

STATISTICAL MODELLING

VIII. Factorial designs at two levels

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In this chapter we discuss the design and analysis of factorial experiments in which all factors have 2 levels.

Definition VIII.1: An experiment that involves k factors all at 2 levels is called a 2^k experiment. ■

These designs represent an important class of designs for the following reasons:

1. They require relatively few runs per factor studied, and although they are unable to explore fully a wide region of the factor space, they can indicate trends and so determine a promising direction for further experimentation.
2. They can be suitably augmented to enable a more thorough local exploration.
3. They can be easily modified to form fractional designs in which only some of the treatment combinations are observed.

4. Their analysis and interpretation is relatively straightforward, compared to the general factorial.

VIII.A Replicated 2^k experiments

(Box, Hunter and Hunter, ch. 10; Cochran & Cox, sec. 5.24–26, Mead, sec. 13.1–3, Mead & Curnow, sec. 6.6)

An experiment involving three factors — a 2^3 experiment — will be used to illustrate.

a) Design of replicated 2^k experiments, including R expressions

The design of this type of experiment is exactly the same as for the general factorial experiments as outlined in VII.A, *Design of factorial experiments*. However, the levels used for the factors are specific to these two-level experiments.

Definition VIII.2: There are three **systems of specifying treatment combinations** in common usage. The first uses a minus sign for the low level of a quantitative factor and a plus for the high level. Qualitative factors are coded arbitrarily but consistently as minus and plus. In the second notation, the upper level of a factor is denoted by a lower case letter used for that factor and the lower level by the absence of this letter. The third notation uses 0 and 1 in place of – and +. ■

We shall use the \pm notation as it relates to the computations for the designs.

Example VIII.1 2^3 pilot plant experiment

An experimenter conducted a 2^3 experiment in which there are two quantitative factors — temperature and concentration — and a single qualitative factor — catalyst. Altogether 16 tests were conducted with the three factors assigned at random so that each occurred just twice. At each test the chemical yield was measured and the data is shown in the following table:

							Replicate	
T	C	K		T	C	K	1	2
–	–	–	1	0	0	0	59	61
+	–	–	t	1	0	0	74	70
–	+	–	c	0	1	0	50	58
+	+	–	tc	1	1	0	69	67
–	–	+	k	0	0	1	50	54
+	–	+	tk	1	0	1	81	85
–	+	+	ck	0	1	1	46	44
+	+	+	tck	1	1	1	79	81

This table also gives the treatment combinations, using the three systems, for the experiment and associated with each observation.

The first consideration in entering the design into R is whether to enter all the values for one rep first or to enter the two reps for a treatment consecutively. For the first

option, the `times` argument would be set to 2, while for the second option we need to set the `each` argument to 2. The following output contains the commands to generate the design for the example using second option and includes the design produced:

```
> #
> #obtain randomized layout
> #
> n <- 16
> mp <- c("-", "+")
> Fac3Pilot.ran <- fac.gen(generate = list(Te = mp, C = mp, K = mp), each = 2,
+                          order="yates")
> Fac3Pilot.unit <- list(Tests = n)
> Fac3Pilot.lay <- fac.layout(unrandomized = Fac3Pilot.unit,
+                             randomized = Fac3Pilot.ran, seed = 897)
> #sort treats into Yates order
> Fac3Pilot.lay <- Fac3Pilot.lay[Fac3Pilot.lay$Permutation,]
> Fac3Pilot.lay
  Units Permutation Tests Te C K
4      4           14    4 - - -
11     11           10   11 - - -
8       8            6    8 + - -
14     14            1   14 + - -
2       2           11    2 - + -
9       9           12    9 - + -
7       7            7    7 + + -
6       6            9    6 + + -
12     12           16   12 - - +
13     13           15   13 - - +
10     10           13   10 + - +
16     16            3   16 + - +
15     15            5   15 - + +
1       1            4    1 - + +
5       5            2    5 + + +
3       3            8    3 + + +
> #add Yield
> Fac3Pilot.dat <- data.frame(Fac3Pilot.lay,
+                             Yield = c(59, 61, 74, 70, 50, 58, 69, 67,
+                                       50, 54, 81, 85, 46, 44, 79, 81))
> Fac3Pilot.dat
  Units Permutation Tests Te C K Yield
4      4           14    4 - - -   59
11     11           10   11 - - -   61
8       8            6    8 + - -   74
14     14            1   14 + - -   70
2       2           11    2 - + -   50
9       9           12    9 - + -   58
7       7            7    7 + + -   69
6       6            9    6 + + -   67
12     12           16   12 - - +   50
13     13           15   13 - - +   54
10     10           13   10 + - +   81
16     16            3   16 + - +   85
15     15            5   15 - + +   46
1       1            4    1 - + +   44
5       5            2    5 + + +   79
3       3            8    3 + + +   81
> #re-sort into randomized order
> Fac3Pilot.dat <- Fac3Pilot.dat[Fac3Pilot.dat$Units,]
> attach(Fac3Pilot.dat)
```

Notes:

- mp stands for minus-plus
- Note Te must be used for Temperature as T is reserved for a function name.
- Note that need to have the treatment factors in Yates order to add the data. ■

b) Analysis of variance

The analysis of replicated 2^k factorial experiments is the same as for the general factorial experiment.

Example VIII.1 2^3 pilot plant experiment (continued)

The features of this experiment are:

1. Observational unit – a test
2. Response variable – Yield
3. Unrandomized factors – Tests
4. Randomized factors – Temp, Conc, Catal
5. Type of study – Three-factor CRD

The experimental structure for this experiment is:

Structure	Formula
unrandomized	16 Tests
randomized	2 Temp*2 Conc*2 Catal

The sources derived from the randomized structure formula are:

$$\begin{aligned}
 \text{Temp*Conc*Catal} &= \text{Temp} + (\text{Conc*Catal}) + \text{Temp}\#(\text{Conc*Catal}) \\
 &= \text{Temp} + \text{Conc} + \text{Catal} + \text{Conc}\#\text{Catal} \\
 &\quad + \text{Temp}\#\text{Conc} + \text{Temp}\#\text{Catal} + \text{Temp}\#\text{Conc}\#\text{Catal}
 \end{aligned}$$

Since all the factors have two levels, the number of levels minus one will in every case be one. Thus, using the cross product rule, the degrees of freedom for any term will be a product of ones and hence be one.

Given that the only random factor is Tests, the following are the symbolic expressions for the maximal expectation and variation models:

$$\begin{aligned}
 \psi &= E[Y] = \text{Temp} \wedge \text{Conc} \wedge \text{Catal} \\
 \text{var}[Y] &= \text{Tests}
 \end{aligned}$$

From this we conclude that the aov function will have a model formula of the form

$$\text{Yield} \sim \text{Temp} * \text{Conc} * \text{Catal} + \text{Error}(\text{Tests})$$

The R output file containing the analysis of the example is:

```

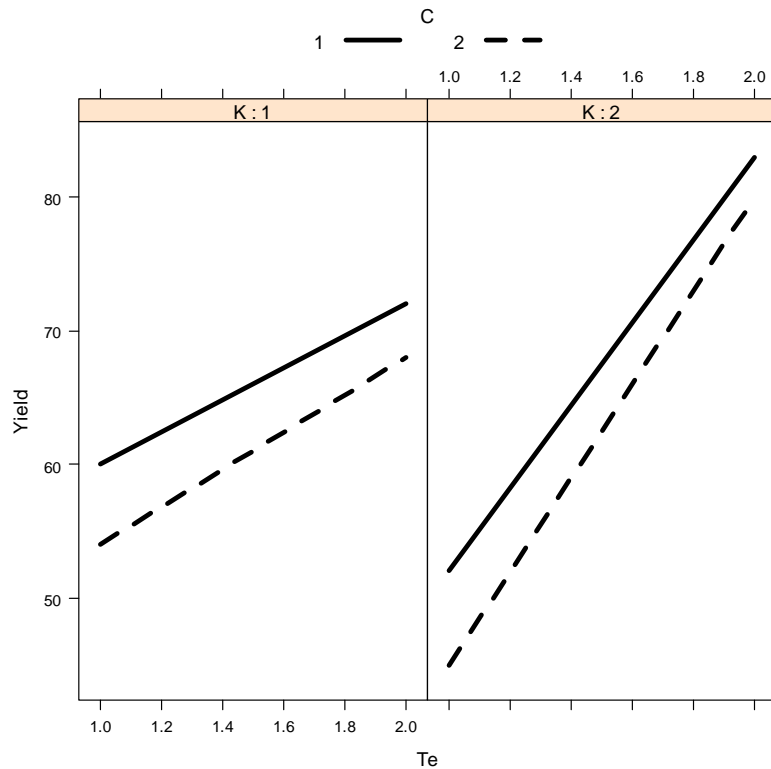
> attach(Fac3Pilot.dat)
> interaction.ABC.plot(Yield, Te, C, K, data=Fac3Pilot.dat,
+ title="Effect of Temperature(Te), Concentration(C) and
+ Catalyst(K) on Yield")
> Fac3Pilot.aov <- aov(Yield ~ Te * C * K + Error(Tests), Fac3Pilot.dat)
> summary(Fac3Pilot.aov)

Error: Tests
      Df    Sum Sq   Mean Sq    F value    Pr(>F)
Te      1      2116      2116      264.500 2.055e-07
C       1       100       100       12.500 0.0076697
K       1         9         9        1.125 0.3198134
Te:C    1         9         9        1.125 0.3198134
Te:K    1       400       400       50.000 0.0001050
C:K     1 6.453e-30 6.453e-30 8.066e-31 1.0000000
Te:C:K  1         1         1        0.125 0.7328099
Residuals 8         64         8

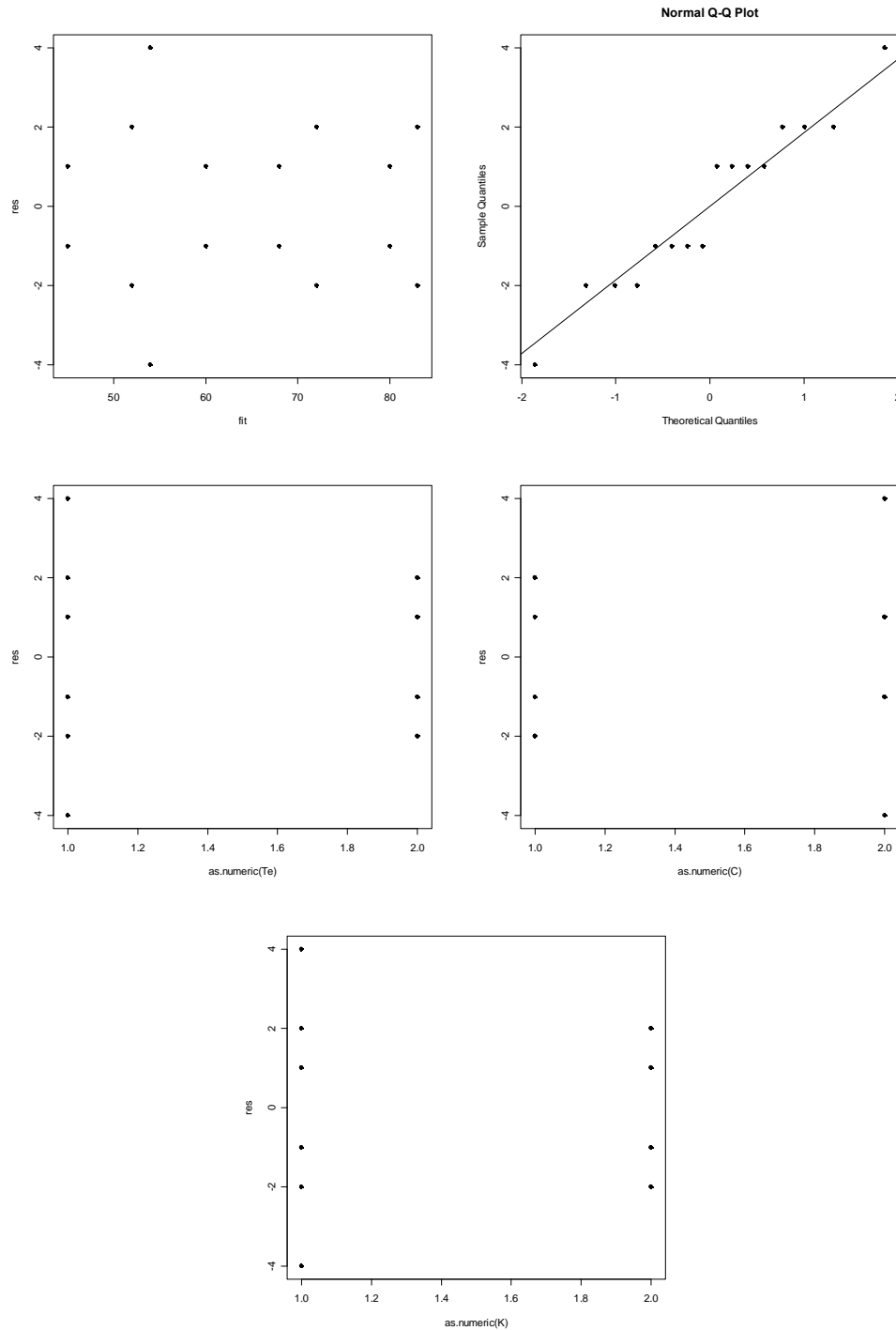
> #
> # Diagnostic checking
> #
> res <- resid.errors(Fac3Pilot.aov)
> fit <- fitted.errors(Fac3Pilot.aov)
>
> plot(fit, res, pch=16)
> plot(as.numeric(Te), res, pch=16)
> plot(as.numeric(C), res, pch=16)
> plot(as.numeric(K), res, pch=16)
> qqnorm(res, pch=16)
> qqline(res)

```

Effect of Temperature(Te), Concentration(C) and Catalyst(K) on Yield



There appears to be a TK interaction.



