An Introduction to Multi-Stratum Factorial Design

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中央研究院統計科學研究所

STATISTICAL SCIENCE CAMP
統計科學營
2023.8.23(三)-8.24(四)

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多 階層 因子 設計

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某一種 收集資料的方法

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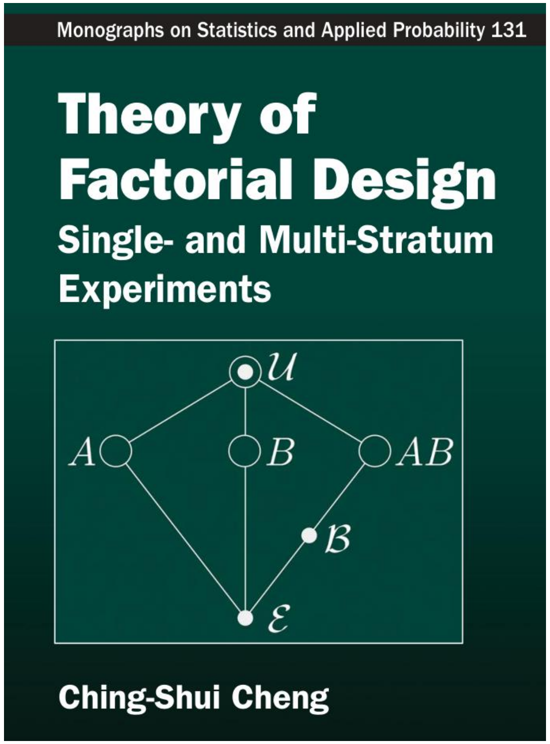
2023.8.23(三)-8.24(四)

Outline

- Data collection & its importance
- Factorial design (因子設計)
- Multi-stratum factorial design
  多 階層 因子 設計



資料收集重要嗎(答案100字以內)

是的，資料收集至關重要。它為決策提供依據，揭示趨勢，改進產品/服務，推動研究創新。透過分析資料，我們可以了解情境，洞察需求，並衡量成效。無論在商業、科學、社會等領域，資料的價值在於引導行動、洞見和發現新的解決方案。然而，資料必須準確、隱私安全，並受到適當的法律和道德框架的保護。

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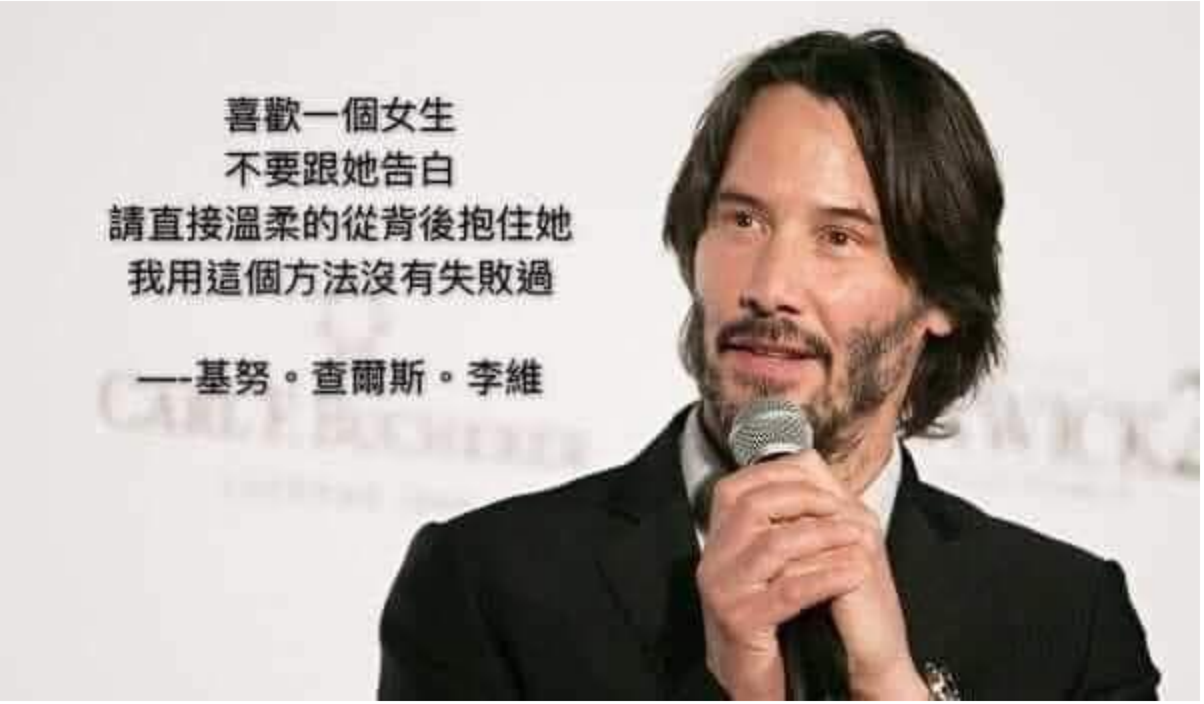
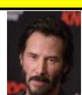
是不是在騙我

我可以向您保證，我這裡的回答是基於我訓練時的知識和資料，並且是以誠實和準確的態度提供給您的。我不會詐騙或欺騙您。如果您有任何疑慮或疑問，請隨時提問，我會盡力為您提供幫助。

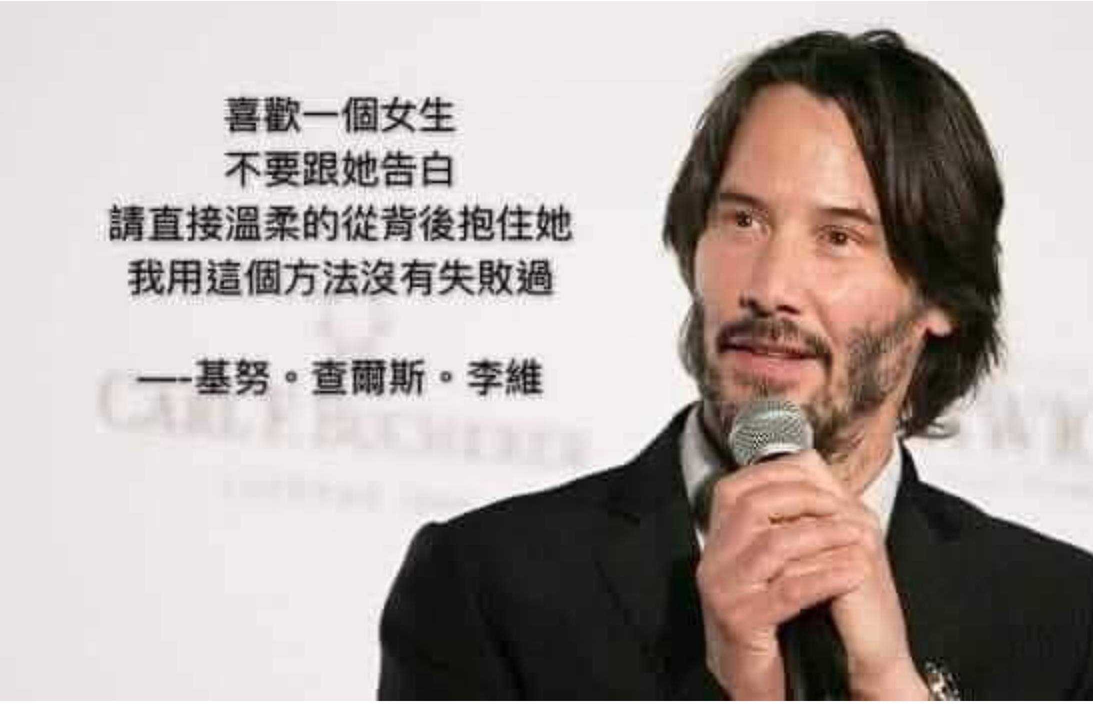
樣本	交往方式	結果

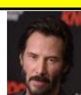
{背後抱住, 直接告白}



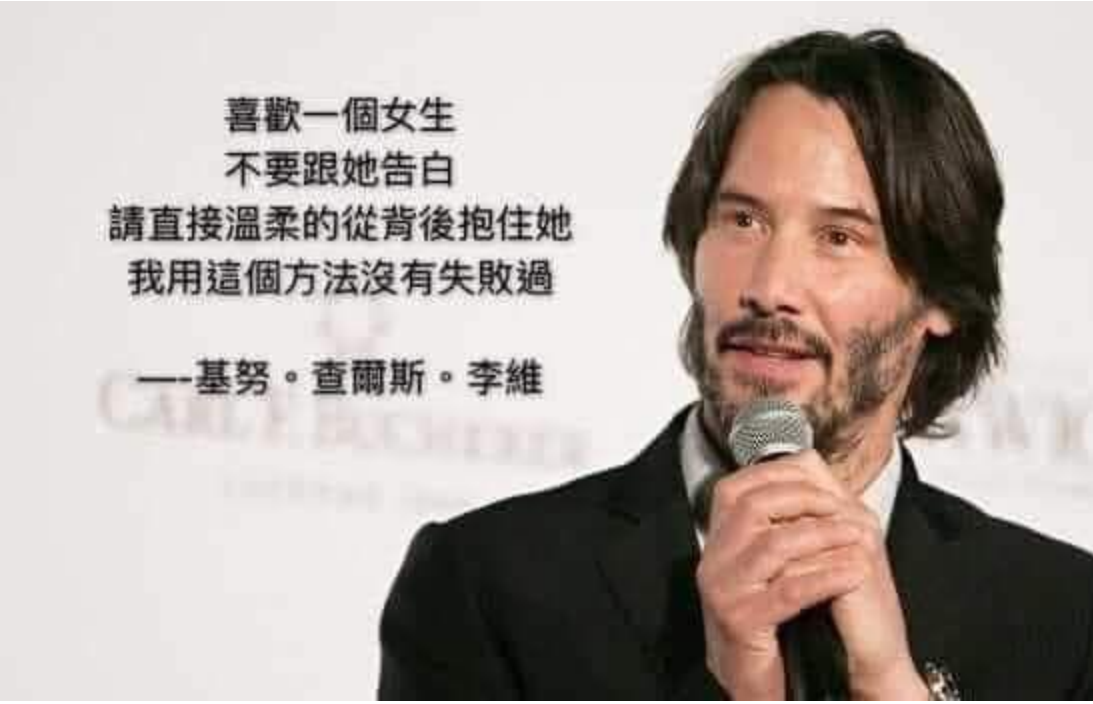
樣本	交往方式	結果
	背後抱住	成功

{背後抱住, 直接告白}



樣本	交往方式	結果
	背後抱住	成功
	直接告白	成功

{背後抱住, 直接告白}



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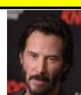
	背後抱住	成功
	直接告白	成功
	背後抱住	警察局

{背後抱住, 直接告白}

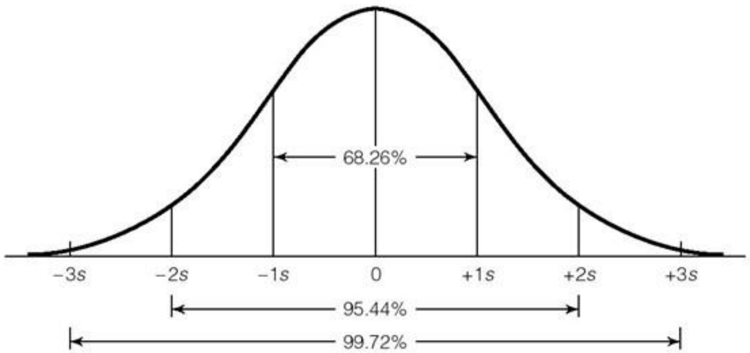
https://news.ebc.net.tw/news/fun/500

「肚臍」的主人接受電子媒體訪問時破梗說，是他的「一指神功」偷點「肚臍」的頭。

再看一次這個點頭短片，主人偷偷跟我們說，其實是他用手，在貓咪的頭後方輕點的傑作。不過無論如何，這隻淡定的小貓，已經成功的吸引大批粉絲，關注他的一舉一動。https://news.ebc.net.tw/news/fun/500

統計模型

- 統計模型由「規律 + 誤差」組成
- 線性迴歸: $y = \beta_0 + \beta_1 x + \varepsilon$
- 常用的假設： ε 來自於常態分佈

