\overline{\mathrm{y}}_i$ is the mean value of y under the i^{th} level of A

ANOVA

- Similarly, calculate S_B and S_C
- $SS_{\varepsilon} = SS_T - SS_{\mathrm{A}} - SS_{\mathrm{B}} - SS_{\mathrm{C}}, f_{\varepsilon} = a - 1$

Source	Degrees of freedom	Sum of squares	Mean square	F ratio
Factor A	$f_A = a-1$	SS_A	$MS_A = SS_A/(a-1)$	MS_A/MS_{ε}
Factor B	$f_B = a-1$	SS_B	$MS_B = SS_B/(a-1)$	MS_B/MS_{ε}
Factor C	$f_C = a-1$	SS_C	$MS_C = SS_C/(a-1)$	MS_C/MS_{ε}
Error	$f_{\varepsilon} = a-1$	SS_{ε}	$MS_{\varepsilon} = SS_{\varepsilon}/(a-1)$	
Total T	$f_T = n-1$	SS_T		

Example

- Orthogonal design: analyze 3 factors (the basic medium, ABA and hormones), and 4 levels of them on the induction effect.

Level Factor	A (the basic medium)	B (ABA, mg/l)	C (hormones, mg/l)
1	A1: AAJ	B1: 2,4-D 2.0	C1: 0.0
2	A2: N6	B2: 2,4-D 3.0	C2: 1.0
3	A3: MS	B3: Dicamba 2.5	C3: 2.0
4	A4: JW	B4: Picloram 2.5	C4: 3.0

$L_{16}(4^5)$

Exp. Unit	A	Blank1	B	C	Blank2	Observation
JW1	1	1	1	1	1	Y1
JW2	1	2	2	2	2	Y2
JW3	1	3	3	3	3	Y3
JW4	1	4	4	4	4	Y4
JW5	2	1	2	3	4	Y5
JW6	2	2	1	4	3	Y6
JW7	2	3	4	1	2	Y7
JW8	2	4	3	2	1	Y8
JW9	3	1	3	4	2	Y9
JW10	3	2	4	3	1	Y10
JW11	3	3	1	2	4	Y11
JW12	3	4	2	1	3	Y12
JW13	4	1	4	2	3	Y13
JW14	4	2	3	1	4	Y14
JW15	4	3	2	4	1	Y15
JW16	4	4	1	3	2	Y16

Exp. Unit	The induction rate (%) of 6 rice varieties						
	Q25	PA64S	MH86	IR64	Q4041	N22	Mean
JW1	23.40	26.50	66.40	49.00	57.30	61.00	47.27
JW2	32.94	40.55	51.05	59.00	61.57	56.09	50.20
JW3	98.06	81.97	89.92	92.15	79.00	82.04	87.19
JW4	24.94	16.35	29.70	29.30	31.40	41.29	28.83
JW5	87.41	67.00	74.86	79.90	63.79	67.20	73.36
JW6	56.40	63.55	63.00	66.31	89.96	90.02	71.54
JW7	19.38	29.35	30.00	29.20	67.26	71.35	41.09
JW8	56.36	53.20	59.77	56.01	60.79	67.00	58.86
JW9	70.96	57.98	77.00	81.30	67.90	77.40	72.09
JW10	65.39	74.80	73.30	84.01	59.00	71.00	71.25
JW11	93.00	79.95	94.57	96.90	71.05	78.07	85.59
JW12	85.50	83.88	90.00	85.00	76.90	79.00	83.38
JW13	54.77	39.00	23.14	35.01	29.00	33.58	35.75
JW14	29.56	19.88	31.07	36.98	51.00	46.01	35.75
JW15	38.55	45.74	68.91	40.01	66.09	50.00	51.55
JW16	56.40	44.94	47.00	37.08	44.07	61.03	48.42

Calculation of SS $\bar{y} = 58.88$

	Factor				
	A	Blank1	B	C	Blank2
T_{1j}	213.49	228.47	252.82	207.49	228.93
T_{2j}	244.85	228.74	258.49	230.4	211.8
T_{3j}	312.31	265.42	253.89	280.22	277.86
T_{4j}	171.47	219.49	176.92	224.01	223.53
$\bar{y}_{1j}$	53.37	42.87	61.21	**78.08 (C1)**	53.37
$\bar{y}_{2j}$	**63.21 (A2)**	44.23	**64.62 (B2)**	63.47	63.21
$\bar{y}_{3j}$	51.87	52.05	57.6	70.06	51.87
$\bar{y}_{4j}$	57.12	54.87	57.19	56.00	57.12
SS_j	2642.87	311.66	1149.58	889.03	635.63
SS_T	5628.77				

The best combination A2-B2-C1 does appear in the 16 trials!