All the residuals plots appear to be satisfactory, Note have not obtained Tukey's one-degree-of-freedom-for-nonadditivity. This is because the design is a CRD and there are no additive expectation terms — a warning message would be produced for this design.

The hypothesis test for this experiment is given below. The hypotheses are the same as for the general three-factor factorial experiment, given in Chapter VII, *Factorial Experiments*. However, here, they have not been given in terms of parameters, but terms being tested.

Step 1: Set up hypotheses

- a) H_0 : A#B#C interaction effect is zero
 H_1 : A#B#C interaction effect is nonzero
- b) H_0 : A#B interaction effect is zero
 H_1 : A#B interaction effect is nonzero
- c) H_0 : A#C interaction effect is zero
 H_1 : A#C interaction effect is nonzero
- d) H_0 : B#C interaction effect is zero
 H_1 : B#C interaction effect is nonzero
- e) H_0 : $\alpha_1 = \alpha_2$
 H_1 : $\alpha_1 \neq \alpha_2$
- f) H_0 : $\beta_1 = \beta_2$
 H_1 : $\beta_1 \neq \beta_2$
- g) H_0 : $\delta_1 = \delta_2$
 H_1 : $\delta_1 \neq \delta_2$

Set $\alpha = 0.05$

Step 2: Calculate test statistics

The analysis of variance table for the three-factor factorial CRD is:

Source	df	SSq	MSq	F	Prob
Tests	15	2699.0			
T	1	2116.0	2116.0	264.5	<0.001
C	1	100.0	100.0	12.5	0.008
T#C	1	9.0	9.0	1.1	0.320
K	1	9.0	9.0	1.1	0.320
T#K	1	400.0	400.0	50.0	<0.001
C#K	1	0.0	0.0	0.0	1.000
T#C#K	1	1.0	1.0	0.1	0.733
Residual	8	64.0	8.0		

Step 3: Decide between hypotheses

For T#C#K interaction: the T#C#K interaction is not significant.

For T#C, T#K and C#K interactions: only the T#K interaction is significant.

For C: the C effect is significant.

Thus, the yield depends on the particular combination of Temperature and Catalyst, whereas Concentration also affects the yield but independently of the other factors. Hence the model that best fits the data is:

$$\psi = E[Y] = C + T \wedge K$$

c) Calculation of responses and Yates effects

When all the factors in a factorial experiment are at 2 levels the calculations for the analysis presented in chapter VII simplify greatly, in particular the calculation of the effects. This is because main effects, elements of \mathbf{a}_e , \mathbf{b}_e and \mathbf{c}_e , which are of the form $\bar{y}_i - \bar{y}_.$, for $i = 1, 2$, where $\bar{y}_. = (\bar{y}_1 + \bar{y}_2)/2$, simplify to

$$\bar{y}_1 - \bar{y}_. = \bar{y}_1 - \frac{\bar{y}_1 + \bar{y}_2}{2} = \frac{\bar{y}_1}{2} - \frac{\bar{y}_2}{2} = \frac{\bar{y}_1 - \bar{y}_2}{2} \quad \text{and} \quad \bar{y}_2 - \bar{y}_. = \frac{\bar{y}_2 - \bar{y}_1}{2} = -(\bar{y}_1 - \bar{y}_2)$$

This is in some ways obvious. It is merely saying that the distance of one of two means from their mean is half the difference between two means. Note there is really only one independent main effect and this is reflected in the fact that they have just one degree of freedom.

Also, two-factor interactions, elements of $(\mathbf{a} \wedge \mathbf{b})_e$, $(\mathbf{a} \wedge \mathbf{c})_e$ and $(\mathbf{b} \wedge \mathbf{c})_e$, are of the form $\bar{y}_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..}$, for $i = 1, 2; j = 1, 2$. For any pair of factors, say B and C, the means can be placed in a 2×2 table as follows.

		C		
		1	2	Mean
B	1	\bar{y}_{11}	\bar{y}_{12}	$\bar{y}_{1.} = (\bar{y}_{11} + \bar{y}_{12})/2$
	2	\bar{y}_{21}	\bar{y}_{22}	$\bar{y}_{2.} = (\bar{y}_{21} + \bar{y}_{22})/2$
Mean		$\bar{y}_{.1} = (\bar{y}_{11} + \bar{y}_{21})/2$	$\bar{y}_{.2} = (\bar{y}_{12} + \bar{y}_{22})/2$	$\bar{y}_{..} = \frac{\bar{y}_{11} + \bar{y}_{12} + \bar{y}_{21} + \bar{y}_{22}}{4}$

Thus, for $i = 1, j = 1$, $\bar{y}_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..}$ simplifies to

$$\begin{aligned} \bar{y}_{11} - \bar{y}_{1.} - \bar{y}_{.1} + \bar{y}_{..} &= \bar{y}_{11} - \frac{\bar{y}_{11} + \bar{y}_{12}}{2} - \frac{\bar{y}_{11} + \bar{y}_{21}}{2} + \frac{\bar{y}_{11} + \bar{y}_{12} + \bar{y}_{21} + \bar{y}_{22}}{4} \\ &= \frac{4\bar{y}_{11} - 2\bar{y}_{11} - 2\bar{y}_{12} - 2\bar{y}_{11} - 2\bar{y}_{21} + \bar{y}_{11} + \bar{y}_{12} + \bar{y}_{21} + \bar{y}_{22}}{4} \\ &= \frac{\bar{y}_{11} - \bar{y}_{12} - \bar{y}_{21} + \bar{y}_{22}}{4} \end{aligned}$$

Similarly,

$$\begin{aligned}\bar{y}_{12} - \bar{y}_{1.} - \bar{y}_{.2} + \bar{y}_{..} &= \frac{-\bar{y}_{11} + \bar{y}_{12} + \bar{y}_{21} - \bar{y}_{22}}{4} \\ \bar{y}_{21} - \bar{y}_{2.} - \bar{y}_{.1} + \bar{y}_{..} &= \frac{-\bar{y}_{11} + \bar{y}_{12} + \bar{y}_{21} - \bar{y}_{22}}{4} \\ \bar{y}_{22} - \bar{y}_{2.} - \bar{y}_{.2} + \bar{y}_{..} &= \frac{\bar{y}_{11} - \bar{y}_{12} - \bar{y}_{21} + \bar{y}_{22}}{4}\end{aligned}$$

Once again there is only one independent quantity and so only one degree of freedom. Notice that what is computed is the difference between $\bar{y}_{12} - \bar{y}_{11}$ and $\bar{y}_{22} - \bar{y}_{21}$. Each of these is the difference between the first and second level of factor B, the simple effects of B, one for the first level and the other for the second level of A.

Indeed all effects in a 2^k experiment have only one degree of freedom, as contemplation of the cross-product rule for crossed factors will reveal. So to accomplish an analysis we actually only need to compute a single value for each effect, instead of a vector of effects. We do not compute exactly the quantities above. However, we do compute quantities that are proportional to them. We compute what are called the responses and, from these, the Yates main and interaction effects.

Definition VIII.3: A **one-factor response** and a **Yates main effect** is the difference between the means for the high and low levels of the factor: $\bar{y}_+ - \bar{y}_-$. ■

Definition VIII.4: A **two-factor response** is the difference of the simple effects: $(\bar{y}_{++} - \bar{y}_{+-}) - (\bar{y}_{-+} - \bar{y}_{--})$. A **two-factor Yates interaction effect** is half the two-factor response. ■

Definition VIII.5: A **three-factor response** is the difference in the response of two factors at each level of the other factor:

$$\begin{aligned}(\bar{y}_{+++} - \bar{y}_{++-} - \bar{y}_{-++} + \bar{y}_{--+}) - (\bar{y}_{+-+} - \bar{y}_{+--} - \bar{y}_{-+-} + \bar{y}_{---}) \text{ or} \\ (\bar{y}_{+++} - \bar{y}_{++-} - \bar{y}_{-++} + \bar{y}_{--+}) - (\bar{y}_{-++} - \bar{y}_{-+-} - \bar{y}_{--+} + \bar{y}_{---}).\end{aligned}$$

A **three-factor Yates interaction** is the half difference in the Yates interaction effects of two factors at each level of the other factor; it is thus one-quarter of the response. ■

Definition VIII.6: Sums of squares can be computed from the Yates effects by squaring them and multiplying by $r2^{k-2}$ where k is the number of factors and r is the number of replicates of each treatment combination. ■

Example VIII.1 2^3 pilot plant experiment (continued)

We obtain the responses and Yates interaction effects for this experiment. This can be conveniently carried out on the means over the replicates.

The treatment means for the example are:

T	C	K	Yield		Mean
			Rep 1	Rep 2	
-	-	-	59	61	60
+	-	-	74	70	72
-	+	-	50	58	54
+	+	-	69	67	68
-	-	+	50	54	52
+	-	+	81	85	83
-	+	+	46	44	45
+	+	+	79	81	80

Thus, for the three factors in this experiment we have the following one-factor responses/main effects:

Temperature,

$$\frac{72 + 68 + 83 + 80}{4} - \frac{60 + 54 + 52 + 45}{4} = 75.75 - 52.75 = 23$$

Concentration,

$$\frac{54 + 68 + 45 + 80}{4} - \frac{60 + 72 + 52 + 83}{4} = 61.75 - 66.75 = -5$$

Catalyst,

$$\frac{52 + 83 + 45 + 80}{4} - \frac{60 + 72 + 54 + 68}{4} = 65.0 - 63.5 = 1.5$$

The two-factor T#K response is the difference between the simple effects of K for each T or the difference between the simple effects of T for each K — it does not matter which. The T#K Yates interaction effect is then half this response.

The simple effect of K

$$\text{at } + (180^{\circ}\text{C}) = \frac{83 + 80}{2} - \frac{72 + 68}{2} = 81.5 - 70 = 11.5$$

$$\text{at } - (160^{\circ}\text{C}) = \frac{52 + 45}{2} - \frac{60 + 54}{2} = 48.5 - 57 = -8.5$$

so that the response is

$$11.5 - (-8.5) = 20$$

and the Yates interaction effect is 10.

The computation for the Yates interaction effect can be gathered together as follows:

$$\frac{1}{2} \left\{ \frac{83 + 80}{2} - \frac{72 + 58}{2} - \frac{52 + 45}{2} + \frac{60 + 54}{2} \right\}$$

which is equal to

$$\frac{83 + 80 + 60 + 54}{4} - \frac{72 + 58 + 52 + 45}{4}$$

Thus, the Yates interaction is just the difference between two averages of four (half) of the observations. Similar results can be demonstrated for the other two two-factor interactions, T#C and C#K.

The three-factor T#C#K response is the half difference between the T#C interaction effects at each level of K. If one follows through the computations, in the same way as for two-factor interaction above, it will be found that the three-factor Yates interaction effect consists of the difference between the following two means of four observations each:

$$\frac{72 + 54 + 52 + 80}{4} - \frac{60 + 68 + 83 + 45}{4} = 64.5 - 64 = 0.5$$

Since, for the example, $k=3$ and $r=2$, the multiplier for the sums of squares is $r2^{k-2} = 2 \times 2^{3-2} = 4$. Hence, the T#C#K sums of squares is:

$$\text{T\#C\#K SSq} = 4 \times 0.5^2 = 1$$

■

Summary of effects

	General Effects (ch.VII)	simplified for 2^k	For 2^k experiments only Response	Yates effects
Main	$\bar{y}_i - \bar{y}_.$	$\frac{\bar{y}_2 - \bar{y}_1}{2}$	$\bar{y}_+ - \bar{y}_-$	$\bar{y}_+ - \bar{y}_-$
Two-factor simple	$\bar{y}_{ij} - \bar{y}_{ik}$	$\bar{y}_{12} - \bar{y}_{11}$ and $\bar{y}_{22} - \bar{y}_{21}$	not applicable	not applicable
Two-factor interaction	$\bar{y}_{ij} - \bar{y}_i - \bar{y}_j + \bar{y}_.$	$\bar{y}_{11} - \bar{y}_{12}$ $\frac{-\bar{y}_{21} + \bar{y}_{22}}{4}$ $\bar{y}_{22} - \bar{y}_{21}$ $= \frac{-\bar{y}_{12} + \bar{y}_{11}}{4}$	$(\bar{y}_{++} - \bar{y}_{+-})$ $-(\bar{y}_{-+} - \bar{y}_{--})$	$(\bar{y}_{++} - \bar{y}_{+-})$ $\frac{-(\bar{y}_{-+} - \bar{y}_{--})}{2}$
Three-factor interaction	\bar{y}_{ijk} $-\bar{y}_{ij} - \bar{y}_{i.k} - \bar{y}_{.jk}$ $+\bar{y}_{i..} + \bar{y}_{.j.} + \bar{y}_{..k}$ $-\bar{y}_.$	not given	$\left(\begin{array}{c} \bar{y}_{+++} - \bar{y}_{+--} \\ -\bar{y}_{-++} + \bar{y}_{--} \end{array} \right)$ $-\left(\begin{array}{c} \bar{y}_{+++} - \bar{y}_{+--} \\ -\bar{y}_{-++} + \bar{y}_{--} \end{array} \right)$	$\left(\begin{array}{c} \bar{y}_{+++} - \bar{y}_{+--} \\ -\bar{y}_{-++} + \bar{y}_{--} \end{array} \right)$ $-\left(\begin{array}{c} \bar{y}_{+++} - \bar{y}_{+--} \\ -\bar{y}_{-++} + \bar{y}_{--} \end{array} \right)$ $\frac{\quad}{4}$

N.B. Can show that every Yates effect is difference between means of half the observations

It turns out that there are easy rules for determining the signs of observations to compute the Yates effects.