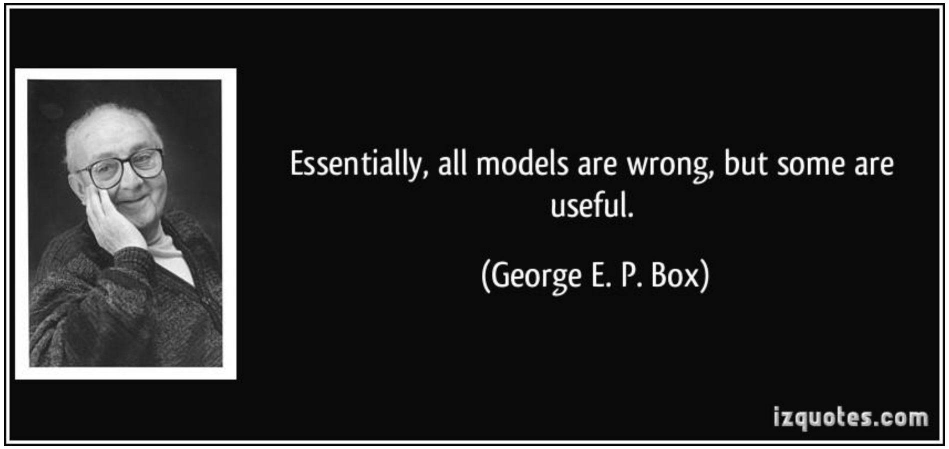


https://homepage.ntu.edu.tw/~clhsieh/biostatistic/4/4-1-1.html

統計模型

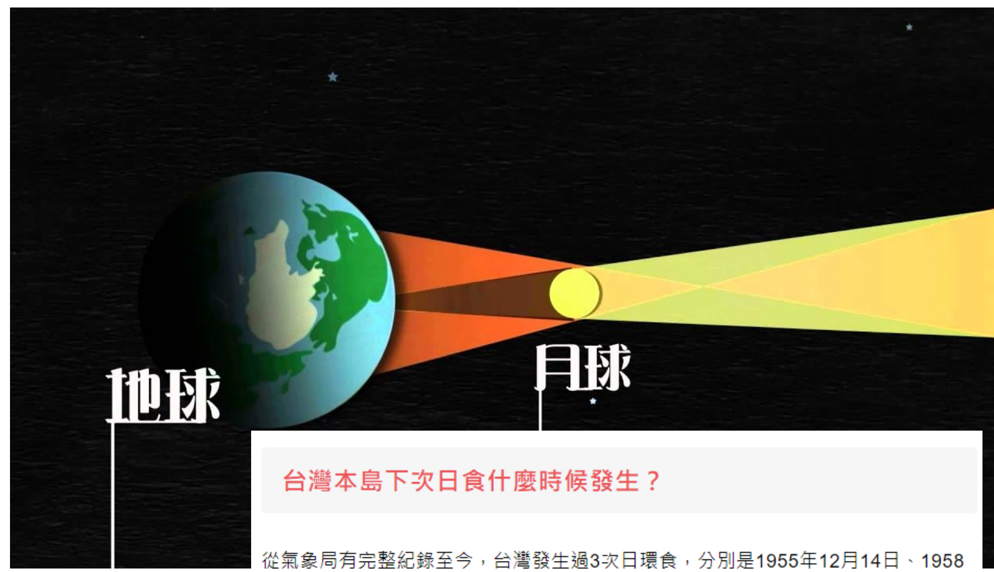
- 「誤差」使得統計模型變得特別
    - 使用隨機變數刻畫誤差
    - 量化不確定性

- 怎麼會用一個錯的模型？



統計模型

- 下面兩個模型都可以解釋太陽為何有時會缺一角，但不見得都Useful



台灣本島下次日食什麼時候發生？

從氣象局有完整紀錄至今，台灣發生過3次日環食，分別是1955年12月14日、1958年4月19日，最近一次是2012年5月21日，台灣本島都可見，今年是第4次。下次日食時間如下：

日偏食：2023年4月20日。

日全食：2070年4月11日，恆春半島可見。

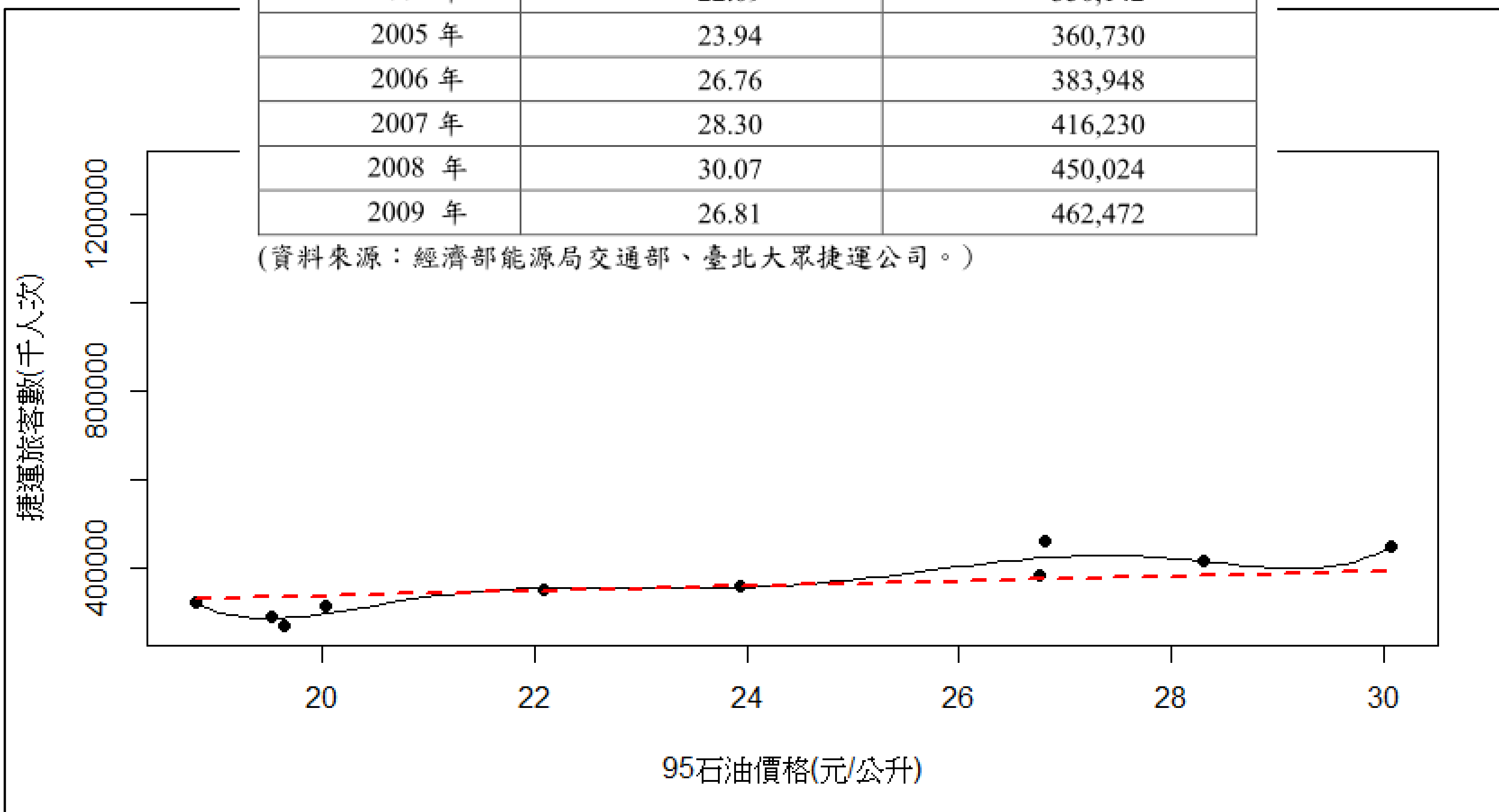
日環食：2215年6月28日，台灣中南部可見。

https://www.cna.com.tw/news/firstnews/202006195013.aspx

表一 台灣區 95 無鉛汽油年均價及捷運旅客數

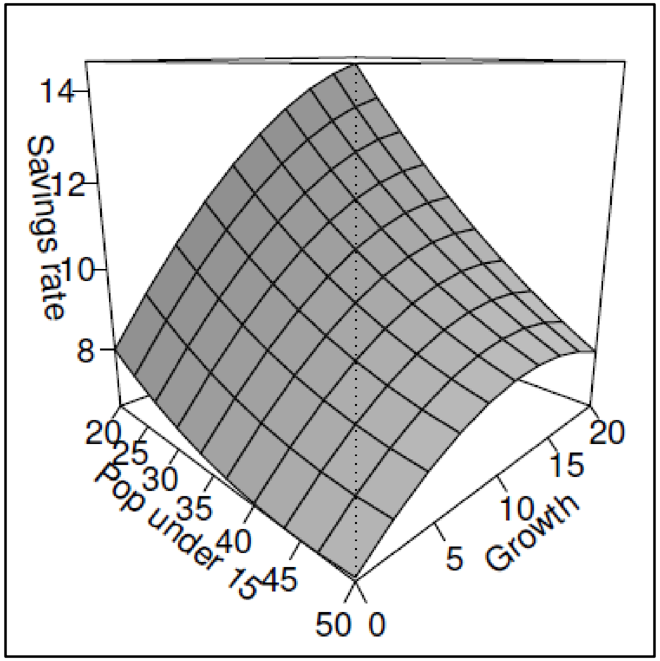
年別	石油價格 (元／公升)	捷運旅客數 (千人次)
2000 年	19.64	268,588
2001 年	19.48	289,643
2002 年	18.80	324,434
2003 年	20.03	316,189
2004 年	22.09	350,142
2005 年	23.94	360,730
2006 年	26.76	383,948
2007 年	28.30	416,230
2008 年	30.07	450,024
2009 年	26.81	462,472

(資料來源：經濟部能源局交通部、臺北大眾捷運公司。)



統計模型

- Polynomial regression (Faraway, 2015, chapter 9)



$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 \boxed{x_1^2} + \beta_4 \boxed{x_2^2} + \beta_5 \boxed{x_1 x_2} + \varepsilon$$

統計模型

- Regression Spline (Faraway, 2015, chapter 9)

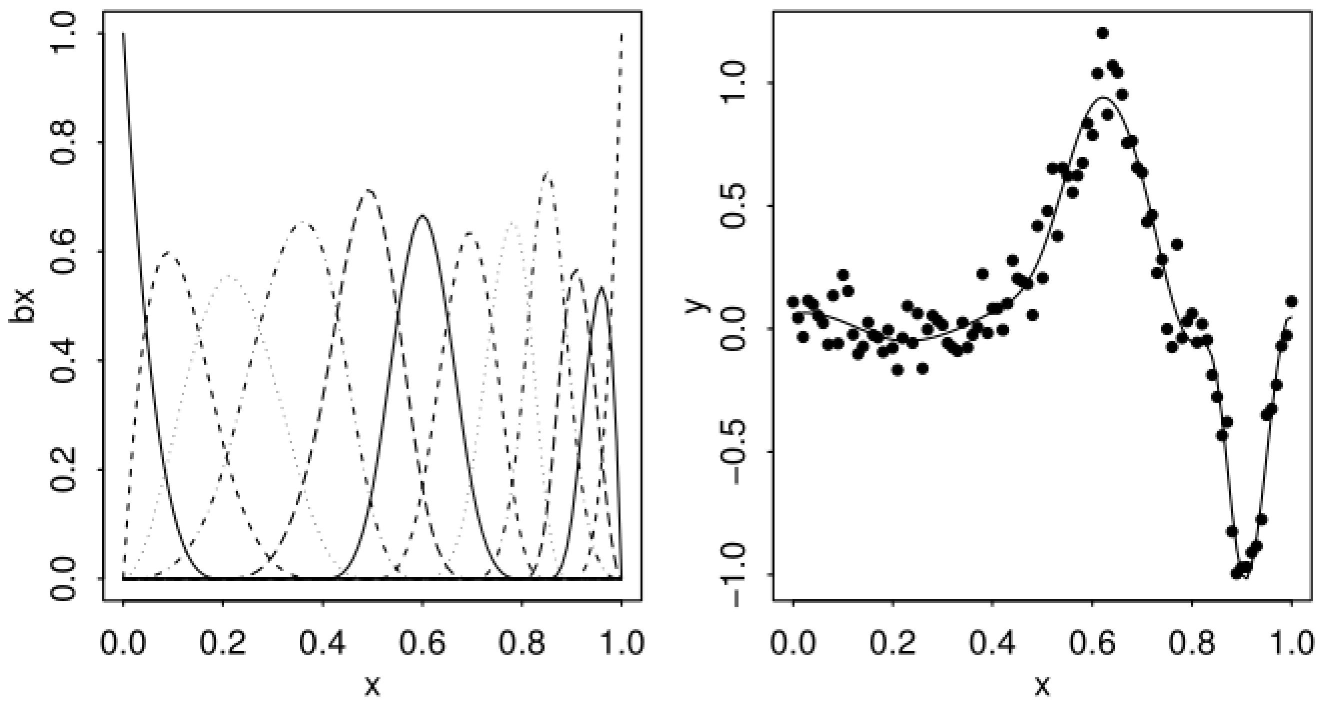


Figure 9.6 Cubic spline basis function on the left, cubic spline fit to the data on the right.

