3. Factorial Experiments

In many experiments, interest lies in the study of the effects of two or more factors simultaneously.

Example 5: Desilylation example from GlaxoSmithKline (Owen et al., 2001[1]) In this experiment the aim was to optimise the desilylation of an ether into an alcohol; a key step in the synthesis of a particular antibiotic. The response is the yield of alcohol, and there are four factors which can be controlled:

	Units	-1 (low)	+1 (high)
Temp	°C	10	20
Time	Hours	19	25
Concentration of solvent	vol	5	7
Equivalents of reagent	equiv.	1	1.33

We use coded units:

-1 for the low level $\qquad\qquad + 1$ for the high level

A treatment (which can be applied to an experimental unit) is now given by a combination of factor values, e.g.

-1, -1, -1, -1 (low, low, low, low; 10, 19, 5, 1)

+1, -1, +1, +1 (high, low, high, high; 20, 19, 7, 1.33).

Another example of a factorial experiment is the helicopter experiment.

3.1. Main Effects and Interactions

What comparisons among the treatments might be of interest here?

Main effects: to measure the average effect of a factor, say A, we can compute

[1]Owen, M.R., Luscombe, C., Lai, L., Godbert, S., Crookes, D.L. and Emiabata-Smith, D. (2001). Efficiency by Design: Optimisation in Process Research. Organic Process Research and Development, 5, 308-323.

$$\begin{aligned}\mathrm{ME}(A) &= \text{average response when } A=+1 - \text{average response when } A=-1 \\ &= \bar{Y}(A+) - \bar{Y}(A-)\,.\end{aligned}$$

For example,

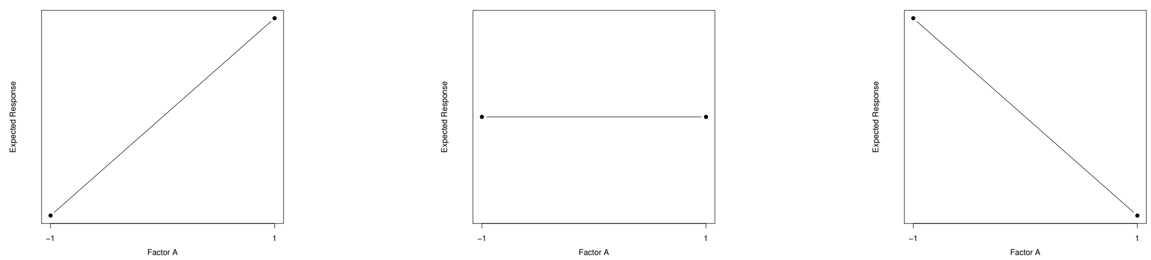
$$\mathrm{ME}(\text{temp}) = \begin{array}{lcl} \text{average response} & - & \text{average response} \\ \text{when temp =+1(20}^\circ C\text{).} & & \text{when temp =-1(10}^\circ C\text{).} \\ \text{Response from all} & & \text{Response from all} \\ \text{treatments of form} & & \text{treatments of form} \\ (+1,*,*,*) & & (-1,*,*,*) \end{array}$$

This is the effect of changing temperature from low to high *averaged across all other factor levels*

Conditional main effects: average effect of a factor, say A, given that another, say B, is fixed to one of its levels

$$\mathrm{ME}(A|B+) = \begin{array}{lcl} \text{average response} & - & \text{average response} \\ \text{when } A=+1 & & \text{when } A=-1 \\ \text{and } B=+1 & & \text{and } B=+1\,, \end{array}$$

The main effect is often displayed as a *main effects plot*, e.g.

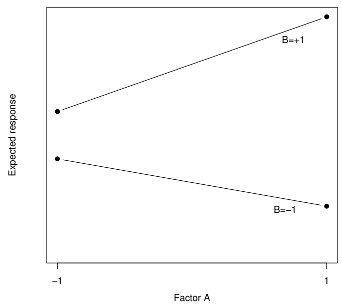


Interactions: We can measure the joint effect of changing two or more factors simultaneously through an interaction.