Definition VIII.7: The **signs for observations in a Yates effect** are obtained from the columns of pluses and minuses that specify the factor combinations for each observation by taking the columns for the factors in the effect and forming their elementwise product. The **elementwise product** is the result of multiplying pairs of elements in the same row as if they were ± 1 and expressing the result as a \pm . ■

Example VIII.1 2^3 pilot plant experiment (continued)

The table of coefficients is:

T	C	K	TC	TK	CK	TCK	Mean
-	-	-	+	+	+	-	60
+	-	-	-	-	+	+	72
-	+	-	-	+	-	+	54
+	+	-	+	-	-	-	68
-	-	+	+	-	-	+	52
+	-	+	-	+	-	-	83
-	+	+	-	-	+	-	45
+	+	+	+	+	+	+	80

Clearly, these can be used to assist in calculating the responses and effects and hence the sums of squares. ■

A table of Yates effects can be obtained in R using `yates.effects`. It is usual to include this after the call to the `summary` function. Note use of `round` function with the `yates.effects` function to obtain nicer output by rounding the effects to 2 decimal places.

```
> round(yates.effects(Fac3Pilot.aov, error.term = "Tests", data=Fac3Pilot.dat), 2)
      Te      C      K  Te:C  Te:K  C:K  Te:C:K
23.0  -5.0   1.5   1.5  10.0   0.0   0.5
```

d) Yates algorithm

A particularly nifty method of performing the calculations is an algorithm due to Yates. It requires that the observations be in Yates order. They are in Yates order when the one column of plus/minuses consists of successive minus and plus signs, a second column of successive pairs of plus and minus signs, the third column of successive quadruplets of plus and minus signs and so forth. Yates algorithm for the example is given in the following table. Beginning with the means, one forms the sum of each successive pair of observations and the successive differences. This operation is repeated recursively until it has been performed k times. The Yates effects described above are then calculated by dividing all except the first by 2^{k-1} ; the first is divided by 2^k . The effect can be identified by the pattern of pluses in its row. Thus, the 5th row contains Yates effect K which is equal to 1.5.

T	C	K	Mean	(1)	(2)	(3)	Estimate
-	-	-	60	132	254	514	64.25
+	-	-	72	122	260	92	23.0
-	+	-	54	135	26	-20	-5.0
+	+	-	68	125	66	6	1.5
-	-	+	52	12	-10	6	1.5
+	-	+	83	14	-10	40	10.0
-	+	+	45	31	2	0	0.0
+	+	+	80	35	4	2	0.5

e) Treatment differences

Mean differences

To examine how the factors affect the response one examines the tables of means corresponding to the terms in the fitted model. That is, tables marginal to significant effects are not examined.

Example VIII.1 2³ pilot plant experiment (continued)

For this example, the fitted model was $\psi = E[Y] = C + T \wedge K$ and so we examine the $T \wedge K$ and C tables of means, **but not the tables of T or K means.**

```
> Fac3Pilot.means <- model.tables(Fac3Pilot.aov, type="means")
> Fac3Pilot.means$tables$"Grand mean"
[1] 64.25
> Fac3Pilot.means$tables$"Te:K"
  K
Te -  +
  - 57.0 48.5
  + 70.0 81.5
> Fac3Pilot.means$tables$"C"
  C
  -  +
66.75 61.75
```

So the table of means for the $T \wedge K$ combinations is:

Catal	1	2
Temp		
1	57.0	48.5
2	70.0	81.5

Thus, it seems that the temperature difference is less without the catalyst than with it.

The table of Concentration means is

Conc	1	2
	66.75	61.75

It is evident that the higher concentration decreases the yield by about 5 units.

So which treatments would give the highest yield? To answer this question we need to check whether or not other treatments are significantly different to the highest yielding combination of temperature and catalyst: both at their higher levels. This is done using Tukey's HSD procedures. The studentized range is

```
> q <- qtukey(0.95, 4, 8)
> q
[1] 4.52881
```

So Tukey's HSD is

$$w(5\%) = \frac{4.52881}{\sqrt{2}} \times \sqrt{\frac{8 \times 2}{4}} = 1.60$$

It is clear that all means are significantly different and so the combination of factors that will give the greatest yield is temperature and catalyst both at the higher levels and concentration at the lower level.

Polynomial models and fitted values

Given that there are only two levels of each factor a linear trend would fit perfectly the means of each factor. Now could fit linear trend (polynomial) models by putting the values of the factor levels for each factor as a column in an \mathbf{X} matrix; a linear interaction term could be fitted by adding to the \mathbf{X} matrix a column obtained by pairwise multiplying the values in the columns for the factors involved in the interaction. However, suppose that instead of putting the actual values of the factor levels into the \mathbf{X} matrix, it was decided to code the values as ± 1 . Interaction terms can still be fitted as the pairwise products of the (coded) elements from the columns for the factors involved in the interaction. Now whether your fit is based on an \mathbf{X} matrix with 0,1 or ± 1 s or the actual factor values, you end up with equivalent fits as the fitted values and F test statistics will be the same for all three parametrizations. The values of the parameter estimates will differ and you will need to put in the values you used in the \mathbf{X} matrix to obtain the estimates. The advantage of using ± 1 is the ease of obtaining the \mathbf{X} matrix and the simplicity of the computations.

Definition VIII.8: The **fitted values** are obtained using the **fitted equation** that consists of the grand mean, the x-term for each significant effect and those for effects of lower degree than the significant sources. An x-term consists of the product of x variables, one for each factor in the term; the x variables take the values -1 and $+1$ according whether the fitted value is required for an observation that received the low or high level of that factor. The coefficient of the term is half the Yates main or interaction effect. ■

The columns of an \mathbf{X} for a particular model can be obtained from the table of coefficients given for working out the sums of squares, with a column added for the grand mean term.

Example VIII.1 2^3 pilot plant experiment (continued)

The full table of coefficients is as follows:

<i>I</i>	T	C	K	TC	TK	CK	TCK
+	-	-	-	+	+	+	-
+	+	-	-	-	-	+	+
+	-	+	-	-	+	-	+
+	+	+	-	+	-	-	-
+	-	-	+	+	-	-	+
+	+	-	+	-	+	-	-
+	-	+	+	-	-	+	-
+	+	+	+	+	+	+	+

For the example, the significant sources are C and T#K so that the \mathbf{X} matrix corresponding to this model would include columns for *I*, T, C, K and TK and the row for each treatment combination would be repeated r times. Thus, the linear trend model that best describes the data from the experiment is:

$$\psi = E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\gamma} = \left(\begin{bmatrix} 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \otimes \mathbf{1}_r \right) \begin{bmatrix} \mu \\ \gamma_T \\ \gamma_C \\ \gamma_K \\ \gamma_{TK} \end{bmatrix}$$

We can write an element of $E[\mathbf{Y}]$ as

$$\psi_{ijkl} = E[Y_{ijkl}] = \mu + \gamma_T x_T + \gamma_C x_C + \gamma_K x_K + \gamma_{TK} x_T x_K$$

where x_T , x_C and x_K takes values ± 1 according to whether the observation took the high or low level of the factor.

An estimator of one of coefficients in the model is half a Yates effect, with the estimator for the first column being the grand mean. The grand mean is obtained in R from the tables of means as shown in the following output:

```
> Fac3Pilot.means$tables$"Grand mean"
64.25
```

For the example, the fitted model is thus

$$\psi = E[Y] = 64.25 + \frac{23.0}{2} x_T + \frac{1.5}{2} x_K + \frac{10.0}{2} x_T x_K - \frac{5.0}{2} x_C$$

The optimum yield occurs for T and K high and C low so it is estimated to be

$$\begin{aligned} \psi &= E[Y] \\ &= 64.25 + 11.5 \times 1 + 0.75 \times 1 + 5 \times 1 \times 1 - 2.5 \times (-1) \\ &= 84 \end{aligned}$$

Also note that a particular table of means can be obtained by using a linear trend model that includes the x -term corresponding to the table of means and any terms of lower degree. Hence, the table of $T \wedge K$ means can be obtained by substituting $x_T = \pm 1$, $x_K = \pm 1$ into

$$\psi = E[Y] = 64.25 + \frac{23.0}{2} x_T + \frac{1.5}{2} x_K + \frac{20.0}{2} x_T x_K$$

VIII.B Economy in experimentation

(Box, Hunter and Hunter, sec.10.8)

In most situations there are more factors to be investigated than can be conveniently accommodated with the time and budget available. Rather than duplicate a 2^3 factorial as was done in the pilot plant study, it is usually better to include a fourth variable and run an unreplicated 2^4 design. Or, as we shall see in later sections, run a half-replicated 2^5 and use 16 runs to investigate 5 factors.

The problem that would appear to arise from this suggestion is that if there is no replication then it will be impossible to measure the uncontrolled variation that has occurred in the experiment. However, when there are 4 or more factors it is unlikely that all factors will affect the response. Further it is usual that the magnitudes of effects are getting smaller as the order of the effect increases. Thus, it is likely that three-factor and higher-order interactions will be small and can be ignored without seriously affecting the conclusions drawn from the experiment.

a) Design of unreplicated 2^k experiments, including R expressions

As there is only a single replicate, these combinations will be completely randomized to the available units, the number of which must be equal to the total number of treatment combinations, 2^k . To generate a design in R, use `fac.gen` to generate the treatment combinations in Yates order and then `fac.layout` with the expressions for a CRD to randomize it. The following instructions would generate the layout for a 2^3 experiment. Note that, in practice, one would need to choose a random number between 0 and 1023 to use as the `seed`— the alternative is to leave the seed out but then the layout cannot be reproduced.

```
> #
> # Unreplicated two-level factorial
> #
> n <- 8
> mp <- c("-", "+")
> Fac3.2Level.Unrep.ran <- fac.gen(list(A = mp, B = mp, C = mp), order="yates")
> Fac3.2Level.Unrep.unit <- list(Runs = n)
> Fac3.2Level.Unrep.lay <- fac.layout(unrandomized = Fac3.2Level.Unrep.unit,
+                                     randomized = Fac3.2Level.Unrep.ran, seed=333)
> remove("Fac3.2Level.Unrep.ran")
```



```
> Fac3.2Level.Unrep.lay
  Units Permutation Runs A B C
1     1           4    1 - - +
2     2           2    2 + - -
3     3           8    3 + + +
4     4           5    4 - - -
5     5           1    5 + + -
6     6           7    6 - + +
7     7           6    7 + - +
8     8           3    8 - + -
```

Example VIII.2 A 2^4 process development study

The data given in the table below are the results, taken from Box, Hunter and Hunter, from a 2^4 design employed in a process development study.

K	T	P	C	Conversion (%)	Order of Runs
-	-	-	-	71	(8)
+	-	-	-	61	(2)
-	+	-	-	90	(10)
+	+	-	-	82	(4)
-	-	+	-	68	(15)
+	-	+	-	61	(9)
-	+	+	-	87	(1)
+	+	+	-	80	(13)
-	-	-	+	61	(16)
+	-	-	+	50	(5)
-	+	-	+	89	(11)
+	+	-	+	83	(14)
-	-	+	+	59	(3)
+	-	+	+	51	(12)
-	+	+	+	85	(6)
+	+	+	+	78	(7)

b) Initial analysis of variance

We could attempt to do an analysis of variance involving all possible interactions between the factors.

Example VIII.2 A 2^4 process development study (continued)

The following R output includes the instructions for performing an initial analysis of this data:

```
> mp <- c("-", "+")
> fnames <- list(Catal = mp, Temp = mp, Press = mp, Conc = mp)
> Fac4Proc.Treats <- fac.gen(generate = fnames, order="yates")
> Fac4Proc.dat <- data.frame(Runs = factor(1:16), Fac4Proc.Treats)
> remove("Fac4Proc.Treats")
> Fac4Proc.dat$Conv <- c(71,61,90,82,68,61,87,80,61,50,89,83,59,51,85,78)
> attach(Fac4Proc.dat)
> Fac4Proc.dat
```

```

  Runs Catal Temp Press Conc Conv
1      1    -    -    -    -    71
2      2    +    -    -    -    61
3      3    -    +    -    -    90
4      4    +    +    -    -    82
5      5    -    -    +    -    68
6      6    +    -    +    -    61
7      7    -    +    +    -    87
8      8    +    +    +    -    80
9      9    -    -    -    +    61
10     10   +    -    -    +    50
11     11   -    +    -    +    89
12     12   +    +    -    +    83
13     13   -    -    +    +    59
14     14   +    -    +    +    51
15     15   -    +    +    +    85
16     16   +    +    +    +    78
>
> Fac4Proc.aov <- aov(Conv ~ Catal * Temp * Press * Conc + Error(Runs),
Fac4Proc.dat)
> summary(Fac4Proc.aov)

Error: Runs

```

	Df	Sum Sq	Mean Sq
Catal	1	256.00	256.00
Temp	1	2304.00	2304.00
Press	1	20.25	20.25
Conc	1	121.00	121.00
Catal:Temp	1	4.00	4.00
Catal:Press	1	2.25	2.25
Temp:Press	1	6.25	6.25
Catal:Conc	1	6.043e-29	6.043e-29
Temp:Conc	1	81.00	81.00
Press:Conc	1	0.25	0.25
Catal:Temp:Press	1	2.25	2.25
Catal:Temp:Conc	1	1.00	1.00
Catal:Press:Conc	1	0.25	0.25
Temp:Press:Conc	1	2.25	2.25
Catal:Temp:Press:Conc	1	0.25	0.25

```

> round(yates.effects(Fac4Proc.aov, error.term="Runs", data=Fac4Proc.dat), 2)

```

Catal	Temp	Press
-8.00	24.00	-2.25
Conc	Catal:Temp	Catal:Press
-5.50	1.00	0.75
Temp:Press	Catal:Conc	Temp:Conc
-1.25	0.00	4.50
Press:Conc	Catal:Temp:Press	Catal:Temp:Conc
-0.25	-0.75	0.50
Catal:Press:Conc	Temp:Press:Conc	Catal:Temp:Press:Conc
-0.25	-0.75	-0.25

