Design and analysis of experiments
Lecture 10

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Factorial designs

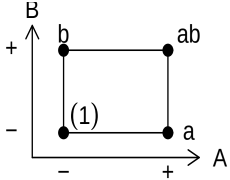
- ANOVA with k factors where each factors has the same number of levels m is called a m^k design
- The number of combinations (i.e. the number of experiments if just one replicate) is m^k:

		Number of levels		
		2	3	4
Number	2	4	9	16
of	3	8	27	64
factors	4	16	81	256

- We will look at 2^k - each factors has two levels, low (-) and high (+).
- These designs are equivalent to multivariate regression with only first order terms.

2^2 designs

	Low	High
A	( )	a
B	( )	b



- The relation between the effects and the levels can be summarised:

	I	A	B	AB
(1)	+	-	-	+
a	+	+	-	-
b	+	-	+	-
ab	+	+	+	+

- Note that column A is created by taking all rows with a and subtracting all rows without a; same for B. The interaction AB is the product of the other two columns.

Effects

- n is the number of observations in each combination.
- Let $(1), a, b, ab$ also denote the sum of the observations in that combination.
- Average: $I = \frac{(1)+a+b+ab}{4n}$
- Main effect A: $A = \frac{a+ab}{2n} - \frac{(1)+b}{2n} = \frac{-(1)+a-b+ab}{2n}$
- Main effect B: $B = \frac{b+ab}{2n} - \frac{(1)+a}{2n} = \frac{-(1)-a+b+ab}{2n}$
- Interaction: $AB = \frac{ab-a}{2n} - \frac{b-(1)}{2n} = \frac{(1)-a-b+ab}{2n}$

Contrasts

- Contrasts: $\text{Contrast}_j = 2n\text{Effect}_j$
- For example: $\text{Contrast}_A = 2nA = -(1) + a - b + ab$
- About contrasts:
  - Theoretical contrast: $\Gamma = \sum c_i \mu_i$
  - Empirical contrast: $C = \sum c_i \bar{y}_{i\bullet}$
  - Here we redefine the empirical contrast: $C = \sum c_i y_{i\bullet} = n \sum c_i \bar{y}_{i\bullet}$
- In the present case $c_i = \pm 1$
- Distribution of empirical contrasts:
  - Normally distributed.
  - Mean: $\mathbb{E}[C] = n\mathbb{E}[\sum c_i \bar{y}_{i\bullet}] = n \sum c_i \mu_i = n\Gamma$
  - Variance: $\text{Var}(C) = \sum c_i^2 \text{Var}(y_{i\bullet}) = \sum c_i^2 n\sigma^2 = N\sigma^2$, where $N = n2^k$

Contrasts

- Standardization:
$$z = \frac{C - \mathbb{E}[C]}{SD(C)}$$
- Hypothesis $H_0 : \Gamma = 0,\ H_1 : \Gamma \neq 0$
- Under H_0: $z_0 = \frac{C}{SD(C)} \sim N(0, 1)$
- $z_0^2 = \frac{C^2}{N\sigma^2}$
- $SS_{\text{Contr}} = \frac{C^2}{N} \sim \sigma^2\chi_1^2$
- From this we can construct the usual F-tests for testing the significance of A, B and AB - note that the 1 degree of freedom comes from the fact that we have 2 levels.
- The balanced design for 2^k is orthogonal, i.e. no worries about order of factors when we do the analysis in R.

ANOVA as regression

- A 2^k design can be expressed as a regression model.
- The 2^2 design:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon$$

- Here A corresponds to $x_1 = \pm 1$ and B corresponds to $x_2 = \pm 1$.
- Going from low to high level, x_i is increased from -1 to 1, i.e. 2 units, thus

$$\begin{aligned}
\hat{\beta}_1 &= \text{Effect}_A/2 \\
\hat{\beta}_2 &= \text{Effect}_B/2 \\
\hat{\beta}_{12} &= \text{Effect}_{AB}/2 \\
\hat{\beta}_0 &= \text{Average}
\end{aligned}$$

Coding

- If the levels x_i are not ± 1 (but still has two values), then we can transform them.
- Coding:

$$x = \frac{\text{value} - \text{mean}}{\text{halfrange}}$$

- This is only for two values!

2^3 designs

- The same ideas can be used when we have three (or more) factors.
- For example (2^3 design, effect A):
  - $\text{Contrast}_A = (a + ab + ac + abc) - ((1) + b + c + bc)$
  - $\text{Effect}_A = \frac{\text{Contrast}_A}{4n} = \frac{\text{Contrast}_A}{N/2}$, where $N = 2^3 n$.
  - $SS_A = \frac{\text{Contrast}_A^2}{N}$
- For 2^k designs ($N = 2^k n$):

$$\text{Effect} = \frac{\text{Contrast}}{2^{k-1}n} = \frac{\text{Contrast}}{N/2}$$

2^3 designs

- Table:

	I	A	B	C	AB	AC	BC	ABC
(1)	+	-	-	-	+	+	+	-
a	+	+	-	-	-	-	+	+
b	+	-	+	-	-	+	-	+
ab	+	+	+	-	+	-	-	-
c	+	-	-	+	+	-	-	+
ac	+	+	-	+	-	+	-	-
bc	+	-	+	+	-	-	+	-
abc	+	+	+	+	+	+	+	+