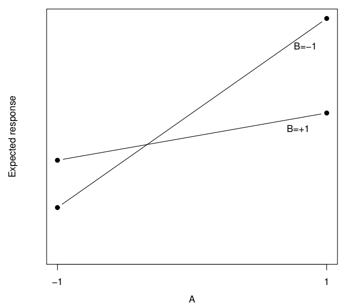
A *two factor interaction* can be interpreted as one-half the difference in the main effect of A when B is set to its high and low levels:

$$\mathrm{Int}(A,B) = \frac{1}{2}\left[\mathrm{ME}(A|B+) - \mathrm{ME}(A|B-)\right] = \frac{1}{2}\left[\mathrm{ME}(B|A+) - \mathrm{ME}(B|A-)\right] ,$$

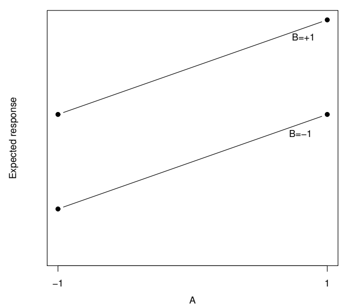
Two factor interactions are often displayed in interaction plots



The above interaction is *antagonistic*: the main effect of A changes sign with B; $\mathrm{ME}(A|B+)\times\mathrm{ME}(A|B-) < 0$.



The above interaction is *synergistic*: the main effect of A has the same sign at $B = -1, +1$; $\mathrm{ME}(A|B+)\times\mathrm{ME}(A|B-) > 0$.



Parallel lines imply there is no interaction; $\mathrm{ME}(A|B+) \approx \mathrm{ME}(A|B-)$.

We can define higher order interactions similarly, e.g. the ABC interaction measures how the AB interaction changes with the levels of C:

$$\begin{aligned}
\text{Int}(A,B,C) &= \frac{1}{2}\left[\text{Int}(A,B|C+) - \text{Int}(A,B|C-)\right] \\
&= \frac{1}{2}\left[\text{Int}(A,C|B+) - \text{Int}(A,C|B-)\right] \\
&= \frac{1}{2}\left[\text{Int}(B,C|A+) - \text{Int}(B,C|A-)\right] .
\end{aligned}$$

So, the next question is: what design should we use to investigate several factors?

3.2. One Factor at a Time

A commonly used approach by some scientists is to:

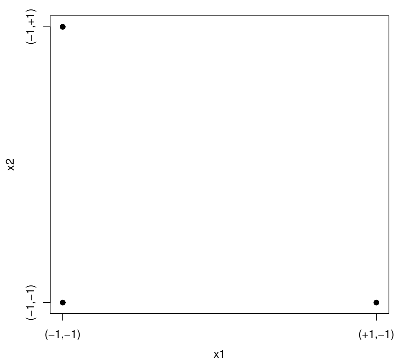
(i) decide which factor is thought to be most important;

(ii) investigate this factor while keeping all others fixed;

(iii) decide on the best setting for this factor;

(iv) move on to the next factor and repeat (ii) and (iii).

For example, with two factors a “one factor at a time” (OFAAT) design might be given by the below three points.



The main effects of the factors can be estimated using the differences in response from *pairs* of points.

There are some problems with OFAAT:

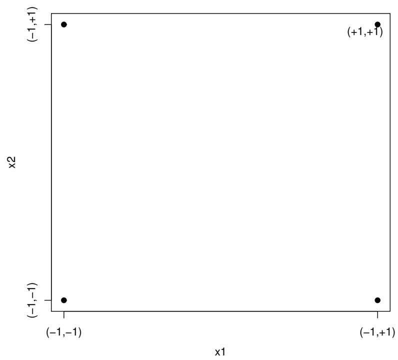
1. only a subset of runs (two) are used to estimate each effect;
2. cannot estimate interactions;
3. lack of coverage
    - what is the effect of factor 1 at different settings of factor 2;
4. therefore can miss optimal settings of factors.

So, OFAAT is generally *not* a good idea.

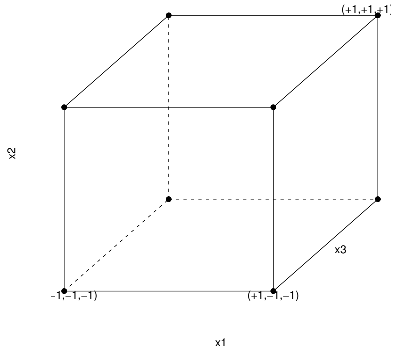
3.3. Factorial Experiments

For m factors, each having two levels, there are 2^m combinations (treatments) of factor values.

If we have sufficient resource, we could run each of these 2^m treatments in our experiment; called a 2^m *full factorial design*. For example, with $m = 2$ factors:



The design points in a two-level factorial design are always the corners of a hypercube; for $m = 3$ factors:



Advantages:

- vary all factors simultaneously, i.e. include points like (+1,+1,+1) which might not be included in a one factor at a time experiment;
- allows estimation of interactions;
- more efficient for estimation of main effects than one factor at a time
  - all observations are used in calculation of each factorial effect;
- better coverage of design space.

Disadvantage:

- can get very big designs for even moderate m.