ANOVA

Source	D.F.	Sum of squares	Mean square	F ratio	P value (F(3,6))
Factor A	3	2642.87	880.96	5.58	0.035971*
Factor B	3	1149.58	383.19	2.43	0.163654
Factor C	3	735.62	245.21	1.55	0.295307
Error: Blank1	3	311.66	103.89		
Error: Blank2	3	635.63	211.88		
Error: Blank 1-2	6	947.29	157.88		
Total T	15	5628.77			

Under significance level 0.05, only factor A is significant.

Another example

- Experiment for the conversion rate of a chemical products

Factor	Level 1	Level 2	Level 3
A: Temperature (℃)	80	85	90
B: Reaction time (min)	90	120	150
C: Catalyst content (%)	5	6	7

$L_9(3^4)$

Exp. Unit	A	B		C	Observation
1	1	1	3	2	31
2	2	1	1	1	54
3	3	1	2	3	38
4	1	2	2	1	53
5	2	2	3	3	49
6	3	2	1	2	42
7	1	3	1	3	57
8	2	3	2	2	62
9	3	3	3	1	64

Calculation of SS

$\bar{y} = 50$

	Factor			
	A	B		C
T_{1j}	141	123	153	171
T_{2j}	165	144	153	135
T_{3j}	144	183	144	144
$\bar{y}_{1j}$	47	41	51	57
$\bar{y}_{2j}$	55	48	51	45
$\bar{y}_{3j}$	48	61	48	48
SS_j	114	618	18	234
SS_T	984			

The best combination is A2B3C1, when ignoring interactions

ANOVA

Source	D.F.	Sum of squares	Mean square	F ratio	P value (F(2,2))
Factor A	2	114	57	6.33	0.136
Factor B	2	618	309	34.33	0.028*
Factor C	2	234	117	13.00	0.071
Error	2	18	9		
Total T	8	984			

Under significance level 0.05, only factor B is significant.

Considering interactions

Considering interactions (example)

Factor	Level 1	Level 2
A: temperature (℃)	60	80
B: reaction time (h)	2.5	3.5
C: ratio of two materials	1.1/1	1.2/1
D: degree of vacuum (kPa)	50	60

- We want to consider A × B

Interaction table of $L_8(2^7)$

Column	1	2	3	4	5	6	7
1	(1)	**3**	2	5	4	7	6
2		(2)	1	6	7	4	5
3			(3)	7	6	5	4
4				(4)	1	2	3
5					(5)	3	2
6						(6)	1
7							(7)

	A	B	A×B	C			D
Column	1	2	3	4	5	6	7

Interactions

- For $L_a(b^c)$, if $a=b^k$, all the columns will be divided into k groups, and the numbers of columns for these groups are b^0, b^1,…, b^{k-1}
- For example, $L_8(2^7)$. Three groups:
- Group 1: column 1;
- Group 2: column 2, 3;
- Group 3: column 4, 5, 6, 7.

Interactions

- If two factors are in the same group, their interaction is in the column of higher group; otherwise, in the column of lower group.
- For example, A is in column 1, B is in column 2, then A x B is in column 3.
- A is in column 2, B is in column 3, then A x B is in column 1.

Table title for interaction in $L_8(2^7)$

No. factors	Column						
	1	2	3	4	5	6	7
3	A	B	A×B	C	A×C	B×C	A×B×C
4	A	B	A×B C×D	C	A×C B×D	B×C A×D	D
4	A	B C×D	A×B	C B×D	A×C	D B×C	A×D
5	A D×E	B C×D	A×B C×E	C B×D	A×C B×E	D A×E B×C	E A×D

A design with interactions

Trial	Temperature (℃)	Reaction time (h)	Ration of two materials	Degree of vacuum (kPa)	Gain *y*
1	60	2.5	1.1/1	50	86
2	60	2.5	1.2/1	60	95
3	60	3.5	1.1/1	60	91
4	60	3.5	1.2/1	50	94
5	80	2.5	1.1/1	60	91
6	80	2.5	1.2/1	50	96
7	80	3.5	1.1/1	50	83
8	80	3.5	1.2/1	60	88