線性模型

Variable 1 x_1	Variable 2 x_2	…..	Variable m x_m	Response y
x_{11}	x_{12}	$\cdots$	x_{1m}	y_1
x_{21}	x_{22}	$\cdots$	x_{2m}	y_2
x_{31}	x_{32}	$\cdots$	x_{3m}	y_3
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
x_{n1}	x_{n2}	$\cdots$	x_{nm}	y_n

n data points

1 response variable
dependent variable
output variable

m explanation variables
predictors
independent variables
inputs
regressors
factors

- General form:

$$y = \sum_{j=0}^{p} \beta_j g_j(x_1, \dots, x_m) + \varepsilon$$

估計參數

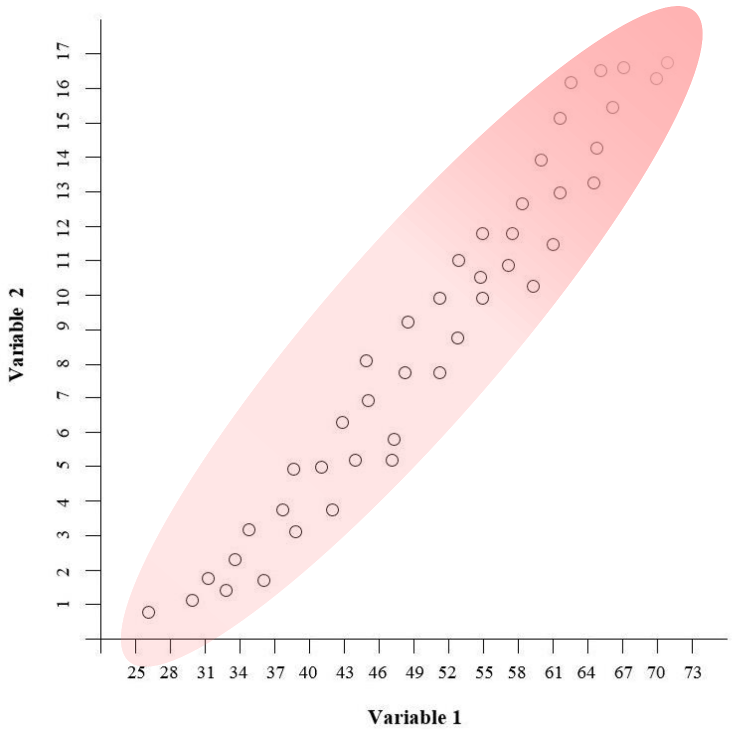
- How to estimate $\boldsymbol{\beta}$ from the data?

$$\text{Minimize} \quad \sum \left\{ y - \sum_{j=0}^{p} \beta_j g_j(x_1, \ldots, x_m) \right\}^2$$

- Matrix notation: $\boldsymbol{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$
- Least squares estimator: $\widehat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{y}$
- $\mathrm{Var}\left(\widehat{\boldsymbol{\beta}}\right) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$

共線性

- $\mathrm{Var}(\widehat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$
- 共線性 (collinearity)



https://www.wikiwand.com/zh-hk/%E5%A4%9A%E9%87%8D%E5%85%B1%E7%BA%BF%E6%80%A7

共線性

- $\mathrm{Var}(\widehat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$
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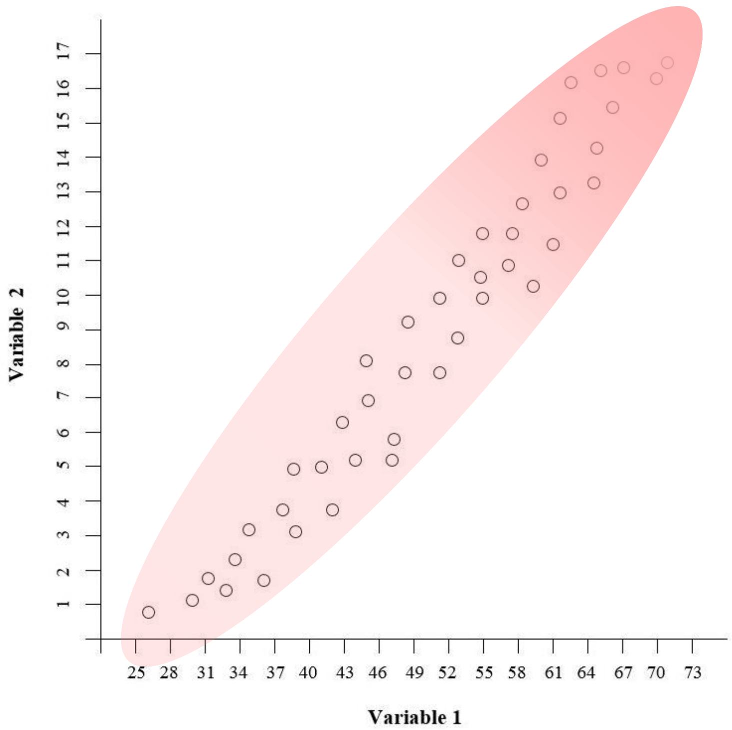


x_1	x_2	Y
⋮	⋮	⋮
⋮	⋮	⋮

資料不足以區分

1. x_1 vs. Y
2. x_2 vs. Y
3. (x_1, x_2) vs. Y

https://www.wikiwand.com/zh-hk/%E5%A4%9A%E9%87%8D%E5%85%B1%E7%BA%BF%E6%80%A7

創造共線性

- Data: Housing Values in Suburbs of Boston
  - Data size: 506
  - *tax*: full-value property-tax rate per \$10,000.
  - …
  - *medv*: median value of owner-occupied homes in \$1000s

```
> library(ISLR2)
> head(Boston)
     crim zn indus chas   nox    rm  age    dis rad tax ptratio lstat medv
1 0.00632 18  2.31    0 0.538 6.575 65.2 4.0900   1 296    15.3  4.98 24.0
2 0.02731  0  7.07    0 0.469 6.421 78.9 4.9671   2 242    17.8  9.14 21.6
3 0.02729  0  7.07    0 0.469 7.185 61.1 4.9671   2 242    17.8  4.03 34.7
4 0.03237  0  2.18    0 0.458 6.998 45.8 6.0622   3 222    18.7  2.94 33.4
5 0.06905  0  2.18    0 0.458 7.147 54.2 6.0622   3 222    18.7  5.33 36.2
6 0.02985  0  2.18    0 0.458 6.430 58.7 6.0622   3 222    18.7  5.21 28.7
```

```
> summary(lm(medv~scale(tax), Boston))

Call:
lm(formula = medv ~ scale(tax), data = Boston)

Residuals:
    Min      1Q  Median      3Q     Max 
-14.091  -5.173  -2.085   3.158  34.058 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  22.5328     0.3616   62.32   <2e-16 ***
scale(tax)   -4.3092     0.3619  -11.91   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 8.133 on 504 degrees of freedom
Multiple R-squared:  0.2195,	Adjusted R-squared:  0.218 
F-statistic: 141.8 on 1 and 504 DF,  p-value: < 2.2e-16
```

```
> summary(lm(medv~s

Call:
lm(formula = medv ~
    data = Boston)

Residuals:
    Min      1Q   M
-13.821  -5.115  -

Coefficients:
                                   Estimate Std. Error t value Pr(>|t|)    
(Intercept)                         22.5635     0.3616  62.402   <2e-16 ***
scale(tax)                         559.4436   360.9669   1.550    0.122    
I(scale(tax) + rnorm(506, sd = 0.001)) -563.7152   360.9427  -1.562    0.119    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 8.122 on 503 degrees of freedom
Multiple R-squared:  0.2233,	Adjusted R-squared:  0.2202 
F-statistic:  72.3 on 2 and 503 DF,  p-value: < 2.2e-16
```

$(\mathbf{X}^T\mathbf{X})^{-1}$ not exist

```
> summary(lm(medv~I(scale(tax))+scale(tax), Boston))

Call:
lm(formula = medv ~ I(scale(tax)) + scale(tax), data = Boston)

Residuals:
    Min      1Q  Median      3Q     Max 
-14.091  -5.173  -2.085   3.158  34.058 

Coefficients: (1 not defined because of singularities)
              Estimate Std. Error t value Pr(>|t|)    
(Intercept)    22.5328     0.3616   62.32   <2e-16 ***
I(scale(tax))  -4.3092     0.3619  -11.91   <2e-16 ***
scale(tax)          NA         NA      NA       NA    
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 8.133 on 504 degrees of freedom
Multiple R-squared:  0.2195,	Adjusted R-squared:  0.218 
F-statistic: 141.8 on 1 and 504 DF,  p-value: < 2.2e-16
```

```
> summary(lm(med

Call:
lm(formula = med

Residuals:
    Min      1Q
-14.091  -5.173

Coefficients: (1
              Estimate Std. Error t value Pr(>|t|)    
(Intercept)    22.5328     0.3616   62.32   <2e-16 ***
scale(tax)     -4.3092     0.3619  -11.91   <2e-16 ***
I(scale(tax))       NA         NA      NA       NA    
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 8.133 on 504 degrees of freedom
Multiple R-squared:  0.2195,	Adjusted R-squared:  0.218 
F-statistic: 141.8 on 1 and 504 DF,  p-value: < 2.2e-16
```

找線性相依

- **Collinearity** can be diagnosed by computing the eigenvalues of $\mathbf{X}^T\mathbf{X}$ (or the singular values of $\mathbf{X}$)

```
> X = model.matrix(lm(medv~scale(tax)+I(scale(tax)+rnorm(506, sd=0.001)), Boston))
> eigen(t(X)%*%X)
eigen() decomposition
$values
[1] 1.009948e+03 5.060000e+02 2.450108e-04

$vectors
              [,1]         [,2]          [,3]
[1,] -1.574971e-05 1.000000e+00 -1.568665e-05
[2,]  7.071250e-01 2.222887e-05  7.070886e-01
[3,]  7.070886e-01 4.401984e-08 -7.071250e-01
```

```
> svd(X)$d
[1] 31.77967612 22.49444376  0.01565282
> svd(X)$v
              [,1]         [,2]          [,3]
[1,]  1.574971e-05 1.000000e+00  1.568665e-05
[2,] -7.071250e-01 2.222887e-05 -7.070886e-01
[3,] -7.070886e-01 4.401984e-08  7.071250e-01
```

$(X^TX)\cdot u \approx 0\cdot u$

$\Rightarrow u^T(X^TX)u \approx 0$

$\Rightarrow (Xu)^T(Xu) \approx 0$

$\Rightarrow X\cdot u \approx 0 \Rightarrow \begin{bmatrix} | & | & | & \cdots & | \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_p \end{bmatrix} \approx 0$

實驗設計

- 預防勝於治療
- 如何預防：妥善規劃該如何收集數據
- 數據品質高，後續的資料分析才輕鬆
- 抽樣調查、實驗設計

實驗設計

- 做實驗常見嗎？
  - 神農嘗百草、費雪的茶和牛奶實驗、先加牛奶還是麥片

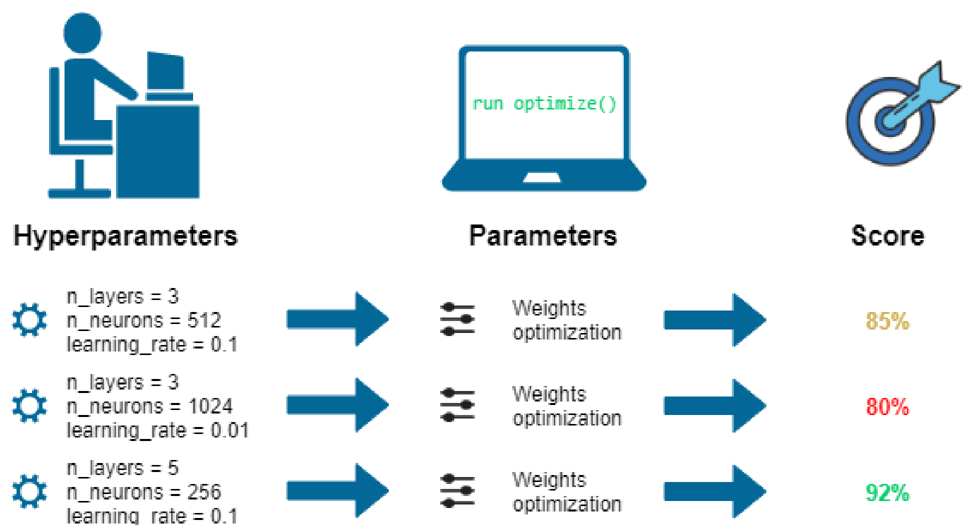
- 妥善規劃實驗重要嗎？
  - 釐清***因子*(*factor*)**與***反應變數*(*response*)**的關聯

- 為什麼要做實驗？
  - 比比看誰最棒 (treatment comparisons)
  - **因子篩選 (factor screening)**
  - 探索黑盒子 (response surface exploration)
  - 系統最佳化 (system optimization)
  - 系統穩健化 (system robustness)

- <u>Various types of experiments:</u>

https://bitesizebio.com/7358/8-steps-to-more-successful-experiments/

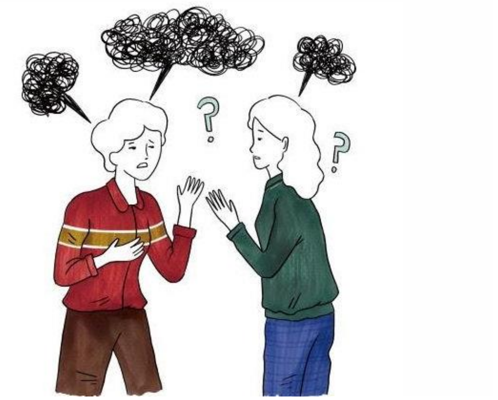
https://www.facebook.com/photo/?fbid=649818645438315&set=pcb.649819665438213



https://www.kdnuggets.com/2020/02/practical-hyperparameter-optimization.html

實驗設計

- 七大手法
  - State Objective
  - Choose Response
  - Choose Factors and Levels
  - Choose Experimental Plan
  - Perform the Experiment
  - Analyze the Data
  - Draw Conclusions and Make Recommendations



https://www.cheers.com.tw/article/article.action?id=5092364

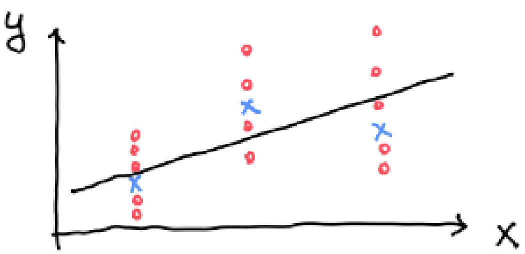
用對方聽得懂的語言，來回反覆溝通，確認雙方需求！

實驗設計

- An ***experimental unit*** (***實驗單位***) refers to a basic unit to which a treatment is applied.