We call these designs 2^m (full) factorial designs. A design may be *unreplicated* (one run of each treatment combination) or *replicated*, with each treatment combination included r times in the experiment

Example 5 cont.: Desilylation Experiment; 2^4 unreplicated factorial design (16 runs, one for each treatment). The design (and responses) is given by:

x_1	x_2	x_3	x_4	Y
-1	-1	-1	-1	82.947
-1	-1	-1	+1	88.667
-1	-1	+1	-1	77.193
-1	-1	+1	+1	84.873
-1	+1	-1	-1	88.073
-1	+1	-1	+1	92.993
-1	+1	+1	-1	83.587
-1	+1	+1	+1	88.707
+1	-1	-1	-1	94.053
+1	-1	-1	+1	94.293
+1	-1	+1	-1	93.007
+1	-1	+1	+1	94.247
+1	+1	-1	-1	93.967
+1	+1	-1	+1	93.407
+1	+1	+1	-1	94.373
+1	+1	+1	+1	94.653

Each row is a treatment combination in our experiment.

3.4. Regression Modelling for Factorial Experiments

We again use a linear model:

$$\begin{aligned} Y_{ij} &= \beta_0 + \sum_{l=1}^{m} \beta_l x_{il} \\ &+ \sum_{k=1}^{m} \sum_{l>k}^{m} \beta_{kl} x_{ik} x_{il} \\ &+ \sum_{k=1}^{m} \sum_{l>k}^{m} \sum_{q>l}^{m} \beta_{klq} x_{ik} x_{il} x_{iq} \\ &+ \cdots + \varepsilon_{ij} \, , \end{aligned} \tag{3.1}$$

for $i = 1, \ldots, 2^m$, $j = 1, \ldots, r$, with

$$x_{ik} = \begin{cases} -1 & \text{if } k\text{th factor is set to low level in run } i \\ +1 & \text{if } k\text{th factor is set to high level in run } i \, . \end{cases}$$

In matrix form:

$$\boldsymbol{Y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}\,,$$

where:

$\boldsymbol{Y}$ - $N \times 1$ response vector, $N = r2^m$;

X - $N \times p$ model matrix;

$\boldsymbol{\beta}$ - $p \times 1$ vector of model parameters;

$\boldsymbol{\varepsilon}$ - iid error vector.

The least squares normal equations are the same as before:

$$X^{\mathrm{T}}X\hat{\boldsymbol{\beta}} = X^{\mathrm{T}}\boldsymbol{Y}\,.$$

For a factorial design,

$$X^{\mathrm{T}}X = NI$$

where I is an $p \times p$ identity matrix. This is because factorial designs are *orthogonal*: for every pair of factors, every combination of levels appears same number of times. Factorial designs are also *balanced*: for each factor column, each level (-1,+1) appears the same number of times. A consequence of orthogonality and balance is that

$$\hat{\boldsymbol{\beta}} = \frac{1}{N}X^{\mathrm{T}}\boldsymbol{Y}\,.$$

That is, all regression parameters are estimated independently and there is no need to make adjustments for other terms in the model; fitting submodels of (3.1) does not change the parameter estimates.

Notice that

$$\hat{\beta}_0 = \frac{1}{N}\sum_{i=1}^{n}\sum_{j=1}^{r} Y_{ij}$$

and in the unreplicated case

$$\hat{\beta}_i = \frac{1}{N}\sum_{j=1}^{N} X_{j,i}Y_j$$

Relationship between regression parameters and factorial effects: fixing $x_2, \ldots, x_m$, the change in expected response from $x_1 = -1$ to $x_1 = +1$ is given by

$$\begin{aligned} \mathrm{E}(Y|x_1 = +1) - \mathrm{E}(Y|x_1 = -1) &= (\beta_0 + \beta_1 + \underbrace{\ldots}_{\text{cancel}}) - (\beta_0 - \beta_1 + \underbrace{\ldots}_{\text{cancel}}) \\ &= 2\beta_1 = \mathrm{ME}(x_1) \\ \Rightarrow \mathrm{ME}(x_i) &= 2\beta_i\,. \end{aligned}$$

Similarly for interactions, e.g. $\bar{Y}(x_1x_2 = +1) - \bar{Y}(x_1x_2 = -1)$,

$$\begin{aligned} \mathrm{E}(Y|x_1x_2 = +1) - \mathrm{E}(Y|x_1x_2 = -1) &= 2\beta_{12} = \mathrm{Int}(x_1, x_2) \\ \Rightarrow \mathrm{Int}(x_i, x_j) &= 2\beta_{ij}\,. \end{aligned}$$