- Again all interactions are obtained as products of the involved factors.
- Also note that $A^2 = B^2 = C^2 = I$, e.g. $(AB) \times (AC) = A^2BC = BC$

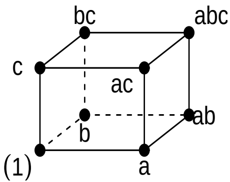
2^3 designs as regression

- We can still formulate this as regression:

$$\begin{aligned} y &= \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \\ &\quad \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 + \epsilon \end{aligned}$$

- Parameters:

$$\hat{\beta} = \frac{\text{Effect}}{2} = \frac{\text{Contrast}}{N}, \qquad \text{except } \hat{\beta}_0 = \bar{y}$$



R

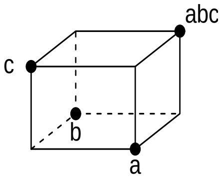
- R-demo, part 1
- Exercise 1

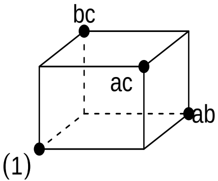
Fractional designs

- When the number of factors grow, we need to do a lot of experiments - sometimes this is not practically possible.
- Also higher order interactions can be difficult to interpret, and may not be very practically relevant.
- In fractional designs we assume that higher order interactions are negligible, and make the design such that we cannot distinguish between various main factors and interactions (from a certain degree and up).
- Confounding: we say that we confound fx the main effect A with the interaction BC if we cannot see the difference between Effect_A and Effect_{BC}.
- Fractional designs are useful when we are really low on resources, but they come at the expense that we cannot estimate some effects, and we cannot check whether they should have been included.
- They are often used as screening experiments or early preliminary experiments to reduce a large number of factors.

The 2^{3-1}_{III} design

- A 2^3 design requires 8 measurements (if only 1 replication is made) - what if we only have resources for 4 measurements?
- In a 2^{3-1}_{III} design we can estimate any main effect, but not interactions - the two-factor interactions have been confounded with the main factors.
- There are two versions of this design depending on which fraction of the full design that has been measured: principal fraction or alternate fraction.





The 2^{3-1}_{III} design

- Defining relation: $I = ABC$ (principal fraction) or $I = -ABC$ (alternate fraction).
- Aliases: the confounded effects are called aliases, fx using $I = ABC$ we get that A and BC are aliases:

$$A = AI = AABC = A^2BC = BC$$

- For a design with $I = ABC$, we take the following table from the 2^3 and only include rows with $ABC = +$:

	I	A	B	C	C= AB	B= AC	A= BC	I= ABC
a	+	+	-	-	-	-	+	+
b	+	-	+	-	-	+	-	+
c	+	-	-	+	+	-	-	+
abc	+	+	+	+	+	+	+	+

- From this, we can see which measurements we should do, estimate contrasts or effects, and see aliases from this, fx

$$\text{Effect}_A = (a - b - c + abc)/2 = \text{Effect}_{BC}$$

Resolution

- Resolution: a design is resolution R if any pair of confounded effects are of orders p_1 and p_2, where $p_1 + p_2 \geq R$.
  - III: Some main effects and pairwise interaction are confounded.
  - IV: Some main effects and third order interactions and/or some pairs of pairwise interactions are confounded.
  - V: And so on... (V is usually the highest)
- A fractional design is only appropriate if only one of the confounded effects can be considered zero, fx $\text{Effect}_A = \text{Effect}_{BC}$ means that we think that there is no significant interaction (we usually expect the higher order terms to be zero).
- There are many fractional design with various degrees of data cost reduction, fx a 2^{7-4}_{III} design required $2^3 = 8$ measurements, compared to a 2^7 design which requires 128 measurements to deal with 7 factors!

Nested designs

- In a two-factor design, it may sometimes be that the different levels in factor B do not correspond to the similar levels when changing the level in another factor A.
- For example: We get four batches of material from three different suppliers, and want to compare them all. However, fx batch j in company 1 does not correspond to batch j in company 2 or 3.
- This can be modelled using a nested design.

Nested designs

- The model:

$$y_{ijk} = \mu + \alpha_i + \beta_{j(i)} + \epsilon_{(ij)k}$$

- We take the random case (fixed or mixed case also available):

$$\alpha_i \sim N(0, \sigma_A^2) \quad \beta_{j(i)} \sim N(0, \sigma_B^2) \quad \epsilon_{(ij)k} \sim N(0, \sigma_E^2)$$

- The expected mean sums of squares are useful for finding variance components:

$$\mathbb{E}[MS_A] = \sigma_E^2 + n\sigma_B^2 + nb\sigma_A^2 \quad \mathbb{E}[MS_{B(A)}] = \sigma_E^2 + n\sigma_B^2 \quad \mathbb{E}[MS_E] = \sigma_E^2$$

- Variance components:

$$\hat{\sigma}_E^2 = MS_E \quad \hat{\sigma}_B^2 = \frac{MS_{B(A)} - MS_E}{n} \quad \hat{\sigma}_A^2 = \frac{MS_A - MS_{B(A)}}{bn}$$

R

- R-demo, part 2
- Exercise 2

Evaluation of the course

- Material for the course:
  - Book
  - Slides
  - R-demoes
- Exercises and homeworks - too difficult/easy?
- Form of lectures - mixture of slides, R-demoes and exercises ok?
- Contents:
  - Too much math or ok?
  - Theory/methods useful for you?
  - Missing something important?
- Any other comments?