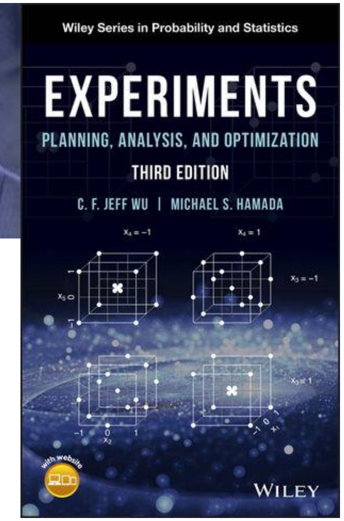
- A ***treatment*** (***處理***) is a factor-level combination applied to the experimental units

- 三大原則
  - Replication
  - Randomization
  - Blocking

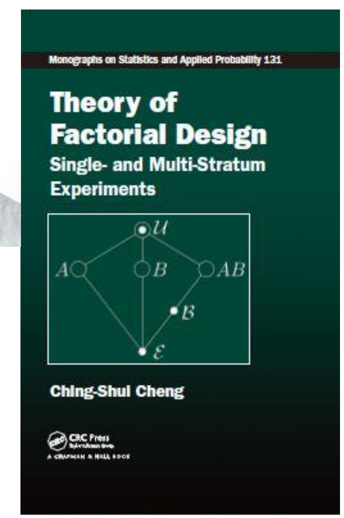


- Multi-stratum: **multiple groups of blocked units**

- C. F. Jeff Wu (吳建福教授)
  - 中央研究院院士 (2000)
  - ISyE, Georgia Tech
  - 美國國家工程研究院院士
  - 吳建福教授訪談

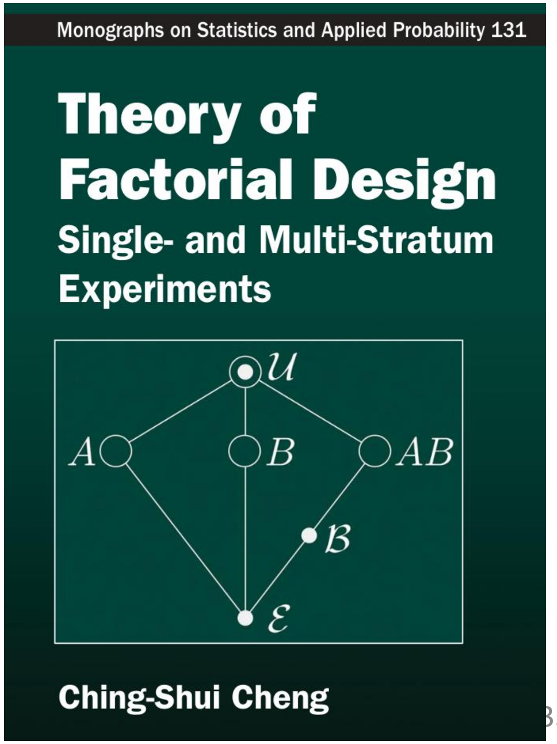


- Ching-Shui Cheng (鄭清水教授)
  - 中央研究院院士 (2016)
  - Stat. Dept., UC Berkeley
  - 我認識一位傳奇鄭清水--黃文璋教授著
  - 清華校史館
  - 中研院新科院士



Outline

- Data collection & its importance
- Factorial design (因子設計)
- Multi-stratum factorial design



完全因子設計

- **Full factorial design**: factorial experiment with all level combinations of factors as the treatments
- 2^k **full factorial design** consists of all 2^k combinations of the k factors taking on two levels

Mutually orthogonal

A	B	C
-	-	-
+	-	-
-	+	-
+	+	-
-	-	+
+	-	+
-	+	+
+	+	+

完全/部分因子設計

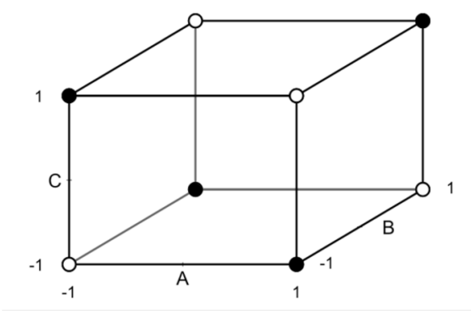
- **Full factorial design**: factorial experiment with all level combinations of factors as the treatments
- 2^k **full factorial design** consists of all 2^k combinations of the k factors taking on two levels

Mutually orthogonal

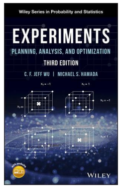
A	B	C
-	-	-
+	-	-
-	+	-
+	+	-
-	-	+
+	-	+
-	+	+
+	+	+

A	B	C	A*B*C
+	-	-	+
-	+	-	+
-	-	+	+
+	+	+	+

$$I = ABC$$



2^{3-1} (regular) fractional factorial design



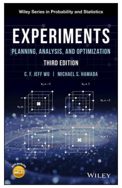
http://www.stat.nthu.edu.tw/~swcheng/Teaching/stat5510/index.php

Table 4.1 Design Matrix and Thickness Data, Adapted Epitaxial Layer Growth Experiment

Run	Factor A	B	C	D	Thickness						$\bar{y}$	s^2	$\ln s^2$
1	−	−	−	+	14.506	14.153	14.134	14.339	14.953	15.455	14.59	0.270	−1.309
2	−	−	−	−	12.886	12.963	13.669	13.869	14.145	14.007	13.59	0.291	−1.234
3	−	−	+	+	13.926	14.052	14.392	14.428					
4	−	−	+	−	13.758	13.992	14.808	13.554					
5	−	+	−	+	14.629	13.940	14.466	14.538					
6	−	+	−	−	14.059	13.989	13.666	14.706					
7	−	+	+	+	13.800	13.896	14.887	14.902					
8	−	+	+	−	13.707	13.623	14.210	14.042					
9	+	−	−	+	15.050	14.361	13.916	14.431					
10	+	−	−	−	14.249	13.900	13.065	13.143					
11	+	−	+	+	13.327	13.457	14.368	14.405					
12	+	−	+	−	13.605	13.190	13.695	14.259	14.428	14.223	13.90	0.229	−1.474
13	+	+	−	+	14.274	13.904	14.317	14.754	15.188	14.923	14.56	0.227	−1.483
14	+	+	−	−	13.775	14.586	14.379	13.775	13.382	13.382	13.88	0.253	−1.374
15	+	+	+	+	13.723	13.914	14.913	14.808	14.469	13.973	14.30	0.250	−1.386
16	+	+	+	−	14.031	14.467	14.675	14.252	13.658	13.578	14.11	0.192	−1.650

Table 4.2 Factors and Levels, Adapted Epitaxial Layer Growth Experiment

Factor	Level −	Level +
A. Susceptor-rotation method	Continuous	Oscillating
B. Nozzle position	2	6
C. Deposition temperature (°C)	1210	1220
D. Deposition time	Low	High



http://www.stat.nthu.edu.tw/~swcheng/Teaching/stat5510/index.php

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6	−	+	−	−	14.059	13.989
7	−	+	+	+	13.800	13.896
8	−	+	+	−	13.707	13.623
9	+	−	−	+	15.050	14.361
10	+	−	−	−	14.249	13.900
11	+	−	+	+	13.327	13.457
12	+	−	+	−	13.605	13.190
13	+	+	−	+	14.274	13.904
14	+	+	−	−	13.775	14.586
15	+	+	+	+	13.723	13.914
16	+	+	+	−	14.031	14.467

A			
−	−	−	+
−	−	−	−
−	−	+	+
−	−	+	−
−	+	−	+
−	+	−	−
−	+	+	+
−	+	+	−

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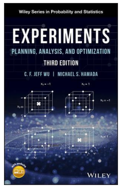
…el

	+
	Oscillating
	6
	1220
	High



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14	+	+	−	−	13.775	14.586
15	+	+	+	+	13.723	13.914
16	+	+	+	−	14.031	14.467

A	*B*		
−	−	−	+
−	−	−	−
−	−	+	+
−	−	+	−
+	+	−	+
+	+	−	−
+	+	+	+
+	+	+	−

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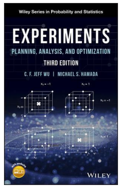

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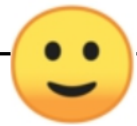

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14	+	+	−	−	13.775	14.586
15	+	+	+	+	13.723	13.914
16	+	+	+	−	14.031	14.467

$A \times B$		C	
−	−	+	+
−	−	+	−
−	+	−	+
−	+	−	−
+	−	−	+
+	−	−	−
+	+	+	+
+	+	+	−

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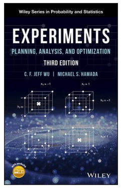
Oscillating
6
1220
High



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13	+	+	−	+	14.274	13.904
14	+	+	−	−	13.775	14.586
15	+	+	+	+	13.723	13.914
16	+	+	+	−	14.031	14.467

$A \times B \times C$ | D

−	−	−	−
−	−	+	+
−	+	−	+
−	+	+	−
+	−	−	+
+	−	+	−
+	+	−	−
+	+	+	+

xial Layer
el
+
Oscillating
6
1220
High

- Why 2^{k}? Why not 3^{k}, 4^{k}, 5^{k}, 6^{k},…?
  - Cost consideration
  - Objective: Screen out inactive factors
  - At an initial stage, a large number of factors involved.

- What input-output relationship can an s-level factor represent?
  - Linear effect ($s = 2$), quadratic effect ($s = 3$)

- Identify factors ➔ Screen out inactive factors using a 2^{k} factorial design ➔ Response surface exploration

- Which is more severe? (<u>miss active factors</u> or <u>include inactive factors</u>)

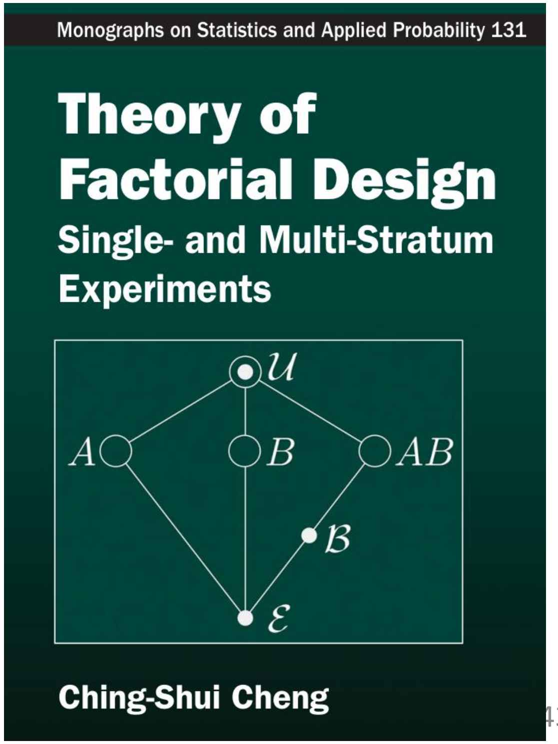
- **Effect Hierarchy Principle**: Lower-order effects are more likely to be important than higher-order effects; effects of the same order are equally likely to be important
  - An empirical principle whose validity has been confirmed in many real experiments
  - Higher-order interactions are more difficult to interpret or justify physically.

- **Effect Sparsity Principle**: The number of relatively important effects in a factorial experiment is small.
  - Based on empirical evidence observed in many investigations, the variation exhibited in the data is primarily attributed to a few effects

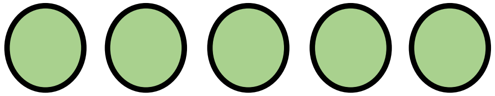
- **Effect Heredity Principle**: In order for an interaction to be significant, at least one of its parent main effects should be significant.