For the desilylation example the least square estimates are

$$\hat{\boldsymbol{\beta}} = \left[\begin{array}{c} 89.94 \\ 4.06 \\ 1.28 \\ -1.11 \\ 1.54 \\ -1.18 \\ 1.18 \\ -1.39 \\ 0.22 \\ -0.32 \\ 0.25 \\ 0.123 \\ 0.10 \\ -0.02 \\ -0.12 \\ 0.10 \end{array}\right] \begin{array}{ll} \beta_0 & \\ \beta_1 & \text{(temp) } x_1 \\ \beta_2 & \text{(time) } x_2 \\ \beta_3 & \text{(conc.) } x_3 \\ \beta_4 & \text{(reagent) } x_4 \\ \beta_{12} & \text{(time}\times\text{temp) } x_1 \times x_2 \\ \beta_{13} & \\ \beta_{14} & \\ \beta_{23} & \\ \beta_{24} & \\ \beta_{34} & \\ \beta_{123} & \text{(temp}\times\text{time}\times\text{conc.) } x_1x_2x_3 \\ \beta_{124} & \\ \beta_{134} & \\ \beta_{234} & \\ \beta_{1234} & \text{(temp}\times\text{time}\times\text{conc.}\times\text{reagent) } x_1x_2x_3x_4 \end{array}$$

The factorial effects are given by $2\boldsymbol{\beta}$; e.g. $\mathrm{ME}(x_1) = 8.12$, $\mathrm{Int}(x_1x_2) = -2.36$.

3.5. Analysis of Variance

Source	df	SS
Regression	$2^m - 1$	$\hat{\boldsymbol{\beta}}^{\mathrm{T}} X^{\mathrm{T}} X \hat{\boldsymbol{\beta}} - N\bar{Y}^2$
x_1	1	$N\hat{\beta}_1^2$ (*)
$\vdots$	$\vdots$	$\vdots$
x_4	1	$N\hat{\beta}_4^2$
x_1x_2	1	$N\hat{\beta}_{12}^2$
$\vdots$	$\vdots$	$\vdots$
$x_1x_2x_3x_4$	1	$N\hat{\beta}_{1234}^2$
Residual	$2^m(r-1)$	$(\boldsymbol{Y} - X\hat{\boldsymbol{\beta}})^{\mathrm{T}}(\boldsymbol{Y} - X\hat{\boldsymbol{\beta}})$
Total	$2^m r - 1$	

As before, the regression sum of squares is given by

$$\begin{aligned} \text{Regression SS} &= \text{RSS(total)} - \text{RSS(residual)} \\ &= \boldsymbol{Y}^{\mathrm{T}}\boldsymbol{Y} - N\bar{Y}^2 - (\boldsymbol{Y} - X\hat{\boldsymbol{\beta}})^{\mathrm{T}}(\boldsymbol{Y} - X\hat{\boldsymbol{\beta}}) = \hat{\boldsymbol{\beta}}^{\mathrm{T}} X^{\mathrm{T}} X \hat{\boldsymbol{\beta}} - N\bar{Y}^2 \,. \end{aligned}$$

Expression (*) in the ANOVA table is formed as

$$\begin{aligned} \mathrm{SS}(x_1) &= \text{RSS(mean)} - \text{RSS}(\text{mean} + x_1) \\ &= \boldsymbol{Y}^{\mathrm{T}}\boldsymbol{Y} - N\bar{Y}^2 - (\boldsymbol{Y} - X_1\hat{\boldsymbol{\beta}}_1)^{\mathrm{T}}(\boldsymbol{Y} - X_1\hat{\boldsymbol{\beta}}_1) \,, \end{aligned}$$

where

$$X_1 = \begin{bmatrix} 1 & -1 \\ 1 & -1 \\ \vdots & \vdots \\ \vdots & -1 \\ \vdots & 1 \\ \vdots & \vdots \\ 1 & 1 \end{bmatrix} \qquad \hat{\boldsymbol{\beta}}_1 = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} .$$

Hence,

$$\mathrm{SS}(x_1) = \hat{\boldsymbol{\beta}}_1^{\mathrm{T}} X_1^{\mathrm{T}} X_1 \hat{\boldsymbol{\beta}}_1 - N\bar{Y}^2 \,.$$

However, the design is orthogonal and so

$$X_1^{\mathrm{T}} X_1 = \begin{bmatrix} N & 0 \\ 0 & N \end{bmatrix} = NI\,,$$

and

$$\mathrm{SS}(x_1) = N \underbrace{\hat{\beta}_0^2}_{\bar{Y}^2} + N\hat{\beta}_1^2 - N\bar{Y}^2 = N\hat{\beta}_1^2\,.$$

Other sums of squares are similar; as they are all independent, it *does not matter* in which order we compare the models.

Note: if $r = 1$ (single replicate design), the Residual df $= 2^m(r-1) = 0$ and RSS $= 0$. This means we cannot conduct hypothesis testing and we have no estimate of σ^2.