Now, as discussed before, a direct estimate of σ_R^2 , the uncontrolled variation, is not available as there were no replicates in the 16 runs.

c) Analysis assuming no 3-factor or 4-factor interactions

However, if we assume that all three-factor and four-factor interactions are negligible, then we could use these to estimate the uncontrolled variation as this is the only reason for them being nonzero. To do this rerun the analysis with the model consisting of a list of factors, separated by pluses, within parentheses and the list raised to the power of 2. The output including commands for this analysis is as follows:

Example VIII.2 A 2⁴ process development study (continued)

```
> # Perform analysis assuming 3- & 4-factor interactions negligible
> Fac4Proc.TwoFac.aov <- aov(Conv ~ (Catal + Temp + Press + Conc)^2 + Error(Runs),
+                               Fac4Proc.dat)
> summary(Fac4Proc.TwoFac.aov)
```

```
Error: Runs
      Df    Sum Sq   Mean Sq    F value    Pr(>F)
Catal   1    256.00    256.00   213.3333 2.717e-05
Temp    1   2304.00   2304.00  1920.0000 1.169e-07
Press   1    20.25     20.25    16.8750 0.0092827
Conc    1    121.00    121.00   100.8333 0.0001676
Catal:Temp  1     4.00     4.00     3.3333 0.1274640
Catal:Press  1     2.25     2.25     1.8750 0.2292050
Catal:Conc  1 5.394e-29 5.394e-29 4.495e-29 1.0000000
Temp:Press  1     6.25     6.25     5.2083 0.0713436
Temp:Conc  1    81.00    81.00    67.5000 0.0004350
Press:Conc  1     0.25     0.25     0.2083 0.6672191
Residuals  5     6.00     1.20
```

>
The analysis is summarized in the following analysis of variance table:

Source	df	SSq	MSq	F	Prob
Runs	15	2801.00			
Catal	1	256.00	256.00	213.33	<0.001
Temp	1	2304.00	2304.00	1920.00	<0.001
Press	1	20.25	20.25	16.87	0.009
Conc	1	121.00	121.00	100.83	<0.001
Catal#Temp	1	4.00	4.00	3.33	0.127
Catal#Press	1	2.25	2.25	1.87	0.229
Catal#Conc	1	0.00	0.00	0.00	1.000
Temp#Press	1	6.25	6.25	5.21	0.071
Temp#Conc	1	81.00	81.00	67.50	<0.001
Press#Conc	1	0.25	0.25	0.21	0.667
Residual	5	6.00	1.20		

This analysis indicates that there is an interaction between Temperature and Concentration and that Catalyst and Pressure also affect the Conversion percentage, although independently of the other factors.

However, there is a problem with this in that the test for main effects has been preceded by a test for interaction terms. Thus, testing is not independent and an allowance needs to be made for this. A further general problem in the use of higher-order interactions for error is that occasionally meaningful higher order interactions occur. The analysis presented above does not confront either of these problems.

d) Probability plot of Yates effects

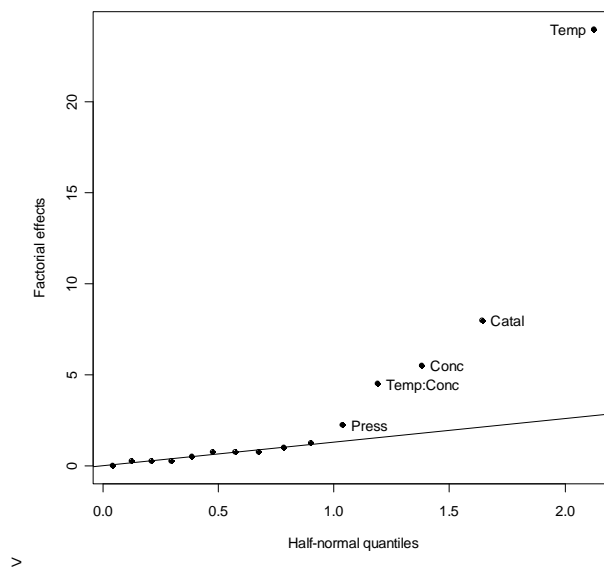
A method that does not require the assumption of zero higher-order interactions and allows for the dependence of the testing is a Normal probability plot of the Yates effects. For these reasons it is the *preferred method*, particularly for unreplicated and fractional experiments. In this plot the Yates effects are plotted against standard normal deviates. This is done on the basis that if there were no effects of the factors, the estimated effects would be just normally distributed uncontrolled variation. Under

these circumstances a straight-line plot of normal deviates versus Yates effects is expected. Significant effects, if any, will appear as outliers in the plot and the nonsignificant effects should lie along a straight line.

The function `qqyeffects` with an `aov.object` as the first argument produces the plot. Label those points that you consider significant by clicking on them (on the side on which you want the label) and then right-click on the graph and select `stop` when you have finished labelling effects. A list of selected effects will be produced and a regression line plotted through the origin and the unselected points.

Example VIII.2 A 2^4 process development study (continued)

```
> #
> #Yates effects probability plot
> #
> qqyeffects(Fac4Proc.aov, error.term="Runs", data=Fac4Proc.dat)
Effect(s) labelled: Press Temp:Conc Conc Catal Temp
```



I have clicked on the five effects with the largest absolute values as these appear to deviate substantially from the straight line going through the remainder of the effects. The large Yates effects correspond to Pressure, Temperature#Concentration, Concentration, Catalyst and Temperature. Hence, Temperature and Concentration interact in their effect on the Conversion percentage and Pressure and Catalyst each affect the response independently of any other factors. The fitted model is

$$\psi = E[Y] = \text{Pressure} + \text{Catalyst} + \text{Temperature} \wedge \text{Concentration}$$

e) Fitted values

Example VIII.2 A 2^4 process development study (continued)

For the example, the grand mean is obtained from the following output

```
> Fac4Proc.means <- model.tables(Fac4Proc.aov, type="means")
> Fac4Proc.means$tables$"Grand mean"
[1] 72.25
```

The fitted equation incorporating the significant effects is:

$$\psi = E[Y] = 72.25 - \frac{8.0}{2} x_K - \frac{2.25}{2} x_P + \frac{24.0}{2} x_T - \frac{5.5}{2} x_C + \frac{4.5}{2} x_T x_C$$

where x_K , x_T and x_C take the values -1 and $+1$.

To predict the response for a particular combination of the treatments, substitute in the appropriate combination of -1 and $+1$. For example, the predicted response for high catalyst, pressure and temperature but a low concentration is calculated as follows:

$$\begin{aligned} E[Y_k] &= 72.25 - \frac{8.0}{2} x_K - \frac{2.25}{2} x_P + \frac{24.0}{2} x_T - \frac{5.5}{2} x_C + \frac{4.5}{2} x_T x_C \\ &= 72.25 - \frac{8.0}{2} (+1) - \frac{2.25}{2} (+1) + \frac{24.0}{2} (+1) - \frac{5.5}{2} (-1) + \frac{4.5}{2} (+1)(-1) \\ &= 72.25 + \frac{-8.0 - 2.25 + 24.0 + 5.5 - 4.5}{2} = 79.625 \end{aligned}$$

f) Diagnostic checking

Having determined the significant terms one can reanalyze with just these terms, and those marginal to them, included in the `model.formula` and obtain the Residuals from this model. The Residuals can be used to do the usual diagnostic checking. For this to be effective requires that the number of fitted effects is small compared to the total number of effects in the experiment and that there is at least 10 degrees of freedom for the Residual line in the analysis of variance.

Example VIII.2 A 2⁴ process development study (continued)

For the example the R output file is as follows:

```
> #
> # Diagnostic checking
> #
> Fac4Proc.Fit.aov <- aov(Conv ~ Temp * Conc + Catal + Press + Error(Runs),
+                               Fac4Proc.dat)
> summary(Fac4Proc.Fit.aov)

Error: Runs
      Df Sum Sq Mean Sq F value    Pr(>F)
Temp   1 2304.00  2304.00 1228.800 8.464e-12
Conc   1  121.00   121.00   64.533 1.135e-05
Catal  1  256.00   256.00  136.533 3.751e-07
Press  1   20.25    20.25   10.800  0.0082
Temp:Conc 1  81.00    81.00   43.200 6.291e-05
Residuals 10  18.75    1.88

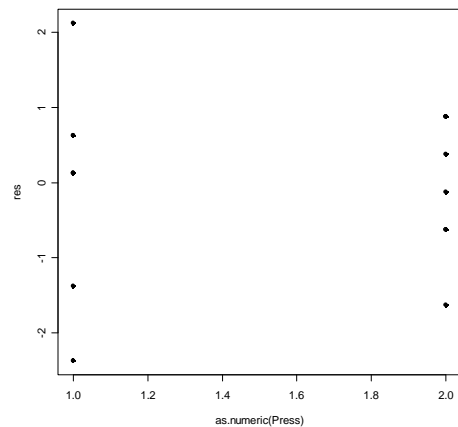
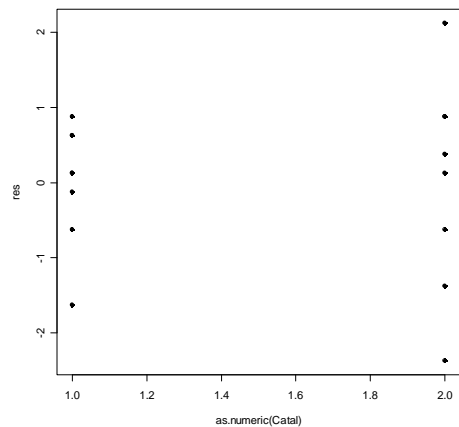
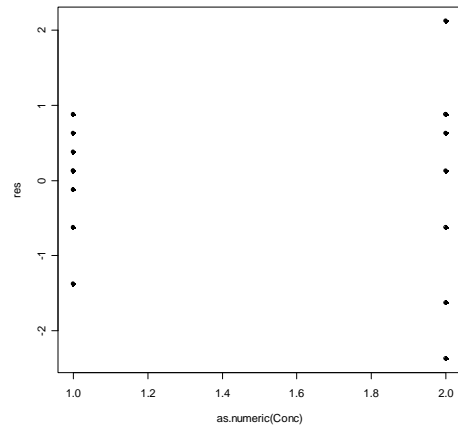
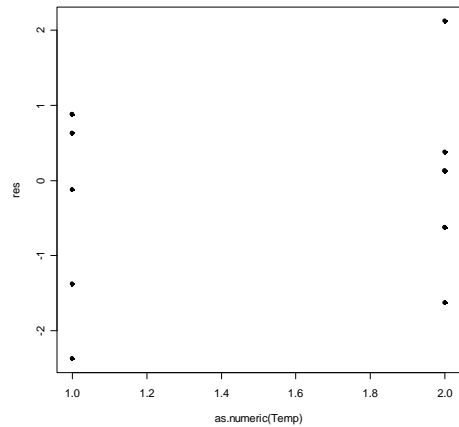
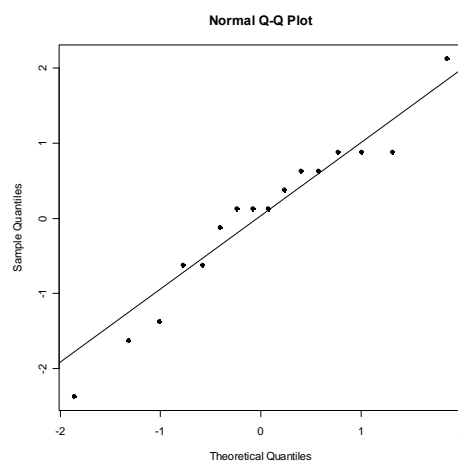
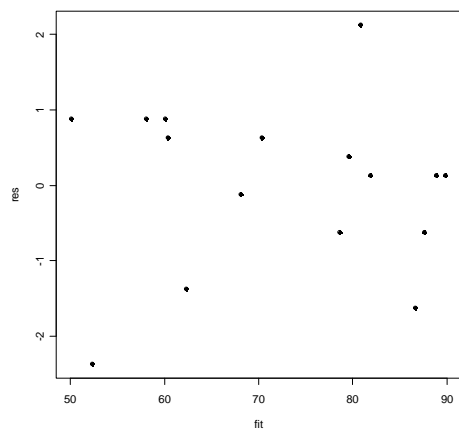
> tukey.1df(Fac4Proc.Fit.aov, Fac4Proc.dat, error.term="Runs")
$Tukey.SS
[1] 1.422313

$Tukey.F
[1] 0.7387496
```

```
$Tukey.p
[1] 0.4123697
```

```
$Devn.SS
[1] 17.32769
```

```
> res <- resid.errors(Fac4Proc.Fit.aov)
> fit <- fitted.errors(Fac4Proc.Fit.aov)
> plot(fit, res, pch=16)
> qqnorm(res, pch=16)
> qqline(res)
> plot(as.numeric(Temp), res, pch=16)
> plot(as.numeric(Conc), res, pch=16)
> plot(as.numeric(Catal), res, pch=16)
> plot(as.numeric(Press), res, pch=16)
```



The residual-versus-fitted-values and residuals-versus-factors plots do not seem to be displaying any particular pattern, although there is evidence of two large residuals, one negative and the other positive. Tukey's one-degree-of-freedom-for-nonadditivity is not significant. The Normal Probability plot shows a straight-line trend. Consequently, the only issue requiring attention is that of the two large residuals.