Outline

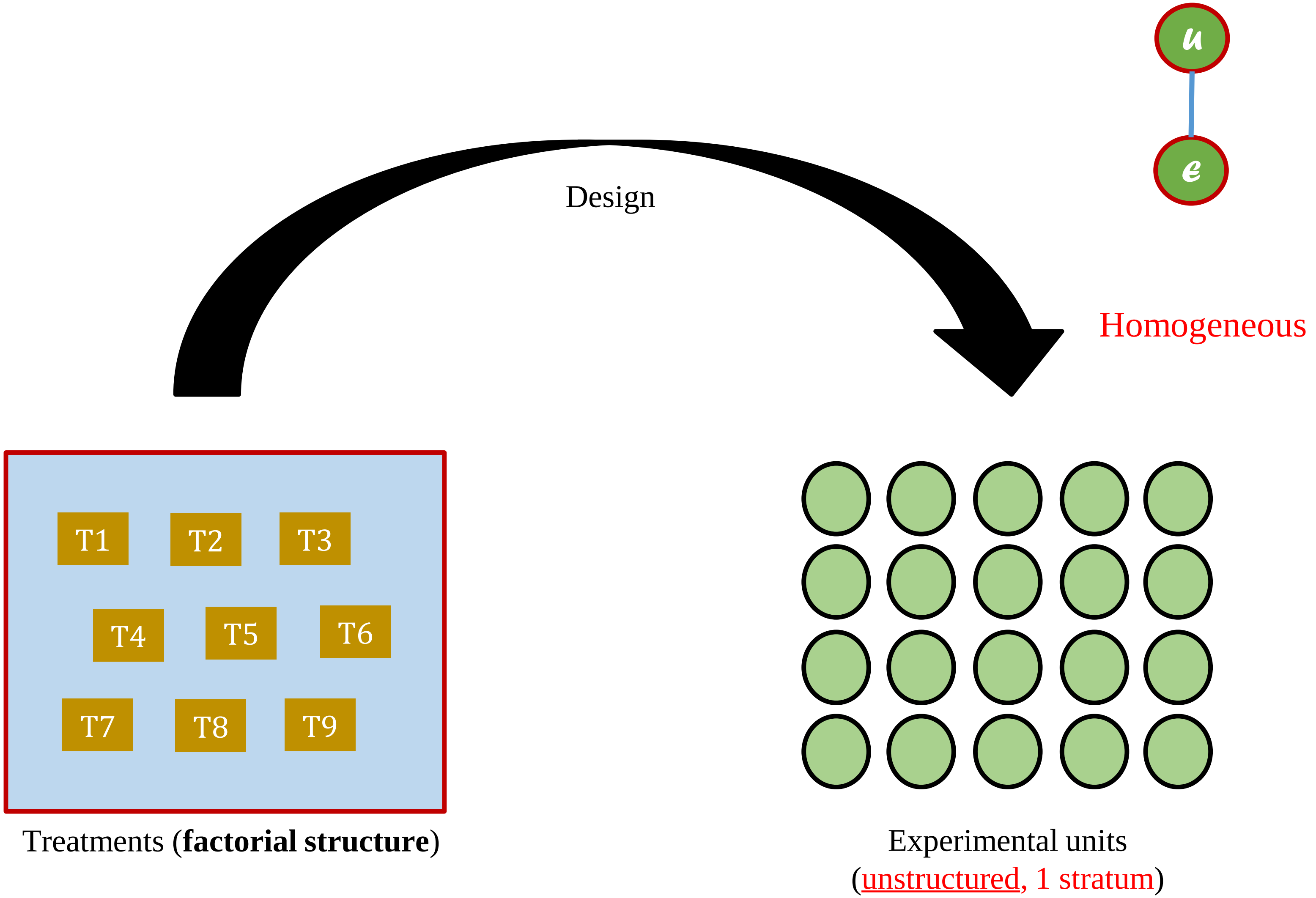
- Data collection & its importance
- Factorial design (因子設計)
- Multi-stratum factorial design



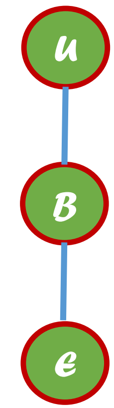
示意圖

- ***Treatments***: T1 T2 T3 T4
- ***Experimental units***: 
- ***Design***: an assignment from treatments to units

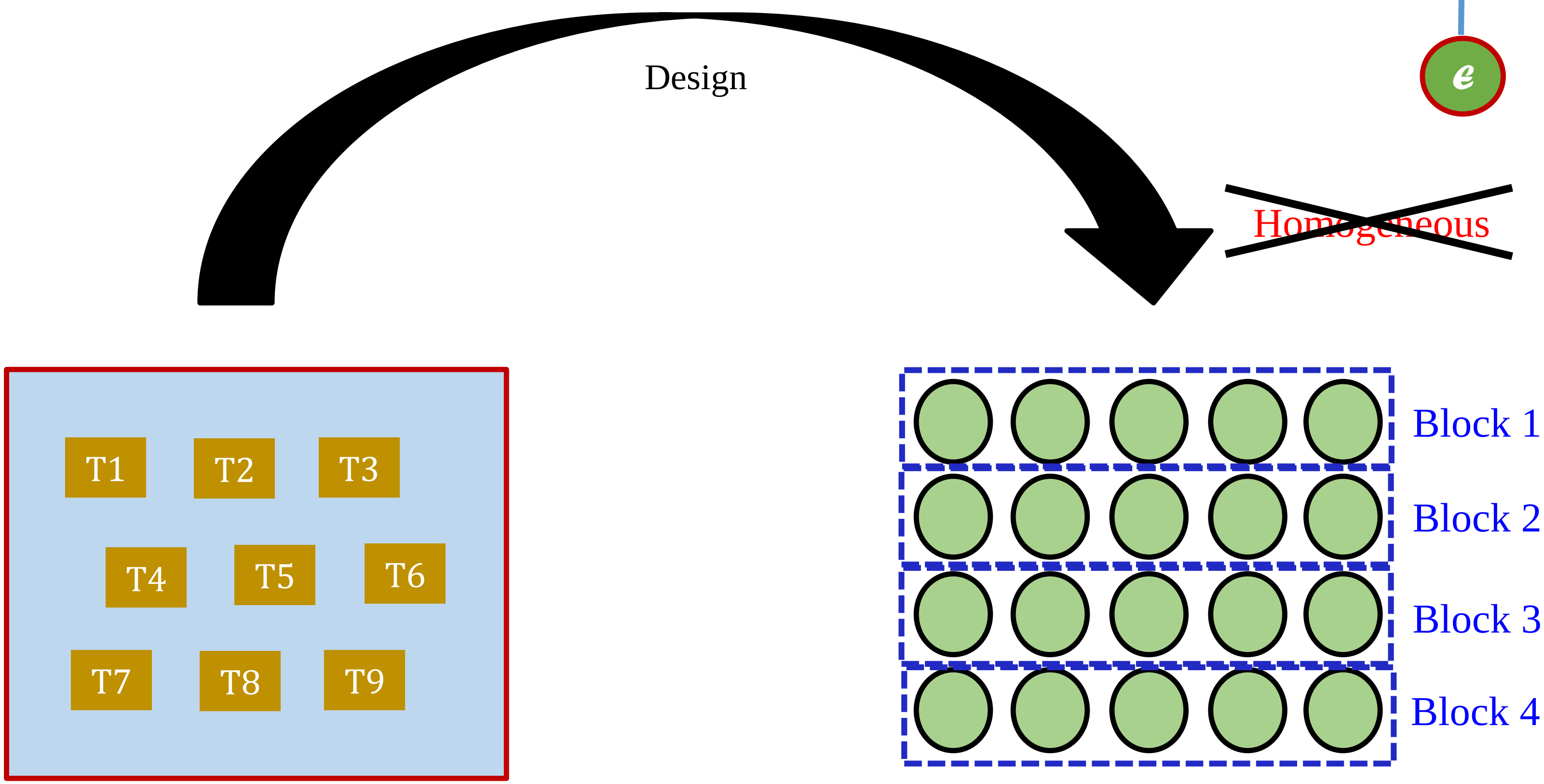
- Experimental units are unstructured with $\mathfrak{B} = \{\mathcal{U}, \mathcal{E}\}$



Block Design -- 區集設計



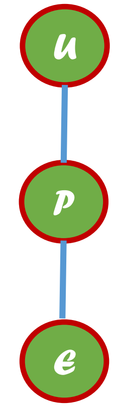
- Experimental units have $\mathfrak{B} = \{\mathcal{U}, \mathcal{B}, \mathcal{E}\}$



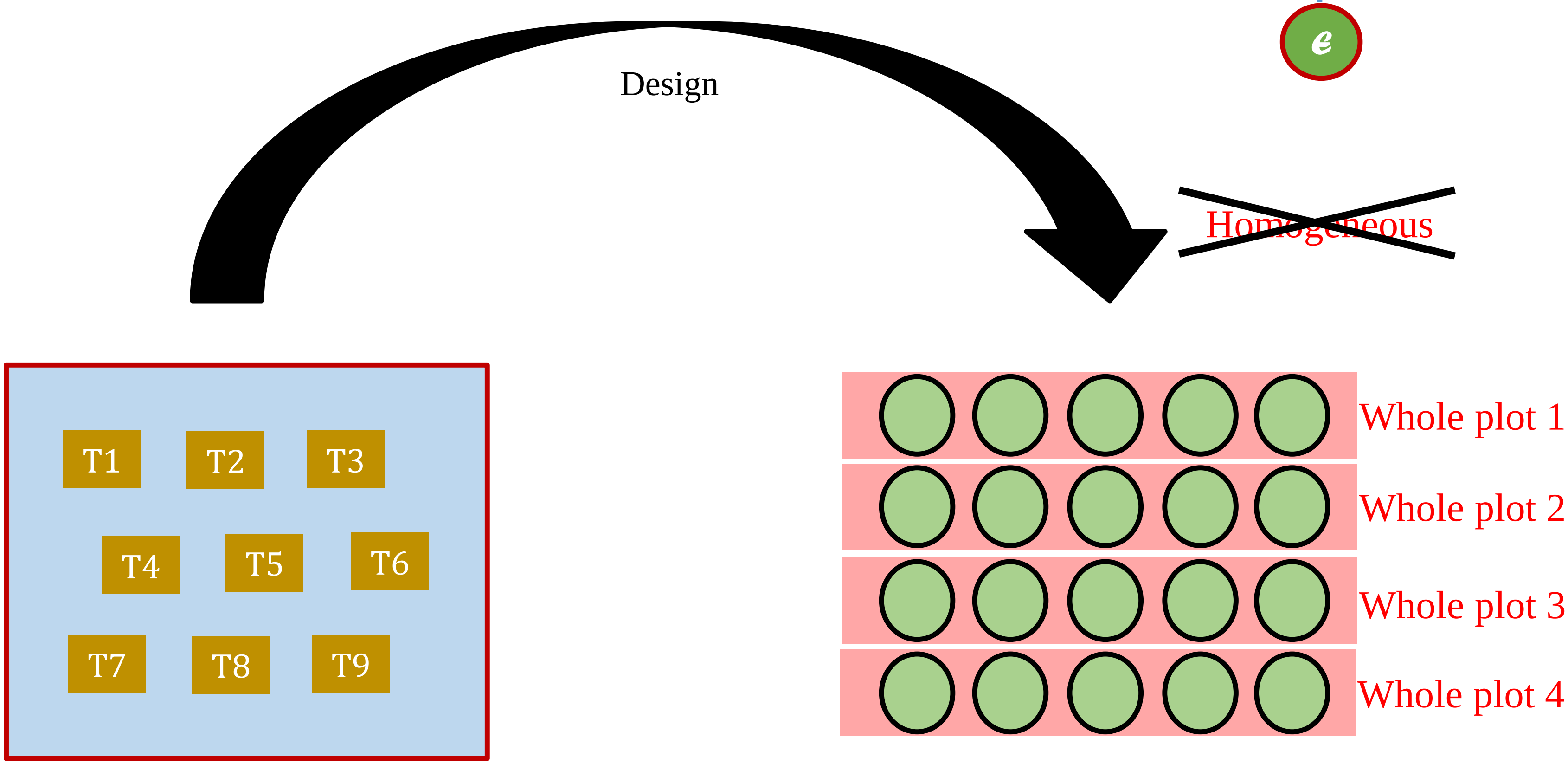
Treatments (**factorial structure**)

Experimental units
(block design , 2 strata)

Split-Plot Design



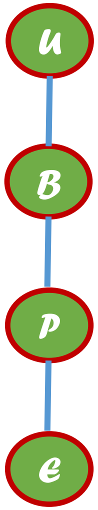
- Experimental units have $\mathfrak{B} = \{\mathcal{U}, \mathcal{P}, \mathcal{E}\}$