Calculation of SS

	A	B	A×B	C			D	
Trial Column	1	2	3	4	5	6	7	*y*
1	1	1	1	1	1	1	1	86
2	1	1	1	2	2	2	2	95
3	1	2	2	1	1	2	2	91
4	1	2	2	2	2	1	1	94
5	2	1	2	1	2	1	2	91
6	2	1	2	2	1	2	1	96
7	2	2	1	1	2	2	1	83
8	2	2	1	2	1	1	2	88
T_1	366	368	352	351	361	359	359	T=724
T_2	358	356	372	373	363	365	365	$\sum y_i^2$ =65668
SS	8	18	50	60.5	0.5	4.5	4.5	SS_T=146

ANOVA

Source	Degrees of freedom	Sum of squares	Mean square	F ratio $F_{0.95}(1, 2)=18.5$
A	1	8.0	8.0	3.2
B	1	18.0	18.0	7.2
C	1	60.5	60.5	24.2*
D	1	4.5	4.5	1.8
A×B	1	50.0	50.0	20.0*
ε	2	5.0	2.5	
Total	7	146.0		

Selecting the best combination of the 4 factors

	A_1	A_2
B_1	(86+95)/2=90.5	(91+96)/2=93.5
B_2	(91+94)/2=92.5	(83+88)/2=85.5

C1<C2, so select C2; D is not significant, so select any level of D. Here we select D2;

So the best combination is A2B1C2D2.

How to design an orthogonal table

- Sum of the degrees of freedom for main effects and interactions is less than the total degree of freedom in the design.
- i.e. $$f_{total} \geq f_A + f_B + f_C + \cdots + f_{A\times B} + f_{A\times C} + f_{B\times C} + \cdots$$
- Notes:

$$f_{total} = (number\ of\ trials) - 1$$

$$f_A = (number\ of\ levels\ of\ A) - 1$$

$$f_{A\times B} = f_A \times f_B$$

Example 1

- A, B, C and D; two levels. Consider interaction A×B, A×C.
- For two levels, $f_A = f_B = f_C = f_D = f_{A\times B} = f_{A\times C} = 1$

$$f_A + f_B + f_C + f_D + f_{A\times B} + f_{A\times C} = 6$$

- So the rows of the table should be $n \geq 6 + 1 = 7$
- Select $L_8(2^7)$

	A	B	A×B	C	A×C	D	
Column	1	2	3	4	5	6	7

Example 2

- A, B, C and D; two levels. Consider interaction A x B, C x D.
- Also $n \geq 6 + 1 = 7$
- But we can not use $L_8(2^7)$. No matter where are the four factors, there may be two interaction or one interaction and one factor which are in the same column. For example:

	A	B	A×B C×D	C			D
Column	1	2	3	4	5	6	7

Example 3

- We should select tables with larger rows. For example, $L_{16}(2^{15})$.
- Basic column of $L_8(2^7)$: 1, 2, 4
- Basic column of $L_{16}(2^{15})$: 1, 2, 4, 8
- Put the factors in the basic column.

	A	B	A×B	C				D				C×D			
Column	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15

Methods for saturated tables

- For tables that

$$f_{total} = f_A + f_B + f_C + \cdots + f_{A\times B} + f_{A\times C} + f_{B\times C} + \cdots$$

- There are some methods:
- 1. Replications.
- 2. Select larger orthogonal tables.
- 3. Regard the column with the smaller SS as the error.
- 4. Regard the design as saturated design.

$L_4(2^2)$: an example in wheat genetics

	Extensibility of 9 replications		Mean	Effect
	BB	bb		
AA	237, 235, 230, 240, 258, 258, 232, 233, 242	241, 236, 238, 253.5, 246.5, 245.5, 224, 220, 200	237.19	17.97
BB	210, 207, 202, 235.5, 225, 235, 219, 211, 209	198, 201, 208, 194.5, 207, 206.5, 151, 152, 151	201.25	-17.97
Mean	228.81	209.64		
Effect	9.58	-9.58		

Interaction	BB	bb
AA	-6.22	6.22
BB	6.22	6.22

ANOVA

Source	D.F.	SS	MS	F	P-value	EMS
Locus Aa	1	11628.03	11628.03	38.43	0.0000	$\sigma_{\varepsilon}^2 + 18\sigma_A^2$
Locus Bb	1	3306.25	3306.25	10.93	0.0024	$\sigma_{\varepsilon}^2 + 18\sigma_B^2$
Interaction	1	1392.78	1393.78	4.61	0.0396	$\sigma_{\varepsilon}^2 + 9\sigma_{AB}^2$
Error	32	9683.67	302.61			σ_{ε}^2
Total	35	26011.72				

Estimation of variance components

Source	Variance	Proportion (%) or heritability in genetics
Locus Aa	629.19	51.58
Locus Bb	166.87	13.68
Interaction	121.24	9.94
Error	302.61	24.81