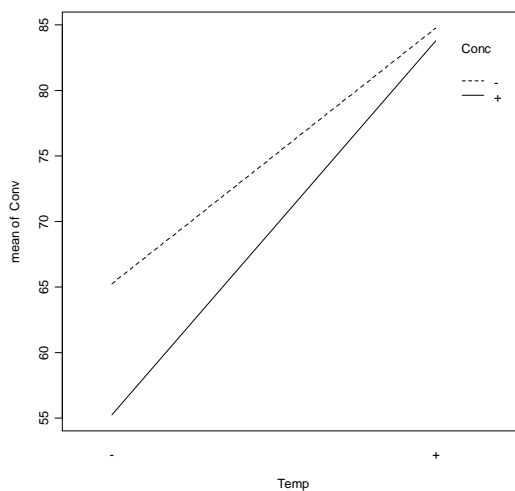
g) Treatment differences

As a result of the analysis we have identified the model that describes the affect of the factors on the response variable and hence the tables of means that need to be examined to determine the exact nature of the effects.

Example VIII.2 A 2⁴ process development study (continued)

The R output that examines the appropriate tables of means is as follows:

```
> #
> # treatment differences
> #
> Fac4Proc.means <- model.tables(Fac4Proc.aov, type="means")
> Fac4Proc.means$tables$"Grand mean"
[1] 72.25
> Fac4Proc.means$tables$"Temp:Conc"
      Conc
Temp -   +
  - 65.25 55.25
  + 84.75 83.75
> Fac4Proc.means$tables$"Catal"
      Catal
  -      +
76.25 68.25
> Fac4Proc.means$tables$"Press"
      Press
  -      +
73.375 71.125
> interaction.plot(Temp, Conc, Conv)
> q <- qtukey(0.95, 4, 10)
> q
[1] 4.326582
```



From the interaction plot, the two treatments that have temperature set high appear to give the greatest conversion rate. However, is there a significant difference between concentration low and high, when temperature is high? Tukey's HSD procedure is used to answer this question.

$$w(5\%) = \frac{4.326582}{\sqrt{2}} \times \sqrt{\frac{1.875 \times 2}{4}} = 2.96$$

From the tables of means, as the difference between the two means is 1.0 and so less than Tukey's HSD, there is no significant difference between them. It is concluded that either setting of concentration can be used. Consequently, the maximum conversion rate will be achieved with both catalyst and pressure set low, temperature set high and either setting of concentration.

VIII.C Confounding in factorial experiments

a) Total confounding of effects

It happens it is not always possible to get a complete set of the treatments into a block or row of an experiment. The incomplete block designs and Youden square designs are available for experiments that involve just a single set of treatments. However, the need for incomplete sets of treatments in a block is even more of a problem with factorial experiments where the number of treatments tends to be larger; on occasion, very large since the number of treatments increases geometrically with the number of factors and levels employed in the experiment. The solution to the problem must take into account the several factors. This turns out to be somewhat of an advantage in that it is possible to have incomplete sets of treatments and retain the orthogonality of the analysis.

Definition VIII.9: A **confounded factorial experiment** is one in which incomplete sets of treatments occur in each block.

The choice of which treatments to put in each block is done by deciding which effect is to be *confounded* with block differences.

Definition VIII.10: A **generator** for a confounded experiment is a relationship that specifies which effect is equal to a particular block contrast.

Example VIII.3 Complete sets of factorial treatments in 2 blocks

Suppose that a trial is to be conducted using a 2^3 factorial design and, to make the eight runs as homogeneous as possible, it desirable that batches of raw material sufficient for a complete set of treatments be blended together. However, suppose that the available blender can only blend sufficient for four runs at a time. This means that two blends will be required for a complete set of treatments.

It seems intuitively reasonable that we should arrange the treatments into two sets in such a way that the effect on the conclusions drawn from the experiment is minimized. Thus, the least serious thing to do is to have the three factor interaction

mixed up or *confounded* with blocks and the other effects unconfounded. To arrange for this to happen is easily done with the table of pluses and minuses. The following is the table for the three factors:

Treatment	A	B	C	AB	AC	BC	ABC
1	-	-	-	+	+	+	-
2	+	-	-	-	-	+	+
3	-	+	-	-	+	-	+
4	+	+	-	+	-	-	-
5	-	-	+	+	-	-	+
6	+	-	+	-	+	-	-
7	-	+	+	-	-	+	-
8	+	+	+	+	+	+	+

Suppose we arrange to have all the treatments with a minus in the ABC column of the table together using one blend and the treatments with a plus in the ABC column using a second blend. Then we have divided the 8 treatments into 2 groups based on the minuses and pluses in the ABC column. In laying out the experiment the two groups are randomly assigned to the two different blends. That is, the allocation to blends might be as shown below:

Treatment	A	B	C	AB	AC	BC	ABC	Group	Blend
1	-	-	-	+	+	+	-	1	2
2	+	-	-	-	-	+	+	2	1
3	-	+	-	-	+	-	+	2	1
4	+	+	-	+	-	-	-	1	2
5	-	-	+	+	-	-	+	2	1
6	+	-	+	-	+	-	-	1	2
7	-	+	+	-	-	+	-	1	2
8	+	+	+	+	+	+	+	2	1

We see that the Blend difference has been associated, and hence confounded, with the ABC effect. The generator for this design is thus $\text{Blend} = \text{ABC}$. Examination of this table reveals that all other effects have two minus and two plus observations in each blend. Hence, they are not affected by blend.

The analysis can still be accomplished using Yates algorithm on the 8 runs with the three treatment factors; it just has to be remembered that the $A\#B\#C$ term is associated with Blend differences.

The experimental structure and the analysis of variance table for this experiment are:

Structure	Formula
Unrandomized	2 Blends/4 Runs
Randomized	2 A*2 B*2 C

Source	df	E[MSq]	
Blends	1		
A#B#C	1	$\sigma_{BR}^2 + 4\sigma_B^2$	$+q_{ABC}(\psi)$
Runs[Blends]	6		
A	1	σ_{BR}^2	$+q_A(\psi)$
B	1	σ_{BR}^2	$+q_B(\psi)$
A#B	1	σ_{BR}^2	$+q_{AB}(\psi)$
C	1	σ_{BR}^2	$+q_C(\psi)$
A#C	1	σ_{BR}^2	$+q_{AC}(\psi)$
B#C	1	σ_{BR}^2	$+q_{BC}(\psi)$

In this experiment, we have gained the advantage of having blocks of size 4 but at the price of being unable to estimate the three-factor interaction. As can be seen from the expected mean squares, Blend variability and the A#B#C interaction cannot be estimated separately. This is not a problem if the interaction can be assumed to be negligible.

Example VIII.4 Repeated two block experiment

It may be considered desirable to increase the size of the experiment to increase the precision with which the effects are estimated. If there are no extra factors available for inclusion, then the basic design could be replicated say r times which requires $2r$ blends. There is a choice as to how the 2 groups of treatments are to be assigned to the blends. For example, the groups of treatments could be assigned completely at random so that each group occurred with r out of the $2r$ blends. Another possibility is that the blends are formed into blocks of two and the groups of treatments randomized to the two blends within each block; to make this worthwhile would need to be able to identify relatively similar pairs of blends, otherwise complete randomization would be preferable. The experimental structure for the completely randomized case is as for the previous experiment, except that there would be $2r$ blends. The analysis would be:

Source	df	E[MSq]	
Blends	$2r-1$		
A#B#C	1	σ_{BR}^2	$+4\sigma_B^2 + q_{ABC}(\psi)$
Residual	$2(r-1)$	σ_{BR}^2	$+4\sigma_B^2$
Runs[Blends]	$6r$		
A	1	σ_{BR}^2	$+q_A(\psi)$
B	1	σ_{BR}^2	$+q_B(\psi)$
A#B	1	σ_{BR}^2	$+q_{AB}(\psi)$
C	1	σ_{BR}^2	$+q_C(\psi)$
A#C	1	σ_{BR}^2	$+q_{AC}(\psi)$
B#C	1	σ_{BR}^2	$+q_{BC}(\psi)$
Residual	$6(r-1)$	σ_{BR}^2	

Example VIII.5 Complete sets of factorial treatments in 4 blocks

Suppose that a 2^3 experiment is to be run but that the blends are only large enough for two runs using one blend. How can we design the experiment best? There will be four groups of treatments which we can represent using two factors at two levels. Let's suppose it is decided to associate the ABC interaction and one of the expendable two-factor interactions, say BC, with the blend differences. The table of coefficients is as follows:

Treatment	A	B	C	B ₁	B ₂	Group	Blend
	1	2	3	4	5		
1	-	-	-	+	-	1	3
2	+	-	-	+	+	2	4
3	-	+	-	-	+	3	1
4	+	+	-	-	-	4	2
5	-	-	+	-	+	3	1
6	+	-	+	-	-	4	2
7	-	+	+	+	-	1	3
8	+	+	+	+	+	2	4

The columns labelled B₁ and B₂ are just the columns of \pm for BC and ABC; that is, the arrangement is generated by B₁ = BC and B₂ = ABC. The treatments in a particular group are determined by placing those with the same combination of \pm for B₁ and B₂ in the same group. The 4 groups are then randomized to the 4 blends.

There is a serious weakness with this design!!! There are 3 degrees of freedom associated with group differences and we know of only two degrees of freedom

confounded with Blends. What has happened to the third degree of freedom? Well, it is obtained as the interaction of B_1 and B_2 . It will be found if you multiply these columns together you obtain the A column. Disaster! a main effect has been confounded with Blends. The experimental structure and analysis of variance table for this experiment are:

Structure	Formula
unrandomized	4 Blends/2 Runs
randomized	2 A*2 B*2 C

Source	df	E[MSq]
Blends	3	
A	1	$\sigma_{BR}^2 + 2\sigma_B^2 + q_A(\psi)$
B#C	1	$\sigma_{BR}^2 + 2\sigma_B^2 + q_{BC}(\psi)$
A#B#C	1	$\sigma_{BR}^2 + 2\sigma_B^2 + q_{ABC}(\psi)$
Runs[Blends]	4	
B	1	$\sigma_{BR}^2 + q_B(\psi)$
A#B	1	$\sigma_{BR}^2 + q_{AB}(\psi)$
C	1	$\sigma_{BR}^2 + q_C(\psi)$
A#C	1	$\sigma_{BR}^2 + q_{AC}(\psi)$

Fortunately, a calculus is available for avoiding such traps.

Theorem VIII.1: Let the columns in a table of \pm s whose rows specify the combinations of the factors in a two-factor experiment be numbered **1, 2, ..., m**. Also, let **I** be the column consisting entirely of +s. The elementwise product of two columns is commutative, the elementwise product of a column with **I** is the column itself and the elementwise product of a column with itself is **I**; that is,

$$ij = ji, li = il = i \text{ and } ii = I \text{ where } i, j = 1, 2, \dots, m$$

Proof: follows directly from a consideration of the results of multiplying ± 1 s together ■

Example VIII.5 Complete sets of factorial treatments in 4 blocks (continued)

Firstly, number the factors as shown in the table. Thus, we can write

$$I = 11 = 22 = 33 = 44 = 55$$

Now in the blocking arrangement just considered **4 = 23** and **5 = 123**.

The **45** column is thus **45 = 23.123 = 12233 = 1II = 1** which shows that **45** is identical to **1** and that the interaction **45** is confounded with **1**.

A better arrangement is obtained by confounding the two block variables with any two of the two-factor interactions. The third degree of freedom is then confounded with the third two-factor interaction. Thus, for $4 = 12$, $5 = 13$, the interaction 45 is confounded with 23 since $45 = 1123 = 23$.

The experimental arrangement is indicated in the following table:

Treatment	A	B	C	B ₁	B ₂	Group
	1	2	3	4	5	
1	–	–	–	+	+	1
2	+	–	–	–	–	2
3	–	+	–	–	+	3
4	+	+	–	+	–	4
5	–	–	+	+	–	4
6	+	–	+	–	+	3
7	–	+	+	–	–	2
8	+	+	+	+	+	1

The groups would be randomized to the blends and the order of the two runs for each blend would be randomized for each blend.

The analysis of variance table for the experiment (same structure as before) is:

Source	df	E[MSq]	
Blends	3		
A#B	1	σ_{BR}^2	$+2\sigma_B^2 + q_{AB}(\psi)$
A#C	1	σ_{BR}^2	$+2\sigma_B^2 + q_{AC}(\psi)$
B#C	1	σ_{BR}^2	$+2\sigma_B^2 + q_{BC}(\psi)$
Runs[Blends]	4		
A	1	σ_{BR}^2	$+q_A(\psi)$
B	1	σ_{BR}^2	$+q_B(\psi)$
C	1	σ_{BR}^2	$+q_C(\psi)$
A#B#C	1	σ_{BR}^2	$+q_{ABC}(\psi)$

The two runs for each group are complimentary in the sense that the plus minus pattern of one run is precisely the opposite to that of the second run. For example, in group 2, the plus and minus signs for the pairs of runs are +— and —++.

Definition VIII.11: Two factor combinations are called a **fold-over pair** if the signs for the factors in one combination are exactly the opposite of those in the other combination. ■

Any 2^k factorial may be broken into 2^{k-1} blocks of size 2 by forming blocks such that each of them consists of a different fold-over pair. Such blocking arrangements leave the main effects of the k factors unconfounded with blocks. However, all two factor interactions are confounded with blocks.