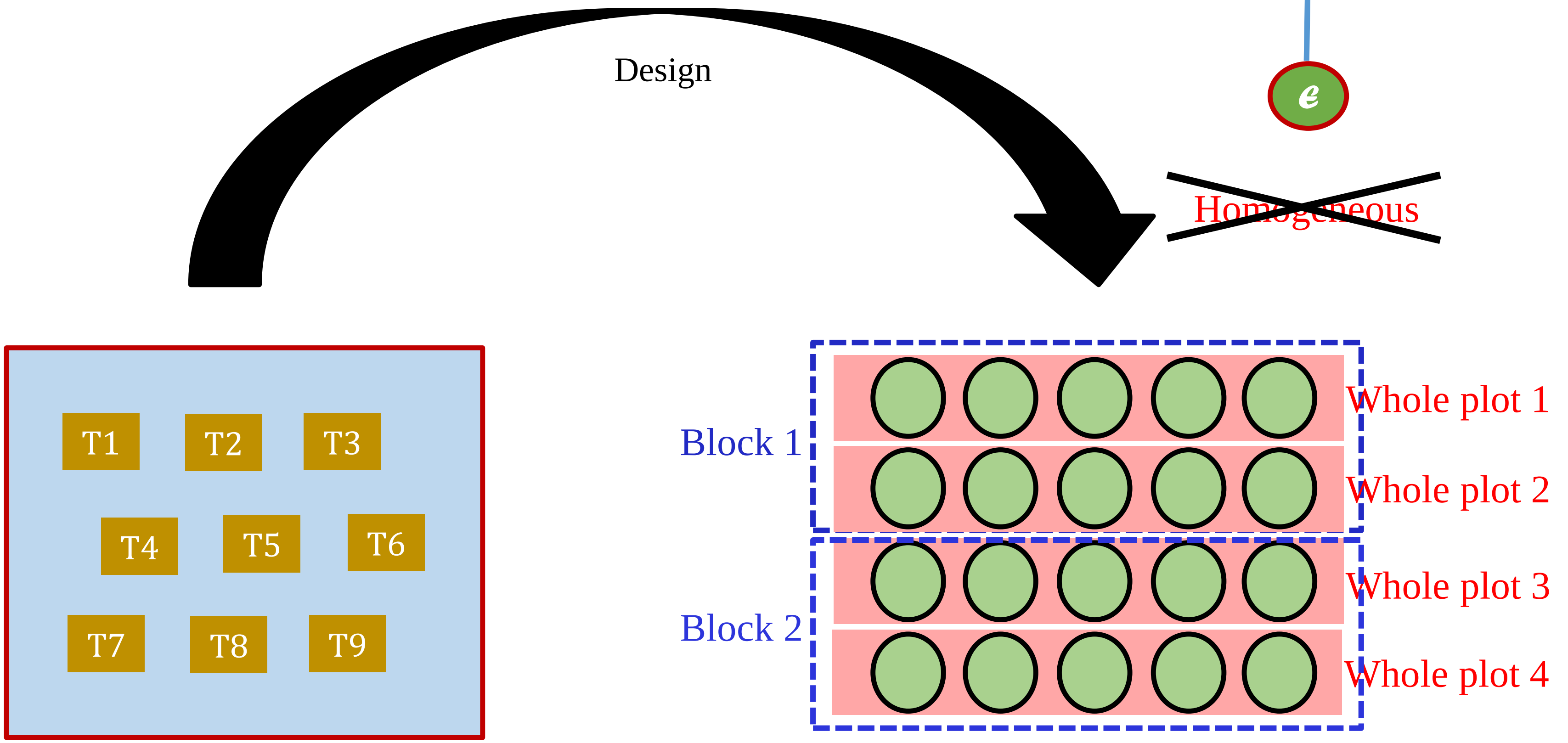


Treatments (**factorial structure**)

Experimental units
(split-plot , 2 strata)

- Experimental units have $\mathfrak{B} = \{\mathcal{U}, \mathcal{B}, \mathcal{P}, \mathcal{E}\}$





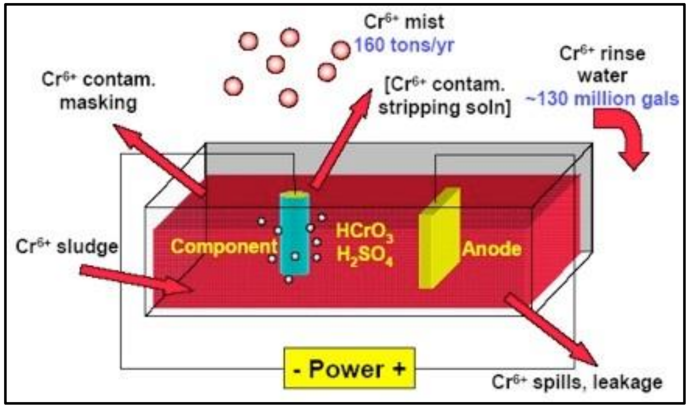
Treatments (**factorial structure**)

Experimental units
(blocked split-plot, 3 strata)

- McLeod and Brewster (2004) discussed an experiment for identifying key factors that would affect the quality of a chrome-plating process.

Chrome plating is a technique of electroplating a thin layer of chromium onto a metal object.

- Six treatment factors (each of two levels):
  - A: chrome concentration
  - B: chrome to sulfate ratio
  - C: bath temperature
  - S: etching current density
  - T: plating current density
  - U: part geometry



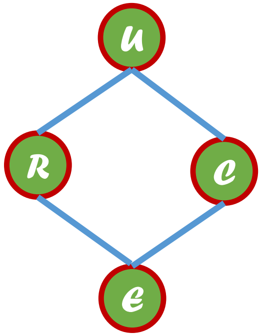
- Two responses: Numbers of pits and cracks

- The experiment is to be run on 16 days, with four days in each of four weeks. Therefore there are a total of 32 runs with the block structure (4 weeks)/(4 days)/(2 runs), and one has to choose 32 out of the $2^6=64$ treatment combinations.

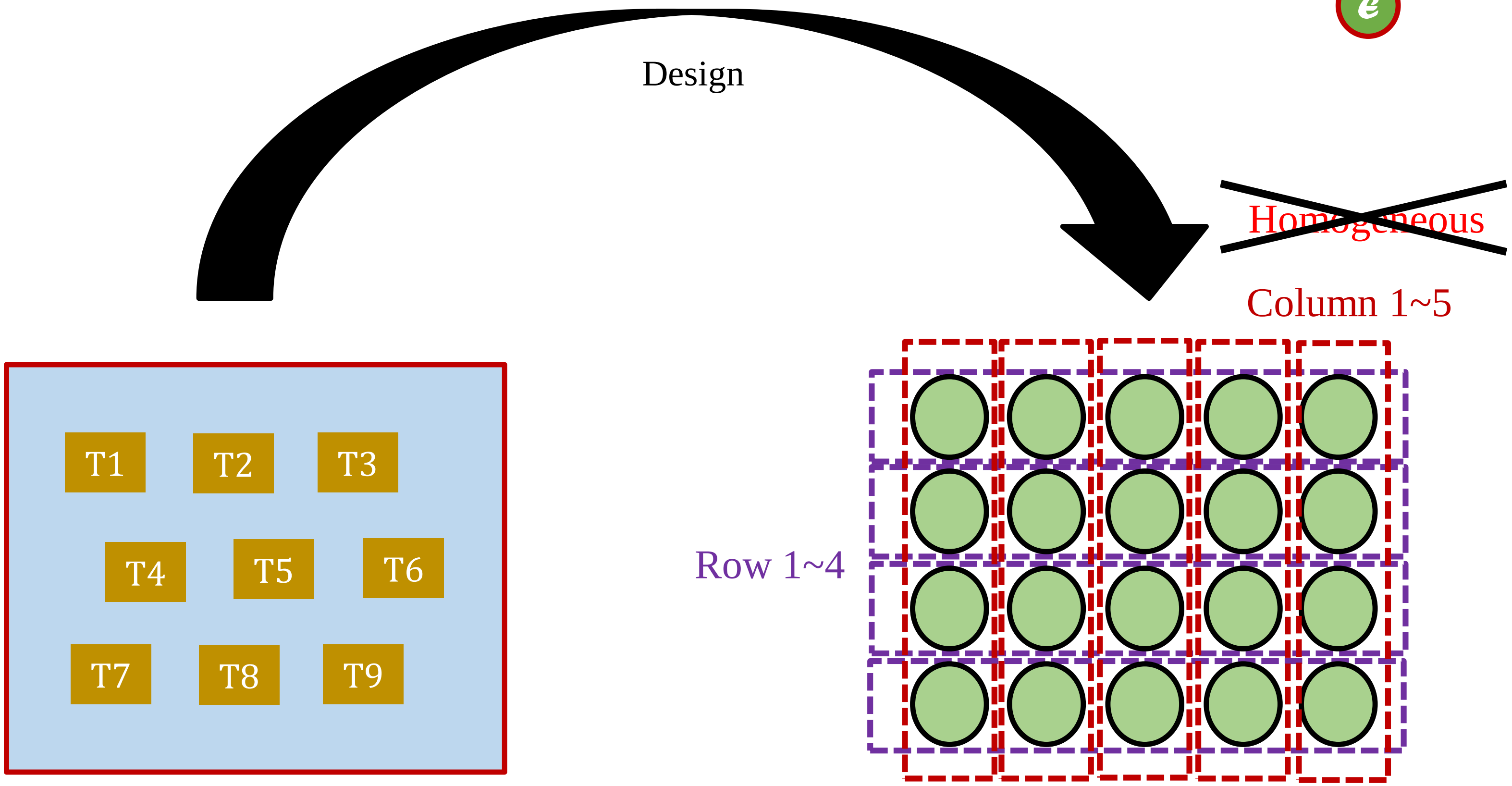
- Weeks, days, and runs can be considered as **blocks**, **whole-plots**, and **subplots**, respectively.

- The three factors A, B, and C must have constant levels on the two experimental runs on the same day, and are called **whole-plot treatment factors**. The other three factors S, T, and U are not subject to this constraint and are called **subplot treatment factors**.

Strip-Plot Design



- Experimental units have $\mathfrak{B} = \{\mathcal{U}, \mathcal{R}, \mathcal{C}, \mathcal{E}\}$

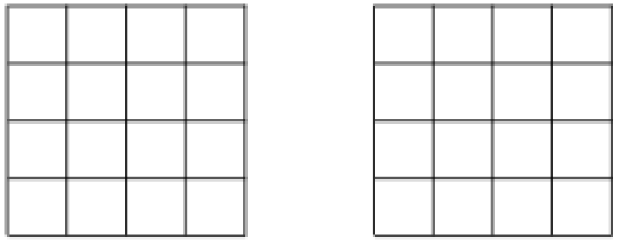


Treatments (**factorial structure**)

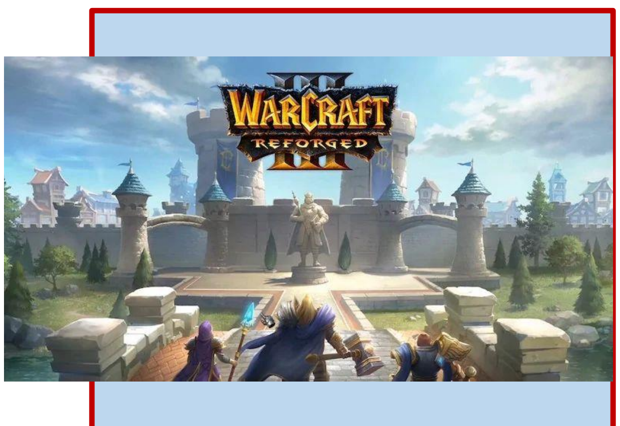
Experimental units
(Strip-plot , 3 strata)

- Miller (1997) described a laundry experiment for investigating methods of reducing the wrinkling of clothes.

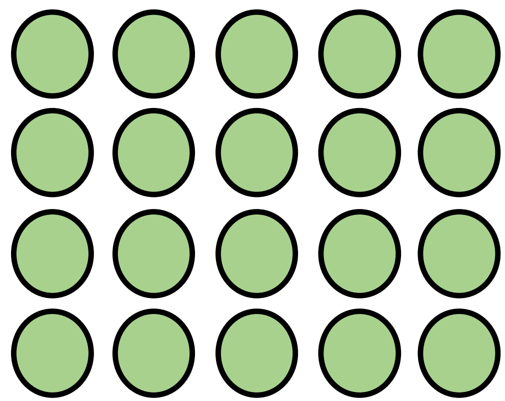
- This results in 32 experimental runs that can be thought to have the following 2/(4×4) block structure, where each cell represents a cloth sample, rows represent sets of samples that are washed together, and columns represent sets of samples that are dried together.



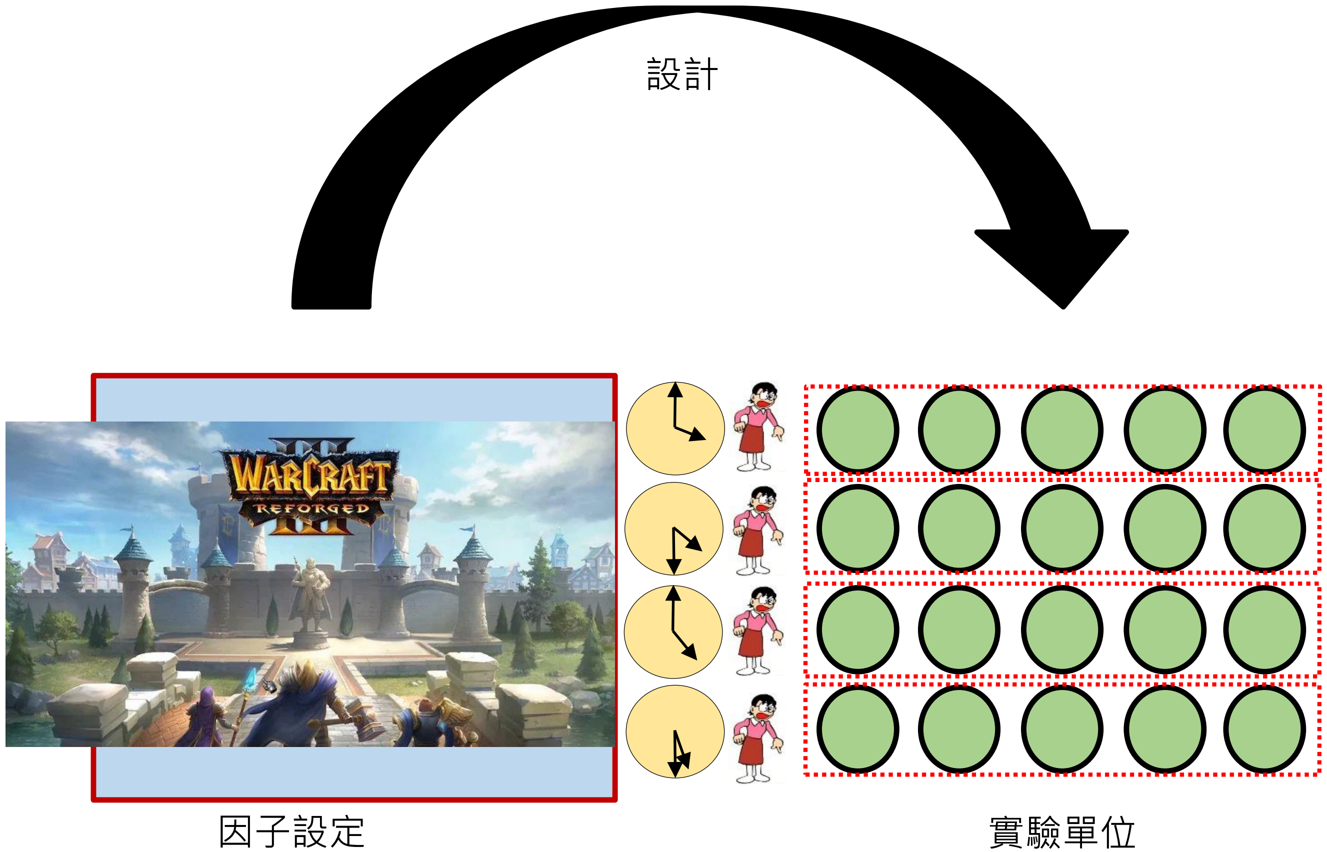
- Ten two-level treatment factors, six of which (A, B, C, D, E, F) are configurations of washers and four (S, T, U, V) are configurations of dryers. One has to choose 32 out of the $2^{10} = 1024$ treatment combinations.