3.6. Three Principles for Factorial Effects

1. Effect hierarchy:

   (i) lower-order effects are more likely to be important than higher-order effects;

   (ii) effects of same order are equally likely to be important.

2. Effect sparsity:

   - the number of important terms in a factorial experiment is likely to be small, relative to total number.

3. Effect heredity:

   - interactions are more likely to be important if at least one parent main effect is also important.

All three are empirical principles and may not always hold; however, they are useful guides and are particularly important for *confounded* and *fractional* factorial designs.

3.7. Blocking and Confounding in Factorial Designs

Recall that blocking is used when there are not enough homogenous, or similar, experimental units to run the whole experiment under similar conditions. For factorial experiments, there are two basic cases:

(I) Each of the b blocks has size $k \geq 2^m$

- a complete replicate of the treatments can be run in each block;
- the analysis is the same as in Section 2.3 but the regression SS can be broken down per factorial effect (see Section 3.5).

(II) Each of the b blocks has size $k < 2^m$, with k a power of two, i.e. $k = 2^{m-q}$ for $q = 1, 2, \ldots, m-1$

- the question then is which treatments to put into each block;
- i.e. we want to place a *fraction* of the treatments in each incomplete block.

Example 6: Consider a 2^3 experiment.

Case (i): two blocks of size $2^{3-1} = 4$. The effect that is likely to be least important is the highest order interaction, $x_1x_2x_3$ and so we could assign treatments to blocks according to the value of this interaction.

The below table shows the design and the model matrix X (having the first column of 1's removed). We assign all runs with $x_1x_2x_3 = -1$ to block 1 and all runs with $x_1x_2x_3 = +1$ to block 2.

Run	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3	$x_1x_2x_3$	Block
1	-1	-1	-1	$+1$	$+1$	$+1$	-1	1
2	-1	-1	$+1$	$+1$	-1	-1	$+1$	2
3	-1	$+1$	-1	-1	$+1$	-1	$+1$	2
4	-1	$+1$	$+1$	-1	-1	$+1$	-1	1
5	$+1$	-1	-1	-1	-1	$+1$	$+1$	2
6	$+1$	-1	$+1$	-1	$+1$	-1	-1	1
7	$+1$	$+1$	-1	$+1$	-1	-1	-1	1
8	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	2

What impact does this have on the analysis of the design?

The block effect is estimated by

$$\bar{Y}(B=2) - \bar{Y}(B=1) = \frac{1}{4}(Y_2 + Y_3 + Y_5 + Y_8) - \frac{1}{4}(Y_1 + Y_4 + Y_6 + Y_7)$$

[The difference in average responses from blocks 1 and 2.]

The three factor interaction also estimated by

$$\text{Int}(x_1, x_2, x_3) = \frac{1}{4}(Y_2 + Y_3 + Y_5 + Y_8) - \frac{1}{4}(Y_1 + Y_4 + Y_6 + Y_7)$$

For this block design, we would use the **same** difference in observations to estimate both these effects, and the block effect is said to be *confounded* with the three factor interaction.

We represent this confounding in shorthand by

$$B = 123\,.$$

We read this as "the block effect is confounded with the three factor interaction $x_1x_2x_3$". Every other column occurs at -1 and +1 in each block an equal number of times, and hence the block effect cancels in all other treatment comparisons. Therefore all other factorial effects are unaffected by the blocking.

Case(ii): four blocks of size $2^{3-2} = 2$. We now split the design into four blocks according to the two interactions: x_1x_2 and x_1x_3. The runs where $(x_1x_2, x_1x_3) = (-1, -1)$ form Block 1, $(-1, +1)$ form Block 2, $(+1, -1)$ form Block 3, and $(+1, +1)$ form Block 4.

Run	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3	$x_1x_2x_3$	Block
1	-1	-1	-1	$+1$	$+1$	$+1$	-1	4
2	-1	-1	$+1$	$+1$	-1	-1	$+1$	3
3	-1	$+1$	-1	-1	$+1$	-1	$+1$	2
4	-1	$+1$	$+1$	-1	-1	$+1$	-1	1
5	$+1$	-1	-1	-1	-1	$+1$	$+1$	1
6	$+1$	-1	$+1$	-1	$+1$	-1	-1	2
7	$+1$	$+1$	-1	$+1$	-1	-1	-1	3
8	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	4

This means that $B_1 = 12$ and $B_2 = 13$. However, when using 4 blocks, there are three comparisons between blocks, so what else has been confounded with blocks? The product between columns x_1x_2 and x_1x_3 is also confounded: x_2x_3.