Example VIII.6: Repeated four block experiment

As before we could replicate the whole experiment so that there are $4r$ blends. The 4 groups of treatments might then be assigned completely at random or in blocks. Suppose that the groups have been assigned completely at random to the $4r$ blends so that each group occurs r times. The analysis would then be:

Source	df	E[MSq]	
Blends	$4r-1$		
A#B	1	σ_{BR}^2	$+2\sigma_B^2 + q_{AB}(\psi)$
A#C	1	σ_{BR}^2	$+2\sigma_B^2 + q_{AC}(\psi)$
B#C	1	σ_{BR}^2	$+2\sigma_B^2 + q_{BC}(\psi)$
Residual	$4(r-1)$	σ_{BR}^2	$+2\sigma_B^2$
Runs[Blends]	$4r$		
A	1	σ_{BR}^2	$+q_A(\psi)$
B	1	σ_{BR}^2	$+q_B(\psi)$
C	1	σ_{BR}^2	$+q_C(\psi)$
A#B#C	1	σ_{BR}^2	$+q_{ABC}(\psi)$
Residual	$4(r-1)$	σ_{BR}^2	

The expected mean squares for this experiment are based on equating the unrandomized and randomized factors with random and fixed factors, respectively. There are thus two sources of uncontrolled variation: differences between blends (σ_{BR}^2) and between runs within blends (σ_B^2). The analysis indicates that the two-factor interactions are going to be affected by blend differences whereas the other effects will not. As blends are likely to be more variable than runs within blends, if blocking is effective as planned, the two-factor interactions are determined with less precision than the other effects. This will be a problem if it is anticipated that there are likely to be two-factor interactions; in such circumstances one needs to consider partial confounding.

b) Partial confounding of effects

In experiments where the complete set of treatments are replicated it is possible to confound different effects in each replicate. This is called *partial confounding*.

Definition VIII.12: Partial confounding occurs when the effects confounded between blocks is different for different groups of blocks

Example VIII.7 Partial confounding in a repeated four block experiment

Suppose that we are wanting to run a four block experiment with repeats such as that discussed in example VIII.6. The total confounding options discussed for that example may be unsatisfactory because of the need to confound two-factor interactions. The use of partial confounding is investigated for this experiment. Consider the following generators for an experiment involving sets of 4 blocks:

Set	Group generators		
I	4 = 12	5 = 13	45 = 23
II	4 = 123	5 = 23	45 = 1
III	4 = 123	5 = 13	45 = 2
IV	4 = 123	5 = 12	45 = 3

Thus the three factor interaction is confounded in three sets, the two factor interactions in 2 sets and the main effects in 1 set. The formation of the groups of treatments is shown in the following table.

Set	Treatment	A 1	B 2	C 3	B ₁ 4	B ₂ 5	Group
					12	13	
I	1	-	-	-	+	+	1
	2	+	-	-	-	-	2
	3	-	+	-	-	+	3
	4	+	+	-	+	-	4
	5	-	-	+	+	-	4
	6	+	-	+	-	+	3
	7	-	+	+	-	-	2
	8	+	+	+	+	+	1
					23	123	
II	1	-	-	-	+	-	5
	2	+	-	-	+	+	6
	3	-	+	-	-	+	7
	4	+	+	-	-	-	8
	5	-	-	+	-	+	7
	6	+	-	+	-	-	8
	7	-	+	+	+	-	5
	8	+	+	+	+	+	6
					13	123	
III	1	-	-	-	+	-	9
	2	+	-	-	-	+	10
	3	-	+	-	+	+	11
	4	+	+	-	-	-	12
	5	-	-	+	-	+	10
	6	+	-	+	+	-	9
	7	-	+	+	-	-	12
	8	+	+	+	+	+	11
					12	123	
IV	1	-	-	-	+	-	13
	2	+	-	-	-	+	14
	3	-	+	-	-	+	14
	4	+	+	-	+	-	13
	5	-	-	+	+	+	15
	6	+	-	+	-	-	16
	7	-	+	+	-	-	16
	8	+	+	+	+	+	15

The groups (pairs) of treatments in this table would then be randomized to the blends and the two treatment combinations in each group randomized to the two runs made for each blend. The layout and data for the experiment are shown in the table below. A layout for such a design can be produced in R. For example, one could obtain the layout for each Set and then combine these into a single `data.frame`.

Blends	Runs	Group	A	B	C	Yield
1	1	15	-	-	+	54.40
	2		+	+	+	81.40
2	1	10	+	-	-	70.60
	2		-	-	+	46.60
3	1	5	-	-	-	61.50
	2		-	+	+	44.50
4	1	9	-	-	-	60.70
	2		+	-	+	82.70
5	1	2	-	+	+	51.90
	2		+	-	-	79.90
6	1	16	-	+	+	43.90
	2		+	-	+	84.90
7	1	7	-	-	+	55.80
	2		-	+	-	59.80
8	1	14	+	-	-	73.50
	2		-	+	-	61.50
9	1	3	+	-	+	81.50
	2		-	+	-	50.50
10	1	11	+	+	+	80.90
	2		-	+	-	51.90
11	1	12	+	+	-	76.40
	2		-	+	+	53.40
12	1	8	+	+	-	68.60
	2		+	-	+	86.60
13	1	13	-	-	-	63.90
	2		+	+	-	69.90
14	1	6	+	-	-	75.90
	2		+	+	+	86.90
15	1	1	+	+	+	83.30
	2		-	-	-	63.30
16	1	4	+	+	-	63.50
	2		-	-	+	44.50

The experimental structure for this experiment is:

Structure	Formula
unrandomized	16 Blends/2 Runs
randomized	2 A*2 B*2 C

The analysis of variance table for this experiment is:

Source	df	MSq	E[MSq]		F	Prob
Blends						
A	1	1161.62	σ_{BR}^2	$+2\sigma_B^2 + q_A(\Psi)$	34.55	<.001
B	1	0.50	σ_{BR}^2	$+2\sigma_B^2 + q_B(\Psi)$	0.01	0.906
C	1	2.20	σ_{BR}^2	$+2\sigma_B^2 + q_C(\Psi)$	0.07	0.804
A#B	1	0.72	σ_{BR}^2	$+2\sigma_B^2 + q_{AB}(\Psi)$	0.02	0.887
A#C	1	289.00	σ_{BR}^2	$+2\sigma_B^2 + q_{AC}(\Psi)$	8.60	0.019
B#C	1	82.81	σ_{BR}^2	$+2\sigma_B^2 + q_{BC}(\Psi)$	2.46	0.155
A#B#C	1	0.20	σ_{BR}^2	$+2\sigma_B^2 + q_{ABC}(\Psi)$	0.01	0.940
Residual	8	33.62	σ_{BR}^2	$+2\sigma_B^2$		
Runs[Blends]						
A	1	3313.50	σ_{BR}^2	$+q_A(\Psi)$	1016.64	<0.001
B	1	150.00	σ_{BR}^2	$+q_B(\Psi)$	46.02	<0.001
C	1	10.67	σ_{BR}^2	$+q_C(\Psi)$	3.27	0.104
A#B	1	9.00	σ_{BR}^2	$+q_{AB}(\Psi)$	2.76	0.131
A#C	1	625.00	σ_{BR}^2	$+q_{AC}(\Psi)$	191.76	<0.001
B#C	1	0.00	σ_{BR}^2	$+q_{BC}(\Psi)$	0.00	1.000
A#B#C	1	0.50	σ_{BR}^2	$+q_{ABC}(\Psi)$	0.15	0.704
Residual	9	3.26	σ_{BR}^2			
Total	31					

Information summary		
Model term	e.f.	nonorthogonal terms
Blends stratum		
A	0.250	
B	0.250	
C	0.250	
A#B	0.500	
A#C	0.500	
B#C	0.500	
A#B#C	0.750	
Runs[Blends] stratum		
A	0.750	Blends
B	0.750	Blends
C	0.750	Blends
A#B	0.500	Blends
A#C	0.500	Blends
B#C	0.500	Blends
A#B#C	0.250	Blends

Clearly, the experiment is balanced; the analysis can be accomplished using Yates algorithm, taking into account the efficiency with which various terms are estimated. Also, diagnostic checking would be performed on the residuals.

VIII.D Fractional factorial designs at two levels

(Box, Hunter & Hunter, ch. 12)

The number of runs required by a full 2^k increases geometrically as k increases. However, it turns out that when k is not small the desired information can often be obtained by performing only a fraction of the full factorial design.

In previous sections it was suggested that there was a great deal of redundancy in a factorial experiment in that higher-order interactions are likely to be negligible and some variables may not affect the response at all. We utilized this fact to suggest that it was not necessary to replicate the various treatments. In this section we go one step further by saying that you need take only a fraction of the full factorial design.

Consider a 2^7 design. A complete factorial arrangement requires $2^7 = 128$ runs. From these runs 128 effects can be calculated as follows:

average	main effects	interactions of order					
		2	3	4	5	6	7
1	7	21	35	35	21	7	1

So there tends to be redundancy in 2^k designs in that there is likely to be an excess number of interactions that can be estimated and sometimes an excess number of

variables studied. Fractional factorial designs exploit this redundancy. To illustrate the ideas the example given by Box, Hunter and Hunter will be presented. It involves a half-fraction of a 2^5 .

Example VIII.8 A complete 2^5 factorial experiment

The data from a complete 2^5 is given in the table below. Note that the results are not in the randomized order that would be order in which the runs were actually conducted. To make it easier to see how the design was constructed, the order of the runs is such that the treatments are in Yates order.

Results from a 2^5 factorial design — chemical experiment

Factor	-	+
1 feed rate (l/min)	10	15
2 catalyst (%)	1	2
3 agitation rate (rpm)	100	120
4 temperature ($^{\circ}$ C)	140	180
5 concentration (%)	3	6

Run	Factor					% reacted
	1	2	3	4	5	
1	-	-	-	-	-	61
*2	+	-	-	-	-	53
*3	-	+	-	-	-	63
4	+	+	-	-	-	61
*5	-	-	+	-	-	53
6	+	-	+	-	-	56
7	-	+	+	-	-	54
*8	+	+	+	-	-	61
*9	-	-	-	+	-	69
10	+	-	-	+	-	61
11	-	+	-	+	-	94
*12	+	+	-	+	-	93
13	-	-	+	+	-	66
*14	+	-	+	+	-	60
*15	-	+	+	+	-	95
16	+	+	+	+	-	98
*17	-	-	-	-	+	56
18	+	-	-	-	+	63
19	-	+	-	-	+	70
*20	+	+	-	-	+	65
21	-	-	+	-	+	59
*22	+	-	+	-	+	55
*23	-	+	+	-	+	67
24	+	+	+	-	+	65
25	-	-	-	+	+	44

*26	+	-	-	+	+	45
*27	-	+	-	+	+	78
28	+	+	-	+	+	77
*29	-	-	+	+	+	49
30	+	-	+	+	+	42
31	-	+	+	+	+	81
*32	+	+	+	+	+	82

The experimental structure for this experiment is the standard structure for a 2^5 CRD; it is:

Structure	Formula
unrandomized	32 Runs
randomized	2 Feed*2 Catal*2 Agitation*2 Temp*2 Conc

The R output for the analysis of this example is as follows:

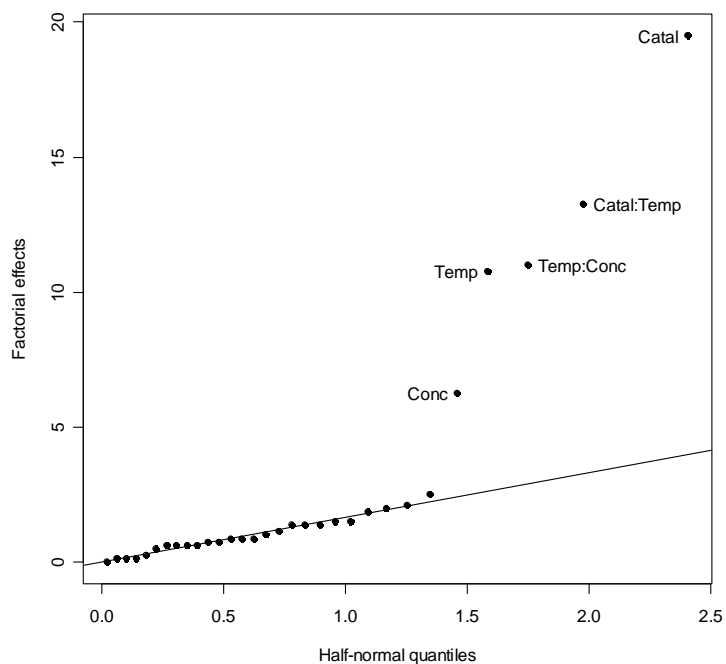
```
> #
> # set up data.frame and analyse
> #
> mp <- c("-", "+")
> fnames <- list(Feed = mp, Catal = mp, Agitation = mp, Temp = mp, Conc = mp)
> Fac5Reac.Treats <- fac.gen(generate = fnames, order="yates")
> Fac5Reac.dat <- data.frame(Runs = factor(1:32), Fac5Reac.Treats)
> remove("Fac5Reac.Treats")
> Fac5Reac.dat$Reacted <- c(61,53,63,61,53,56,54,61,69,61,94,93,66,60,95,98,
+ 56,63,70,65,59,55,67,65,44,45,78,77,49,42,81,82)
> Fac5Reac.dat
  Runs Feed Catal Agitation Temp Conc Reacted
1     1   -    -         -      -    -      61
2     2   +    -         -      -    -      53
3     3   -    +         -      -    -      63
4     4   +    +         -      -    -      61
5     5   -    -         +      -    -      53
6     6   +    -         +      -    -      56
7     7   -    +         +      -    -      54
8     8   +    +         +      -    -      61
9     9   -    -         -      +    -      69
10    10  +    -         -      +    -      61
11    11  -    +         -      +    -      94
12    12  +    +         -      +    -      93
13    13  -    -         +      +    -      66
14    14  +    -         +      +    -      60
15    15  -    +         +      +    -      95
16    16  +    +         +      +    -      98
17    17  -    -         -      -    +      56
18    18  +    -         -      -    +      63
19    19  -    +         -      -    +      70
20    20  +    +         -      -    +      65
21    21  -    -         +      -    +      59
22    22  +    -         +      -    +      55
23    23  -    +         +      -    +      67
24    24  +    +         +      -    +      65
25    25  -    -         -      +    +      44
26    26  +    -         -      +    +      45
27    27  -    +         -      +    +      78
28    28  +    +         -      +    +      77
29    29  -    -         +      +    +      49
30    30  +    -         +      +    +      42
31    31  -    +         +      +    +      81
32    32  +    +         +      +    +      82
```

```
> Fac5Reac.aov <- aov(Reacted ~ Feed * Catal * Agitation * Temp * Conc +
Error(Runs), Fac5Reac.dat)
> summary(Fac5Reac.aov)
```