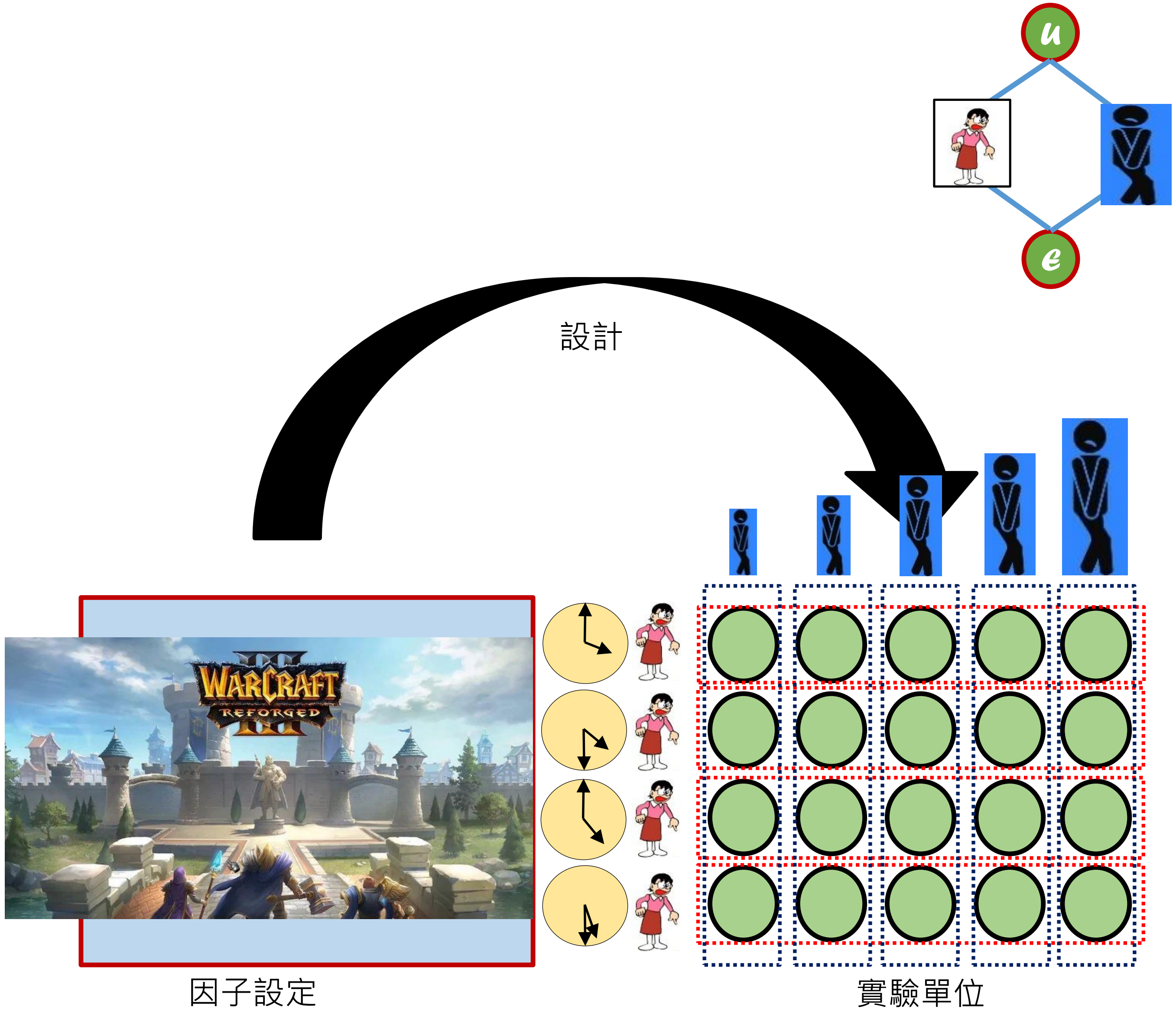


因子設定



實驗單位


設計
WARCRAFT
REFORGED
因子設定
實驗單位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設計
WARCRAFT
REFORGED
因子設定
實驗單位

The Annals of Statistics
2018, Vol. 46, No. 4, 1779–1806
https://doi.org/10.1214/17-AOS1603

Q: 給定實驗成本下，如何衡量不同的「多階層因子設計」的優劣？

A BAYESIAN APPROACH TO THE SELECTION OF TWO-LEVEL MULTI-STRATUM FACTORIAL DESIGNS

BY MING-CHUNG CHANG AND CHING-SHUI CHENG

Academia Sinica and University of California, Berkeley

In a multi-stratum factorial experiment, there are multiple error terms (strata) with different variances that arise from complicated structures of the experimental units. For unstructured experimental units, minimum aberration is a popular criterion for choosing regular fractional factorial designs. One difficulty in extending this criterion to multi-stratum factorial designs is that the formulation of a word length pattern based on which minimum aberration is defined requires an order of desirability among the relevant words, but a natural order is often lacking. Furthermore, a criterion based only on word length patterns does not account for the different stratum variances. Mitchell, Morris and Ylvisaker [*Statist. Sinica* **5** (1995) 559–573] proposed a framework for Bayesian factorial designs. A Gaussian process is used as the prior for the treatment effects, from which a prior distribution of the factorial effects is induced. This approach is applied to study optimal and efficient multi-stratum factorial designs. Good surrogates for the Bayesian criteria that can be related to word length and generalized word length patterns for regular and nonregular designs, respectively, are derived. A tool is developed for eliminating inferior designs and reducing the designs that need to be considered without requiring any knowledge of stratum variances. Numerical examples are used to illustrate the theory in several settings.

Model

N experimental units with the block structure $\mathfrak{B} = \{\mathcal{F}_0, \mathcal{F}_1, ..., \mathcal{F}_m\}$

Let $\mathcal{F}_0 = \mathcal{U}$ and $\mathcal{F}_m = \mathcal{E}$

n two-level treatment factors, two levels: -1 and 1

Factorial effects: $\beta_S, S \subseteq \{1, ..., n\}$; $\boldsymbol{\beta} = (\beta_\phi, \beta_{\{1\}}, ..., \beta_{\{1,...,n\}})^T$

Model

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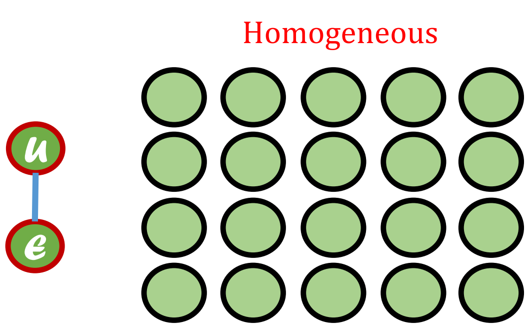
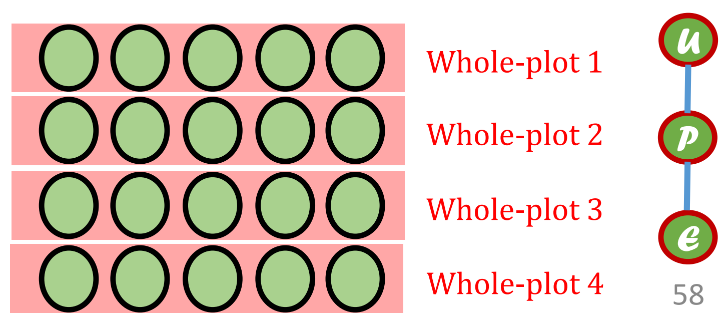
Factorial effects: $\beta_S, S \subseteq \{1, \ldots, n\}$; $\boldsymbol{\beta} = (\beta_\phi, \beta_{\{1\}}, \ldots, \beta_{\{1,\ldots,n\}})^T$

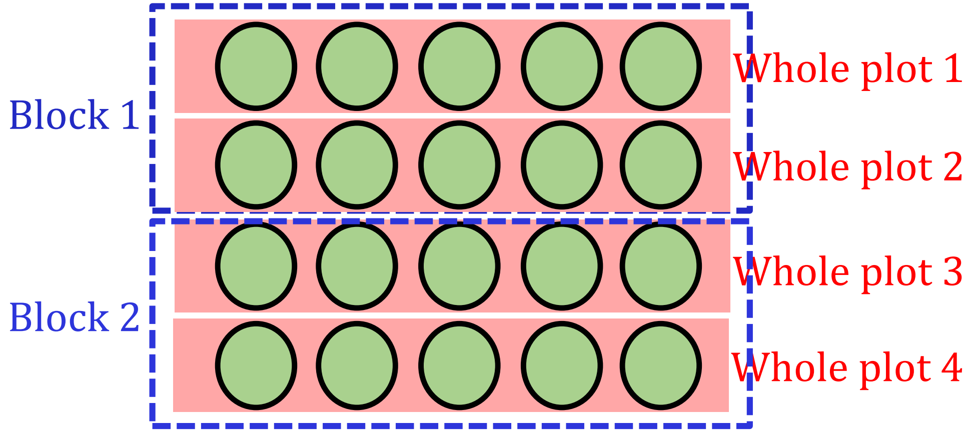
$$\mathbf{y} = \mathbf{U}\boldsymbol{\beta} + \textstyle\sum_{i=0}^{m} \mathbf{X}_{\mathcal{F}_i}\boldsymbol{\gamma}^{\mathcal{F}_i}$$

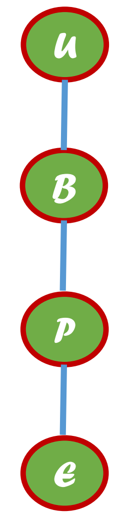
$\mathbf{U}$ is an $N \times 2^n$ full model matrix and $\boldsymbol{\gamma}^{\mathcal{F}_i} = (\gamma_1^{\mathcal{F}_i}, \ldots, \gamma_{n_{\mathcal{F}_i}}^{\mathcal{F}_i})^T \sim \mathrm{N}(\mathbf{0}, \sigma_{\mathcal{F}_i}^2 \mathbf{I}_{n_{\mathcal{F}_i}})$

$\mathbf{X}_{\mathcal{F}}$: an $N \times n_{\mathcal{F}}$ *incidence* matrix with 0's and 1's such that the (i,j)-th entry is 1 if the i-th unit has level j of $\mathcal{F}$









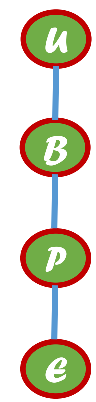
Experimental units
(blocked split-plot, 3 strata)

$$\boldsymbol{y} = \mathbf{U}\boldsymbol{\beta} + \mathbf{1}_{20}\underset{\sigma^2_{\mathcal{U}}}{\underset{\updownarrow}{\gamma^{\mathcal{U}}}} + \begin{bmatrix} \mathbf{1}_{10} & \mathbf{0}_{10} \\ \mathbf{0}_{10} & \mathbf{1}_{10} \end{bmatrix} \underset{\sigma^2_{\mathcal{B}}}{\underset{\updownarrow}{\begin{bmatrix} \gamma_1^{\mathcal{B}} \\ \gamma_2^{\mathcal{B}} \end{bmatrix}}} + \begin{bmatrix} \mathbf{1}_5 & \mathbf{0}_5 & \mathbf{0}_5 & \mathbf{0}_5 \\ \mathbf{0}_5 & \mathbf{1}_5 & \mathbf{0}_5 & \mathbf{0}_5 \\ \mathbf{0}_5 & \mathbf{0}_5 & \mathbf{1}_5 & \mathbf{0}_5 \\ \mathbf{0}_5 & \mathbf{0}_5 & \mathbf{0}_5 & \mathbf{1}_5 \end{bmatrix} \underset{\sigma^2_{\mathcal{P}}}{\underset{\updownarrow}{\begin{bmatrix} \gamma_1^{\mathcal{P}} \\ \gamma_2^{\mathcal{P}} \\ \gamma_3^{\mathcal{P}} \\ \gamma_4^{\mathcal{P}} \end{bmatrix}}} + \mathbf{I}_{20}\underset{\sigma^2_{\mathcal{E}}}{\underset{\updownarrow}{\boldsymbol{\gamma}^{\mathcal{E}}}}$$