Denote this as

$$B_1 = 12 \qquad B_2 = 13$$

and

$$\begin{aligned} B_3 = B_1B_2 &= 1213 \\ &= 1 \times 1 \times 2 \times 3 \qquad \text{elementwise multiplication of columns} \\ &= I \times 23 \qquad \text{any column multiplied by itself is a column of 1s} \\ &= 23 \end{aligned}$$

Hence, we confound $B_1 = 12$, $B_2 = 13$, $B_3 = 23$.

Question: What happens if you choose to confound 123? Any other choice of interaction effect to also confound with blocks (e.g. 12) will result in a main effect (e.g. 3) also being confounded with blocks.

In general, to arrange a 2^m design in $b = 2^q$ blocks of size $k = 2^{m-q}$:

- choose q independent factorial effects (columns) for the *defining blocks*. Typically choose higher order interactions (effect hierarchy).

$$B_1 = v_1, \ldots, B_q = v_q$$

  - v_i is the factorial effect confounded with block effect B_i.

- all the products of $v_1, \ldots, v_q$ are also confounded:

$$\begin{aligned} B_1B_2 &= v_1v_2 \\ B_1B_3 &= v_1v_3 \qquad \text{- elementwise multiplication} \\ \vdots &= \vdots \\ B_1B_2\ldots B_q &= v_1v_2\ldots v_q \end{aligned}$$

For example, a 2^8 design in $2^3 = 8$ blocks of size $2^{8-3} = 2^5 = 32$:

$$B_1 = 13578 \qquad B_2 = 23678 \qquad B_3 = 24578\,.$$

We obtain the other confounded effects by elementwise multiplication of columns:

$$\begin{aligned} B_1 B_2 &= 1256 \\ B_1 B_3 &= 1234 \\ B_2 B_3 &= 3456 \\ B_1 B_2 B_3 &= 14678 \end{aligned}$$

The analysis is straightforward and the same as Section 3.5 **but** remember the df, SS and regression coefficients for confounded interactions are now *blocking* terms. For example, for our earlier 2^3 example in $2^{3-2} = 4$ blocks of size 2:

Source	df	SS
x_1	1	$8\hat{\beta}_1^2$
x_2	1	$8\hat{\beta}_2^2$
x_3	1	$8\hat{\beta}_3^2$
$x_1x_2x_3$	1	$8\hat{\beta}_{123}^2$
Blocks	3	$8\hat{\beta}_{12}^2 + 8\hat{\beta}_{13}^2 + 8\hat{\beta}_{23}^2$
$(=x_1x_2, x_1x_3, x_2x_3)$		
Total	7	$\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{Y} - N\bar{Y}^2$

The blocks are orthogonal to all unconfounded factorial effects, so order of models in the ANOVA is unimportant.

4. Fractional Factorial designs at Two Levels

Example 7: Consider a chemistry experiment to investigate the effect of 5 factors on the production of bacteriocin from bacteria in controlled laboratory cultures.

The factors are:

Factor	Name	Units	Low level	Upper level
x_1	Glucose	wt/vol	1%	2%
x_2	Initial inoculum size	$\log_{10}$CFU/ml	5	7
x_3	Aeration	l/min	0	1
x_4	Temperature	°C	25	30
x_5	Sodium	wt/vol	3%	5%

Factorial designs can become very big with only a moderate number of factors

$$\begin{aligned} 2^3 &= 8 \\ 2^4 &= 16 \\ 2^5 &= 32 \\ \vdots &= \vdots \\ 2^{10} &= 1024 \end{aligned}$$

etc..

Resource constraints may mean that not all 2^m treatment combinations can be run. Also, lots of the degrees of freedom are used to estimate high-order interactions, e.g. in a 2^5 experiment, 16 degrees of freedom are used to estimate 3 factor and higher interactions. The principle of effect hierarchy suggests this is probably wasteful.

We can run smaller experiments by selecting a subset, or fraction, of the treatment combinations, of size 2^{m-q}:

(a) split the experiment into blocks, where each block contains the number of runs we wish to use, and

(b) only use *one* of these blocks (it does not generally matter which).

For example, in Example 7: five factors in 16 runs

$$2^{5-1} = 16 \qquad q = 1\,.$$

Consider $2^q = 2$ blocks, confounding interaction 1234.