Error: Runs

	Df	Sum Sq	Mean Sq
Feed	1	15.12	15.12
Catal	1	3042.00	3042.00
Agitation	1	3.12	3.12
Temp	1	924.50	924.50
Conc	1	312.50	312.50
Feed:Catal	1	15.12	15.12
Feed:Agitation	1	4.50	4.50
Catal:Agitation	1	6.12	6.12
Feed:Temp	1	6.13	6.13
Catal:Temp	1	1404.50	1404.50
Agitation:Temp	1	36.12	36.12
Feed:Conc	1	0.12	0.12
Catal:Conc	1	32.00	32.00
Agitation:Conc	1	6.12	6.12
Temp:Conc	1	968.00	968.00
Feed:Catal:Agitation	1	18.00	18.00
Feed:Catal:Temp	1	15.13	15.13
Feed:Agitation:Temp	1	4.50	4.50
Catal:Agitation:Temp	1	10.13	10.13
Feed:Catal:Conc	1	28.12	28.12
Feed:Agitation:Conc	1	50.00	50.00
Catal:Agitation:Conc	1	0.13	0.13
Feed:Temp:Conc	1	3.13	3.13
Catal:Temp:Conc	1	0.50	0.50
Agitation:Temp:Conc	1	0.13	0.13
Feed:Catal:Agitation:Temp	1	4.565e-28	4.565e-28
Feed:Catal:Agitation:Conc	1	18.00	18.00
Feed:Catal:Temp:Conc	1	3.12	3.12
Feed:Agitation:Temp:Conc	1	8.00	8.00
Catal:Agitation:Temp:Conc	1	3.13	3.13
Feed:Catal:Agitation:Temp:Conc	1	2.00	2.00

```
> qqyeffects(Fac5Reac.aov, error.term="Runs", data=Fac5Reac.dat)
Effect(s) labelled: Conc Temp Temp:Conc Catal:Temp Catal
```



```

> round(yates.effects(Fac5Reac.aov, error.term="Runs", data=Fac5Reac.dat), 2)
      Feed          Catal
      -1.37         19.50
      Agitation      Temp
      -0.62         10.75
      Conc           Feed:Catal
      -6.25         1.37
      Feed:Agitation Catal:Agitation
      0.75         0.87
      Feed:Temp      Catal:Temp
      -0.88         13.25
      Agitation:Temp Feed:Conc
      2.12         0.12
      Catal:Conc     Agitation:Conc
      2.00         0.87
      Temp:Conc      Feed:Catal:Agitation
      -11.00        1.50
      Feed:Catal:Temp Feed:Agitation:Temp
      1.38         -0.75
      Catal:Agitation:Temp Feed:Catal:Conc
      1.13         -1.87
      Feed:Agitation:Conc Catal:Agitation:Conc
      -2.50        0.13
      Feed:Temp:Conc  Catal:Temp:Conc
      0.63         -0.25
      Agitation:Temp:Conc Feed:Catal:Agitation:Temp
      0.13         0.00
      Feed:Catal:Agitation:Conc Feed:Catal:Temp:Conc
      1.50         0.62
      Feed:Agitation:Temp:Conc Catal:Agitation:Temp:Conc
      1.00        -0.63
Feed:Catal:Agitation:Temp:Conc
      -0.50
> Fac5Reac.Fit.aov <- aov(Reacted ~ Temp * (Catal + Conc) + Error(Runs),
+                           Fac5Reac.dat)
> summary(Fac5Reac.Fit.aov)

Error: Runs
      Df Sum Sq Mean Sq F value    Pr(>F)
Temp    1  924.5   924.5  83.317 1.368e-09
Catal    1 3042.0  3042.0 274.149 2.499e-15
Conc     1  312.5   312.5  28.163 1.498e-05
Temp:Catal 1 1404.5  1404.5 126.575 1.726e-11
Temp:Conc  1  968.0   968.0  87.237 8.614e-10
Residuals 26  288.5    11.1
> #
> # Diagnostic checking
> #
> tukey.1df(Fac5Reac.Fit.aov, Fac5Reac.dat, error.term="Runs")
$Tukey.SS
[1] 10.62126

$Tukey.F
[1] 0.9555664

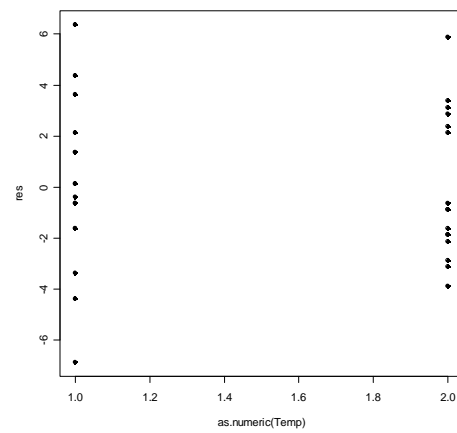
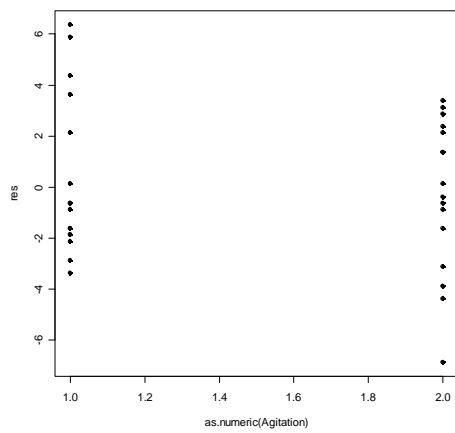
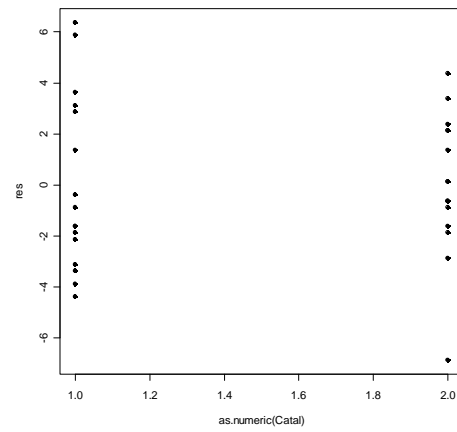
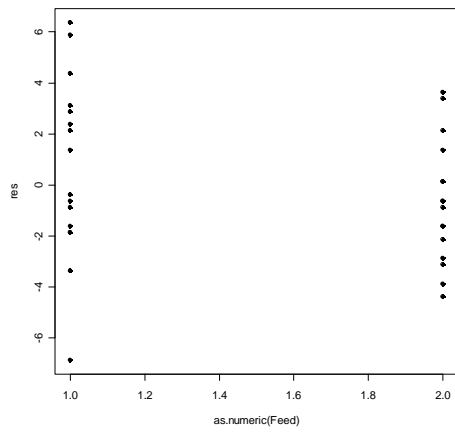
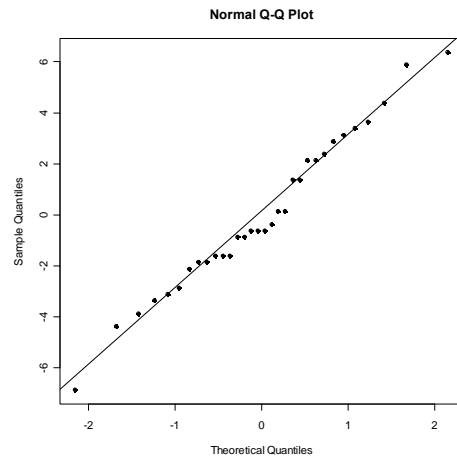
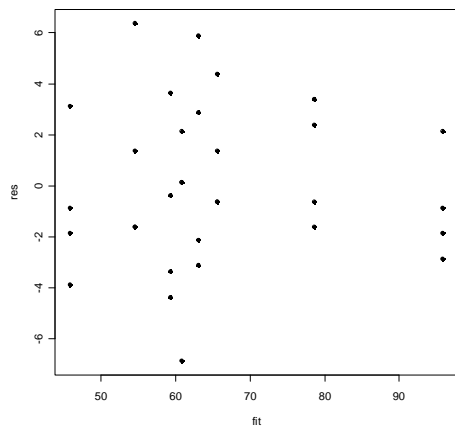
$Tukey.p
[1] 0.3376716

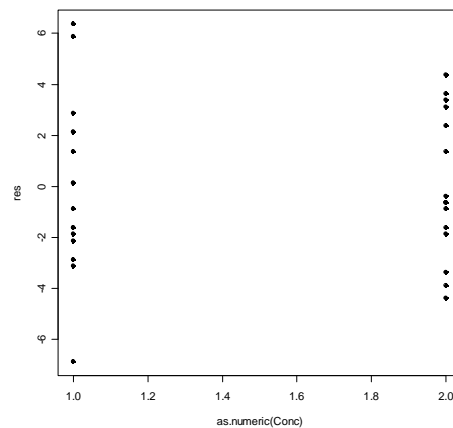
$Devn.SS
[1] 277.8787

> res <- resid.errors(Fac5Reac.Fit.aov)
> fit <- fitted.errors(Fac5Reac.Fit.aov)
> plot(fit, res, pch=16)
> qqnorm(res, pch=16)
> qqline(res)
> plot(as.numeric(Feed), res, pch=16)
> plot(as.numeric(Catal), res, pch=16)

```

```
> plot(as.numeric(Agitation), res, pch=16)  
> plot(as.numeric(Temp), res, pch=16)  
> plot(as.numeric(Conc), res, pch=16)
```





From this we conclude that the main effects Catal, Temp and Conc and the two-factor interactions Catal#Temp and Temp#Conc are the only effects distinguishable from noise. Consequently we conclude that Catalyst and Temperature interact in their effect on the % Reacted as do Concentration and Temperature. The fitted model is

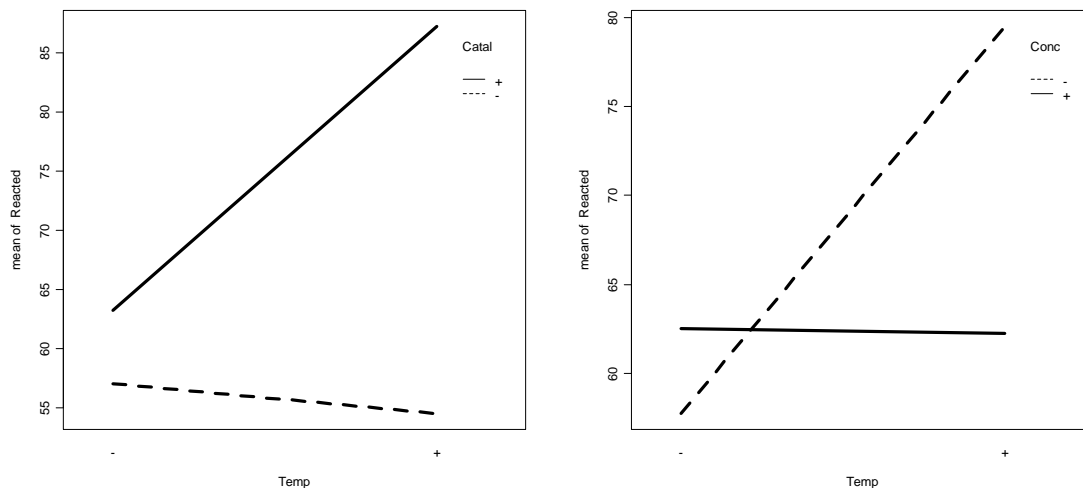
$$\psi = E[Y] = \text{Catalyst} \wedge \text{Temperature} + \text{Concentration} \wedge \text{Temperature}$$

The residuals plots are fine and so also is the normal probability plot. Tukey's one-degree-of-freedom-for-nonadditivity is not significant. So there is no evidence that the assumptions are unmet.

```
> #
> # treatment differences
> #
> interaction.plot(Temp, Catal, Reacted, lwd=4)
> interaction.plot(Temp, Conc, Reacted, lwd=4)
> Fac5Reac.means <- model.tables(Fac5Reac.Fit.aov, type="means")
> Fac5Reac.means$tables$"Temp:Catal"
  Catal
Temp -   +
  - 57.00 63.25
  + 54.50 87.25
> Fac5Reac.means$tables$"Temp:Conc"
  Conc
Temp -   +
  - 57.75 62.50
  + 79.50 62.25
> q <- qtTukey(0.95, 4, 26)
> q
[1] 3.87964
```

Tukey's HSD is

$$w(5\%) = \frac{3.87964}{\sqrt{2}} \times \sqrt{\frac{11.1 \times 2}{8}} = 4.57$$



a) Half-fractions of full factorial experiments

Definition VIII.13: A $\frac{1}{p}$ th fraction of a 2^k experiment is designated a 2^{k-p} experiment. The number of runs in the experiment is equal to the value of 2^{k-p} . ■

Construction of half-fractions

Rule VIII.1: A 2^{k-1} experiment is constructed as follows:

1. Write down a complete design in $k-1$ factors.
2. Compute the column of signs for factor k by forming the elementwise product of the columns of the complete design. That is, $\mathbf{k} = \mathbf{123}\dots(\mathbf{k}-1)$. ■

Example VIII.9 A half-fraction of a 2^5 factorial experiment

Now, the full factorial experiment analysed in example VIII.8 required 32 runs. Suppose that the experimenter had chosen to make only the 16 runs marked with asterisks in the above table — that is, the $2^4 = 16$ runs specified by rule VIII.1 for a 2^{5-1} design:

1. A full 2^4 design was chosen for the four factors **1**, **2**, **3** and **4**.
2. The column of signs for the four-factor interaction was computed and these were used to define the levels of factor **5**. Thus, $\mathbf{5} = \mathbf{1234}$.