Design Selection

$$B_{k,i}(d) = \frac{1}{N}\sum_{S:|S|=k} \|\mathbf{P}_{W_{\mathcal{F}_i}} \mathbf{u}_S\|^2$$

k階效應投影在$\mathcal{F}_i$上的共線性強度



$$\xi_{\mathcal{F}} = \sum_{\mathcal{G}\in\mathfrak{B}:\mathcal{G}\preceq\mathcal{F}} \frac{N}{n_{\mathcal{G}}}\sigma_{\mathcal{G}}^2$$

$\mathcal{F}$這個stratum的強度

$$\Rightarrow \left(\sum_{i=0}^{m-1}\left(\frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}}\right)B_{1,i}(d), \ldots, \sum_{i=0}^{m-1}\left(\frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}}\right)B_{n,i}(d)\right)$$

Sequential minimization, from left to right

Theorem. A necessary and sufficient condition for a design d^* to have minimum aberration with respect to the wordlength pattern

$$W(d) = \left(\sum_{i=0}^{m-1}\left(\frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}}\right)B_{1,i}(d), \ldots, \sum_{i=0}^{m-1}\left(\frac{1}{\xi_{\mathcal{F}_m}} - \frac{1}{\xi_{\mathcal{F}_i}}\right)B_{n,i}(d)\right)$$

for all $\boldsymbol{\xi}$ is that for **each nonempty set** $\mathfrak{G} \subseteq \mathfrak{B} \setminus \{\mathcal{F}_m\}$ that satisfy

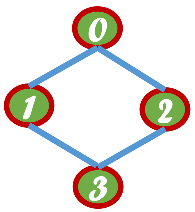
$$\mathcal{F} \in \mathfrak{G}, \mathcal{F}' \in \mathfrak{B}, \text{ and } \mathcal{F} \prec \mathcal{F}' \Rightarrow \mathcal{F}' \in \mathfrak{G}, \qquad (**)$$

d^* has minimum aberration with respect to

$$W_{\mathfrak{G}}(d) = \left(\sum_{i:\mathcal{F}_i \in \mathfrak{G}} B_{1,i}(d), \ldots, \sum_{i:\mathcal{F}_i \in \mathfrak{G}} B_{n,i}(d)\right).$$

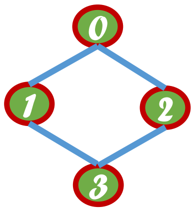
$$W_{\mathfrak{G}_1} = (B_{1,0}, B_{2,0}, \ldots, B_{n,0})$$
$$W_{\mathfrak{G}_2} = (B_{1,0} + B_{1,1}, B_{2,0} + B_{2,1}, \ldots, B_{n,0} + B_{n,1})$$

$$W_{\mathfrak{G}_1} = (B_{1,0}, B_{2,0}, ..., B_{n,0})$$
$$W_{\mathfrak{G}_2} = (B_{1,0} + B_{1,1}, B_{2,0} + B_{2,1}, ..., B_{n,0} + B_{n,1})$$

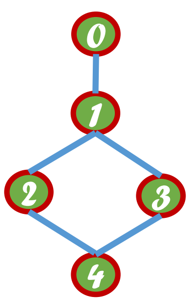


$$W_{\mathfrak{G}_1} = (B_{1,0}, B_{2,0}, ..., B_{n,0})$$
$$W_{\mathfrak{G}_2} = (B_{1,0} + B_{1,1}, B_{2,0} + B_{2,1}, ..., B_{n,0} + B_{n,1})$$
$$W_{\mathfrak{G}_3} = (B_{1,0} + B_{1,2}, B_{2,0} + B_{2,2}, ..., B_{n,0} + B_{n,2})$$
$$W_{\mathfrak{G}_4} = (B_{1,0} + B_{1,1} + B_{1,2}, B_{2,0} + B_{2,1} + B_{2,2}, ..., B_{n,0} + B_{n,1} + B_{n,2})$$

$$W_{\mathfrak{G}_1} = (B_{1,0}, B_{2,0}, ..., B_{n,0})$$
$$W_{\mathfrak{G}_2} = (B_{1,0} + B_{1,1}, B_{2,0} + B_{2,1}, ..., B_{n,0} + B_{n,1})$$



$$W_{\mathfrak{G}_1} = (B_{1,0}, B_{2,0}, ..., B_{n,0})$$
$$W_{\mathfrak{G}_2} = (B_{1,0} + B_{1,1}, B_{2,0} + B_{2,1}, ..., B_{n,0} + B_{n,1})$$
$$W_{\mathfrak{G}_3} = (B_{1,0} + B_{1,2}, B_{2,0} + B_{2,2}, ..., B_{n,0} + B_{n,2})$$
$$W_{\mathfrak{G}_4} = (B_{1,0} + B_{1,1} + B_{1,2}, B_{2,0} + B_{2,1} + B_{2,2}, ..., B_{n,0} + B_{n,1} + B_{n,2})$$



$$W_{\mathfrak{G}_1} = (B_{1,0}, B_{2,0}, ..., B_{n,0})$$
$$W_{\mathfrak{G}_2} = (B_{1,0} + B_{1,1}, B_{2,0} + B_{2,1}, ..., B_{n,0} + B_{n,1})$$
$$W_{\mathfrak{G}_3} = (B_{1,0} + B_{1,1} + B_{1,2}, B_{2,0} + B_{2,1} + B_{2,2}, ..., B_{n,0} + B_{n,1} + B_{n,2})$$
$$W_{\mathfrak{G}_4} = (B_{1,0} + B_{1,1} + B_{1,3}, B_{2,0} + B_{2,1} + B_{2,3}, ..., B_{n,0} + B_{n,1} + B_{n,3})$$
$$W_{\mathfrak{G}_5} = (B_{1,0} + B_{1,1} + B_{1,2} + B_{1,3}, B_{2,0} + B_{2,1} + B_{2,2} + B_{2,3}, ..., B_{n,0} + B_{n,1} + B_{n,2} + B_{n,3})$$

Statistica Sinica **32** (2022), 251-269
doi:https://doi.org/10.5705/ss.202019.0416

A UNIFIED FRAMEWORK FOR MINIMUM ABERRATION

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Abstract: Minimum aberration is a popular method of selecting fractional factorial designs. Numerous extensions to the original methods have benefited fields of experimental design such as multi-stratum designs, multi-group designs, and multi-platform designs. However, most of these extensions are ad hoc, developed on case-by-case bases without strong statistical justifications or a unified rationale. As such, we provide a new perspective on minimum aberration using a Bayesian approach. Our theory includes a unified framework for minimum aberration and is easily applied to many situations. Furthermore, it enables experimenters to derive their own aberration criteria. Several theoretical results and three numerical illustrations are provided.

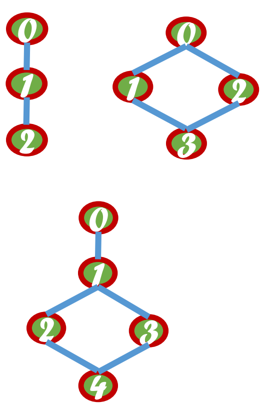
Key words and phrases: Bayesian, blocking, fractional factorial, mixed-level, multi-group, multi-platform, multi-stratum, split-plot, strip-plot.

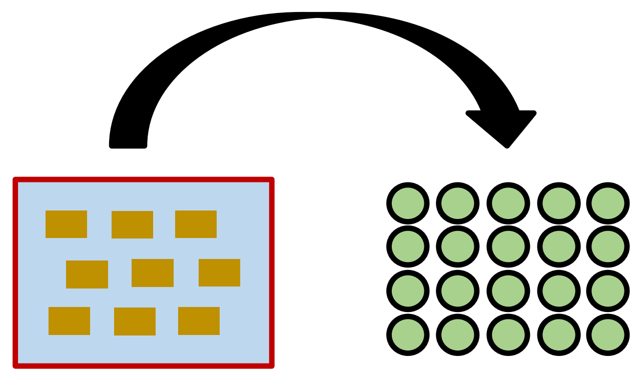
- Chang and Cheng (2018) + Chang (2022)
  - Factors
    - Mixed-level
    - Quantitative and qualitative
    - Effect hierarchy
    - Effect heredity
  - Treatments
    - Regular factorials
    - Nonregular factorials
    - Supersaturated designs
  - Experimental units
    - Block design
    - Split-plot
    - Strip-plot
    - Simple block structures
    - Orthogonal block structures

Regular		
A	B	C
+	-	-
-	+	-
-	-	+
+	+	+

Nonregular		
A	B	C
+	-	+
-	+	-
-	-	+
+	+	+

Supersaturated		
A	B	C
+	-	-
-	+	-





Summary

- 分析數據是統計科學的看家本領
- 實驗設計就是在探討如何收集高品質的數據
- 當無法主動收集資料，而只能被動接受資料時，資料品質難以控制，因此需要大數據
- 當可以有系統的收集資料時，資料品質高，因此只需要小數據

Summary

- 實驗設計有很多細目，因子設計特別適合做**因子篩選**。
- **多階層因子**設計專門處理有異質性的實驗單位
- 不同的目的有不同的實驗設計手法
  - 反應曲面探索適合用**space-filling設計**
- 溝通永遠都是統計科學家不可或缺的技能

「統計科學」擁有見微知著的本領
「實驗設計」散發挑選微量資料的美感

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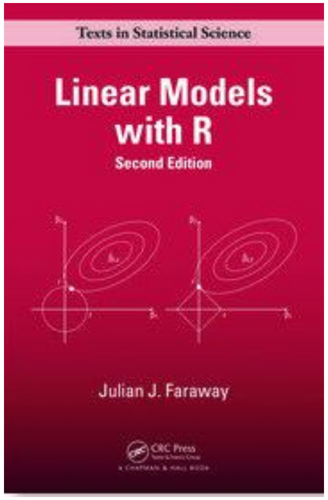

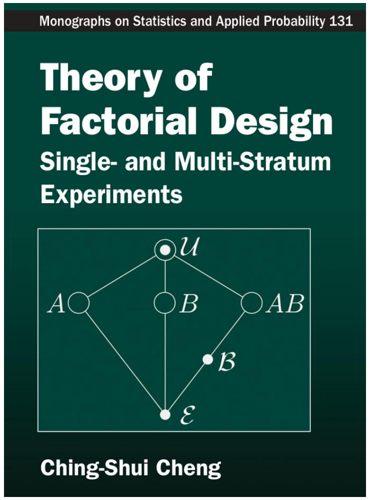

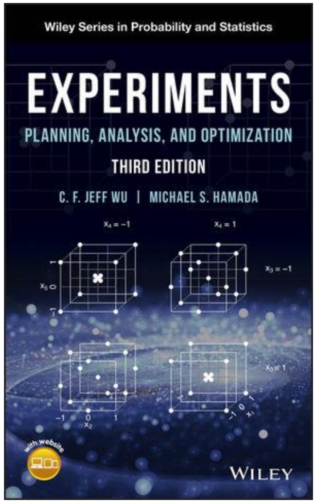

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- **Ming-Chung Chang*** (2022). A unified framework for minimum aberration, *Statistica Sinica*, 32, 251-269.

在鉻電鍍過程中，以下是與不同參數相關的術語的解釋，以及它們對鉻電鍍的意義：

A. **鉻濃度（Chrome Concentration）**：這是指電解液中的鉻離子的濃度。鉻濃度的控制對於獲得均勻和穩定的鍍層至關重要。較高的鉻濃度通常會導致更快的電鍍速度，但也可能導致鍍層失去均勻性。

B. **鉻與硫酸比例（Chrome to Sulfate Ratio）**：這是指鉻酸鹽（鉻離子）與硫酸之間的比例。適當的鉻與硫酸比例有助於維持電解液的穩定性，影響鍍層的均勻性和質量。

C. **電鍍液溫度（Bath Temperature）**：這是指電解液的溫度。溫度可以影響電鍍速度和鍍層的質量。較高的溫度通常會導致更快的電鍍速度，但可能需要更仔細的控制以避免鍍層失去均勻性。

S. **蝕刻電流密度（Etching Current Density）**：這是在電鍍過程之前進行的蝕刻階段中使用的電流密度。蝕刻用於準備基材表面，以確保鍍層附著良好。適當的蝕刻可以清除雜質和不良表面，提高鍍層的附著力。

T. **電鍍電流密度（Plating Current Density）**：這是在電鍍過程中使用的電流密度。它決定了鉻離子在基材上沉積的速率。適當的電流密度可以影響鍍層的均勻性和外觀。

U. **零件幾何形狀（Part Geometry）**：零件的形狀和幾何結構對電鍍過程和鍍層的均勻性有重要影響。複雜的幾何形狀可能導致鍍層在某些區域更難以均勻沉積。

綜合來看，這些參數在鉻電鍍過程中相互作用，影響著鍍層的質量、均勻性和附著力。合理地控制這些參數可以確保獲得所需的電鍍效果，使得鍍層在外觀、性能和耐用性方面都達到預期標準。

Regenerate