The fraction is given by

Block 1					Block 2				
x_1	x_2	x_3	x_4	x_5	x_1	x_2	x_3	x_4	x_5
-1	-1	-1	+1	-1	-1	-1	-1	-1	-1
-1	-1	-1	+1	+1	-1	-1	-1	-1	+1
-1	-1	+1	-1	-1	-1	-1	+1	+1	-1
-1	-1	+1	-1	+1	-1	-1	+1	+1	+1
-1	+1	-1	-1	-1	-1	+1	-1	+1	-1
-1	+1	-1	-1	+1	-1	+1	-1	+1	+1
-1	+1	+1	+1	-1	-1	+1	+1	-1	-1
-1	+1	+1	+1	+1	-1	+1	+1	-1	+1
+1	-1	-1	-1	-1	+1	-1	-1	+1	-1
+1	-1	-1	-1	+1	+1	-1	-1	+1	+1
+1	-1	+1	+1	-1	+1	-1	+1	-1	-1
+1	-1	+1	+1	+1	+1	-1	+1	-1	+1
+1	+1	-1	+1	-1	+1	+1	-1	-1	-1
+1	+1	-1	+1	+1	+1	+1	-1	-1	+1
+1	+1	+1	-1	-1	+1	+1	+1	+1	-1
+1	+1	+1	-1	+1	+1	+1	+1	+1	+1

The $2^q - 1 = 1$ effects confounded with blocks give the *defining relation*:

$$I = 1234\,.$$

The 1234 interaction is *aliased* with the mean; this interaction column is *constant* in the fraction.

As we only have $N = 2^{m-q} = 2^{5-1} = 16$ runs, we can only estimate 16 factorial effects out of the total of $2^m = 2^5 = 32$. The alias scheme will tell us what factorial effects we can estimate.

Using elementwise multiplication of columns, we can derive the *aliasing scheme*:

$$\left.\begin{array}{rcl} I &=& 1234 \\ 1 &=& 234 \\ 2 &=& 134 \\ 3 &=& 124 \\ 4 &=& 123 \\ 5 &=& 12345 \\ 12 &=& 34 \\ 13 &=& 24 \\ 14 &=& 23 \\ 15 &=& 2345 \\ 25 &=& 1345 \\ 35 &=& 1245 \\ 45 &=& 1235 \\ 235 &=& 145 \\ 125 &=& 345 \\ 135 &=& 245 \end{array}\right\} \text{16 ``effects'' (``alias strings'') that can be estimated}$$

Example 8: Consider the 2^{5-1} Bacteria experiment with a different defining relation $I = 12345$. The fraction is given by

Block 1					Block 2				
x_1	x_2	x_3	x_4	x_5	x_1	x_2	x_3	x_4	x_5
-1	-1	-1	-1	-1	-1	-1	-1	-1	+1
-1	-1	-1	+1	+1	-1	-1	-1	+1	-1
-1	-1	+1	-1	+1	-1	-1	+1	-1	-1
-1	-1	+1	+1	-1	-1	-1	+1	+1	+1
-1	+1	-1	-1	+1	-1	+1	-1	-1	-1
-1	+1	-1	+1	-1	-1	+1	-1	+1	+1
-1	+1	+1	-1	-1	-1	+1	+1	-1	+1
-1	+1	+1	+1	+1	-1	+1	+1	+1	-1
+1	-1	-1	-1	+1	+1	-1	-1	-1	-1
+1	-1	-1	+1	-1	+1	-1	-1	+1	+1
+1	-1	+1	-1	-1	+1	-1	+1	-1	+1
+1	-1	+1	+1	+1	+1	-1	+1	+1	-1
+1	+1	-1	-1	-1	+1	+1	-1	-1	+1
+1	+1	-1	+1	+1	+1	+1	-1	+1	-1
+1	+1	+1	-1	+1	+1	+1	+1	-1	-1
+1	+1	+1	+1	-1	+1	+1	+1	+1	+1

The aliasing scheme is

$$
\begin{aligned}
I &= 12345 \\
1 &= 2345 \\
2 &= 1345 \\
3 &= 1245 \\
4 &= 1235 \\
5 &= 1234 \\
12 &= 345 \\
13 &= 245 \\
14 &= 235 \\
15 &= 234 \\
23 &= 145 \\
24 &= 135 \\
25 &= 134 \\
34 &= 125 \\
35 &= 124 \\
45 &= 123
\end{aligned}
$$

This design has no pairs of two factor interactions aliased together and is the more common half-fraction. It is appropriate when there is no prior information on importance of effects. The original design from Example 7 might be used if factor 5 and its interactions are thought likely to be important before the experiment is run; two-factor interactions involving factor 5 aliased with 4 factor interactions.

The general case of fractional factorial designs:

- A 2^{m-q} fraction has q *defining words* $v_1, \ldots, v_q$

  e.g. 2^{6-2}

$$
\left.\begin{aligned}
v_1 &= 1234 \\
v_2 &= 3456
\end{aligned}\right\} \text{“words” of length 4}
$$

- The *defining relation* is a list of all $2^q - 1$ effects aliased with the mean (formed through all products of the defining words) e.g.

$$\begin{aligned} I &= v_1 = v_2 = v_1 v_2 \\ I &= 1234 = 3456 = 1256 \end{aligned}$$

- The alias scheme is a list of 2^{m-q} alias strings, each of which can be estimated in the experiment

  e.g.

$$\text{16 alias strings} \begin{cases} I &= 1234 = 3456 = 1256 \\ 1 &= 234 = 13456 = 256 \\ 2 &= 134 = 23456 = 156 \leftarrow \text{ elementwise multiplication of} \\ \vdots &= \vdots \qquad\qquad\qquad\qquad\qquad \text{columns} \\ 56 &= 123456 = 34 = 12 \end{cases}$$

- We can estimate one effect from each string, assuming all others are negligible; e.g. if we want to estimate interaction 56, we must assume 34 and 12 are zero.
- All effects in the same alias string are aliased, or confounded, together and cannot be independently estimated.
- To find the treatments in the fraction, we just need to solve, e.g. $v_1 = -1, v_2 = -1, \ldots, v_q = -1$ or any other set $v_1 = \pm 1, v_2 = \pm 1, \ldots, v_q = \pm 1$.

  e.g. $x_1 x_2 x_3 x_4 = -1, x_3 x_4 x_5 x_6 = -1$

4.1. Resolution of a Design

The *resolution* of a 2^{m-q} design is the length of the shortest word in the defining relation. For example,

2^{6-2} $I = 1234 = 3456 = 1256$ - resolution IV

2^{3-1} $I = 123$ - resolution III.

Designs of the following resolution are particularly common:

Resolution III: no main effect is aliased with any other main effect but at least one main effect is aliased with a two-factor interaction.

Resolution IV: no main effect is aliased with any other main effect or any two-factor interaction. Some two-factor interactions are aliased together.

Resolution V: no main effect or two-factor interaction is aliased with any other main effect or two-factor interaction.

In general, resolution R implies no effect involving i factors is aliased with effects involving less than $R-i$ factors.

Example 7 is a design with resolution IV, whilst Example 8 has resolution V.

4.2. Minimum Aberration

For a 2^{m-q} design, let A_i denote the number of words of length i in the defining relation, and let

$$W = (A_3, \dots, A_m)$$

be the *wordlength pattern.*

Example 9: 2^{7-2} experiment - two designs, d_1 and d_2.

$d_1 : I = 4567 = 12346 = 12357$

$d_2 : I = 1236 = 1457 = 234567$

Both designs are resolution IV but have different wordlength patterns:

$W(d_1) = (0, 1, 2, 0, 0)$

$W(d_2) = (0, 2, 0, 1, 0)$.

Minimum Aberration: for any two 2^{m-q} designs d_1 and d_2, let r be the smallest integer such that $A_r(d_1) \neq A_r(d_2)$. Then d_1 is said to have *less aberration* than d_2 if

$$A_r(d_1) < A_r(d_2)\,.$$

If no design has less aberration than d_1, then d_1 has *minimum aberration.*

Example 9 cont.

$$A_3(d_1) = A_3(d_2) = 0$$
$$A_4(d_1) = 1 < A_4(d_2) = 2$$

Hence, d_1 has less aberration than d_2. In fact d_1 has minimum aberration

Minimum aberration designs can obtained from tables in books (e.g. Wu and Hamada) or from software (e.g. SAS).

4.3. Blocking Fractional Factorial Designs

This is achieved as in Chapter 5, **except** when we choose a factorial effect to confound with blocks, we also confound all effects in that alias string.

Example 10: a 2^{6-2} design with defining relation

$$I = 1235 = 1246 = 3456\,.$$

Choose two effects to confound with blocks:

$$\begin{aligned} B_1 &= 134 \\ B_2 &= 234 \\ B_1B_2 &= 12\,. \end{aligned}$$

We also confound all aliases of these effects:

$$\begin{aligned} B_1 &= 134 = 245 = 236 = 156 \\ B_2 &= 234 = 145 = 136 = 256 \\ B_1B_2 &= 12 = 35 = 46 = 123456 \end{aligned}$$

The breakdown of the degrees of freedom is given in the following table. We cannot estimate any effects confounded with blocks.

Source	df
1=235=246=13456	1
2=135=146=23456	1
3=125=12346=456	1
4=12345=126=356	1
5=123=12456=346	1
6=12356=124=345	1
13=25=2346=1456	1
14=26=2345=1356	1
15=23=2456=1346	1
16=24=2356=1345	1
34=56=1245=1236	1
36=45=1256=1234	1
Blocks	3
134=245=236=156	
234=145=136=256	
12=35=46=123456	
Total	15