Consequently, the only data available would be that given in the table below; this data has been arranged in Yates order for factors 1–4, not in randomized order. Also, given are the coefficients of the contrasts for all the two-factor interactions.

**Results from a half-fraction of a 2⁵ factorial design
— chemical experiment**

Factor	–	+
1 feed rate (l/min)	10	15
2 catalyst (%)	1	2
3 agitation rate (rpm)	100	120
4 temperature (°C)	140	180
5 concentration (%)	3	6

Run	Factor					Interactions										% reacted
	1	2	3	4	5	12	13	14	15	23	24	25	34	35	45	
17	–	–	–	–	+	+	+	+	–	+	+	–	+	–	–	56
2	+	–	–	–	–	–	–	–	–	+	+	+	+	+	+	53
3	–	+	–	–	–	–	+	+	+	–	–	–	+	+	+	63
20	+	+	–	–	+	+	–	–	+	–	–	+	+	–	–	65
5	–	–	+	–	–	+	–	+	+	–	+	+	–	–	+	53
22	+	–	+	–	+	–	+	–	+	–	+	–	–	+	–	55
23	–	+	+	–	+	–	–	+	–	+	–	+	–	+	–	67
8	+	+	+	–	–	+	+	–	–	+	–	–	–	–	+	61
9	–	–	–	+	–	+	+	–	+	+	–	+	–	+	–	69
26	+	–	–	+	+	+	–	+	+	+	–	–	–	–	+	45
27	–	+	–	+	+	–	+	–	–	–	+	+	–	–	+	78
12	+	+	–	+	–	+	–	+	–	–	+	–	–	+	–	93
29	–	–	+	+	+	+	–	–	–	–	–	–	+	+	+	49
14	+	–	+	+	–	–	+	+	–	–	–	+	+	–	–	60
15	–	+	+	+	–	–	–	–	+	+	+	–	+	–	–	95
32	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	82

Aliasing in half-fractions

As one would expect there is no such thing as a free lunch. We have gained by only having to run half the combinations, but what has been lost? The short answer is that various effects have been aliased.

Definition VIII.14: Two effects are said to be **aliased** when they are mixed up because of the deliberate use of only a fraction of the treatments. ■

Compare this to confounding, where certain treatment effects are mixed up with block effects. That is, the inability to separate the effects arises from different actions. In one case, it is because of the treatment combinations that the investigator chooses to observe; in the other case, it arises from the assigning of treatments to physical units.

In the table above, only the columns for the main effects and two-factor interactions are presented. What about the 10 three-factor interactions, the 5 four-factor interactions and the 1 five-factor interaction? Consider the three factor interaction **123**; its coefficients are:

$$\mathbf{123} = -++-+--+---+---+$$

but we notice this is identical to the column **45** in the above table. That is, $\mathbf{123} = \mathbf{45}$ and these two interactions are aliased.

Now suppose we use l_{45} to denote the linear function of the observations which we used to estimate the **45** interaction:

$$l_{45} = (-56+53+63-65+53-55-67+61-69+45+78-93+49-60-95+82)/8 = -9.5$$

Now, l_{45} estimates the sum of the effects **45** and **123** from the complete design. It is said that $l_{45} \rightarrow \mathbf{45} + \mathbf{123}$. That is, it is the sum of the parameters for **45** and **123** that is estimated by l_{45} . The complete aliasing pattern for this design is as follows:

Aliasing pattern for a 2^{5-1} design

Relationship between column pairs	Aliasing pattern
1 = 2345	$l_1 \rightarrow \mathbf{1} + \mathbf{2345}$
2 = 1345	$l_2 \rightarrow \mathbf{2} + \mathbf{1345}$
3 = 1245	$l_3 \rightarrow \mathbf{3} + \mathbf{1245}$
4 = 1235	$l_4 \rightarrow \mathbf{4} + \mathbf{1235}$
5 = 1234	$l_5 \rightarrow \mathbf{5} + \mathbf{1234}$
12 = 345	$l_{12} \rightarrow \mathbf{12} + \mathbf{345}$
13 = 245	$l_{13} \rightarrow \mathbf{13} + \mathbf{245}$
14 = 235	$l_{14} \rightarrow \mathbf{14} + \mathbf{235}$
15 = 234	$l_{15} \rightarrow \mathbf{15} + \mathbf{234}$
23 = 145	$l_{23} \rightarrow \mathbf{23} + \mathbf{145}$
24 = 135	$l_{24} \rightarrow \mathbf{24} + \mathbf{135}$
25 = 134	$l_{25} \rightarrow \mathbf{25} + \mathbf{134}$
34 = 125	$l_{34} \rightarrow \mathbf{34} + \mathbf{125}$
35 = 124	$l_{35} \rightarrow \mathbf{35} + \mathbf{124}$
45 = 123	$l_{45} \rightarrow \mathbf{45} + \mathbf{123}$
(I = 12345)	$[l_1 \rightarrow \text{average} + \frac{1}{2}(\mathbf{12345})]$

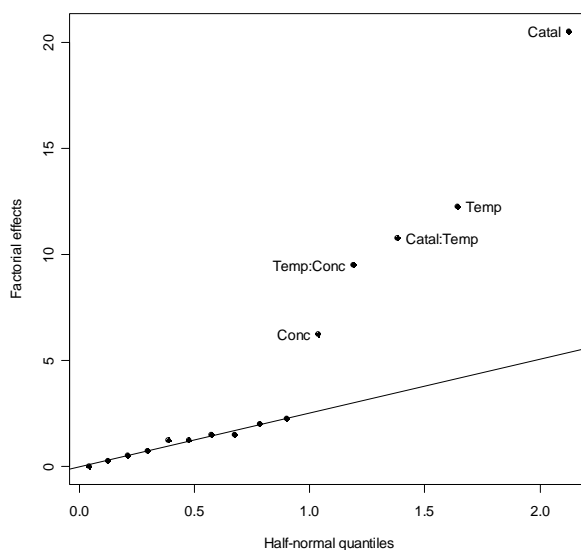
Evidently our analysis would be justified if it could be assumed that the three-factor and four-factor interactions could be ignored.

Analysis of half-fractions

The analysis of this set of 16 runs can still be accomplished using Yates algorithm since there are 4 factors for which it represents a full factorial. However, R will perform the analysis producing lines for a set of unaliased terms. The experimental structure is the same as for the full factorial. The R output for the analysis is as follows:

```
> mp <- c("-", "+")
> fnames <- list(Feed = mp, Catal = mp, Agitation = mp, Temp = mp)
> Frf5Reac.Treats <- fac.gen(generate = fnames, order="yates")
> attach(Frf5Reac.Treats)
> Frf5Reac.Treats$Conc <-
+   factor(mpone(Feed)*mpone(Catal)*mpone(Agitation)*mpone(Temp), labels = mp)
> detach(Frf5Reac.Treats)
> Frf5Reac.dat <- data.frame(Runs = factor(1:16), Frf5Reac.Treats)
> remove("Frf5Reac.Treats")
> Frf5Reac.dat$Reacted <- c(56,53,63,65,53,55,67,61,69,45,78,93,49,60,95,82)
> Frf5Reac.dat
  Runs Feed Catal Agitation Temp Conc Reacted
1     1   -    -         -     -    +     56
2     2   +    -         -     -    -     53
3     3   -    +         -     -    -     63
4     4   +    +         -     -    +     65
5     5   -    -         +     -    -     53
6     6   +    -         +     -    +     55
7     7   -    +         +     -    +     67
8     8   +    +         +     -    -     61
9     9   -    -         -     +    -     69
10    10  +    -         -     +    +     45
11    11  -    +         -     +    +     78
12    12  +    +         -     +    -     93
13    13  -    -         +     +    +     49
14    14  +    -         +     +    -     60
15    15  -    +         +     +    -     95
16    16  +    +         +     +    +     82
> Frf5Reac.aov <- aov(Reacted ~ Feed * Catal * Agitation * Temp * Conc +
+                      Error(Runs), Frf5Reac.dat)
> summary(Frf5Reac.aov)

Error: Runs
      Df    Sum Sq   Mean Sq
Feed   1    16.00    16.00
Catal  1  1681.00  1681.00
Agitation 1 5.966e-30 5.966e-30
Temp    1    600.25   600.25
Conc    1    156.25   156.25
Feed:Catal 1     9.00     9.00
Feed:Agitation 1     1.00     1.00
Catal:Agitation 1     9.00     9.00
Feed:Temp 1     2.25     2.25
Catal:Temp 1    462.25   462.25
Agitation:Temp 1     0.25     0.25
Feed:Conc 1     6.25     6.25
Catal:Conc 1     6.25     6.25
Agitation:Conc 1    20.25    20.25
Temp:Conc 1    361.00   361.00
> qqyeffects(Frf5Reac.aov, error.term = "Runs", data=Frf5Reac.dat)
Effect(s) labelled: Conc Temp:Conc Catal:Temp Temp Catal
```



```
> round(yates.effects(Frf5Reac.aov, error.term="Runs", data=Frf5Reac.dat), 2)
      Feed      Catal      Agitation      Temp      Conc
-2.00    20.50      0.00    12.25    -6.25
Feed:Catal  Feed:Agitation  Catal:Agitation
 1.50      0.50      1.50
Feed:Temp   Catal:Temp   Agitation:Temp   Feed:Conc   Catal:Conc
-0.75     10.75      0.25      1.25      1.25
Agitation:Conc  Temp:Conc
 2.25      -9.50
```

Note that `fac.gen` is used to generate the first four of the five factors as this design is complete in these four factors — the fifth factor is then generated as the product of the first four factors.

The values of the Yates effects for the fractional set are similar to those obtained in the analysis of the complete set. The normal plot for the fraction draws attention to precisely the same set of effects as that for the full factorial: Conc, Temp, Catal, Temp#Conc and Temp#Catal. Again, the fitted model is

$$\psi = E[Y] = \text{Catalyst} \wedge \text{Temperature} + \text{Concentration} \wedge \text{Temperature}$$

and essentially the same information has been obtained with only half the effort.

The following R output gives the analysis for the significant effects (and effects marginal to them), along with the diagnostic checking:

```
> Frf5Reac.Fit.aov <- aov(Reacted ~ Temp * (Catal + Conc) + Error(Runs),
+                               Frf5Reac.dat)
> summary(Frf5Reac.Fit.aov)

Error: Runs
      Df  Sum Sq Mean Sq F value    Pr(>F)
Temp    1   600.25   600.25  85.445 3.253e-06
Catal    1  1681.00  1681.00  239.288 2.600e-08
Conc     1   156.25   156.25  22.242 0.0008212
Temp:Catal  1   462.25   462.25  65.801 1.043e-05
Temp:Conc  1   361.00   361.00  51.388 3.037e-05
Residuals 10    70.25     7.03
```

```

> #
> # Diagnostic checking
> #
> tukey.1df(Frf5Reac.Fit.aov, Frf5Reac.dat, error.term="Runs")
$Tukey.SS
[1] 5.767756

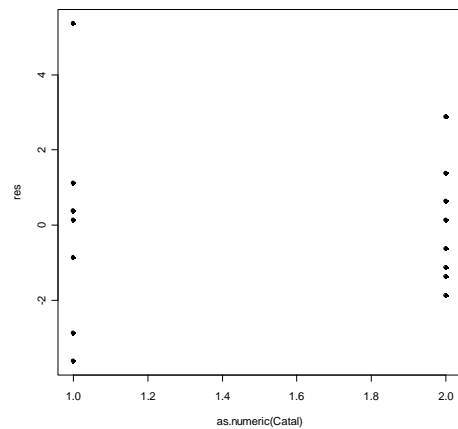
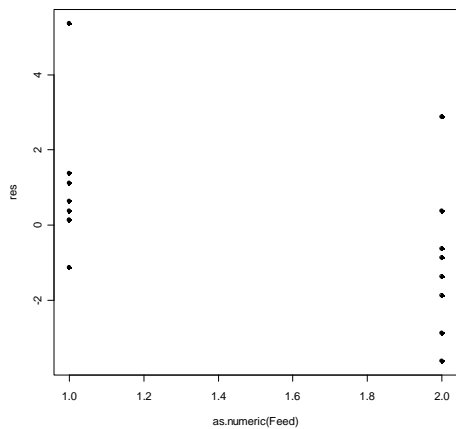
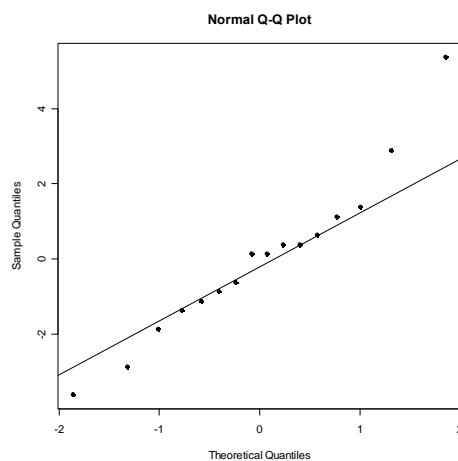
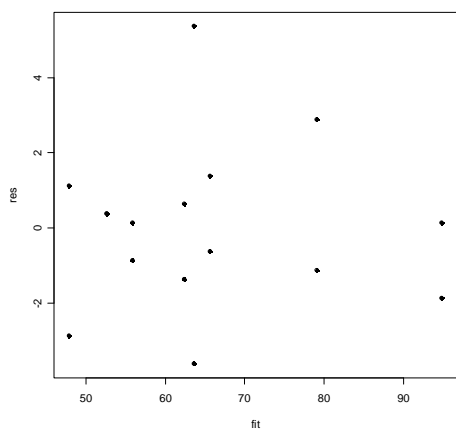
$Tukey.F
[1] 0.8050248

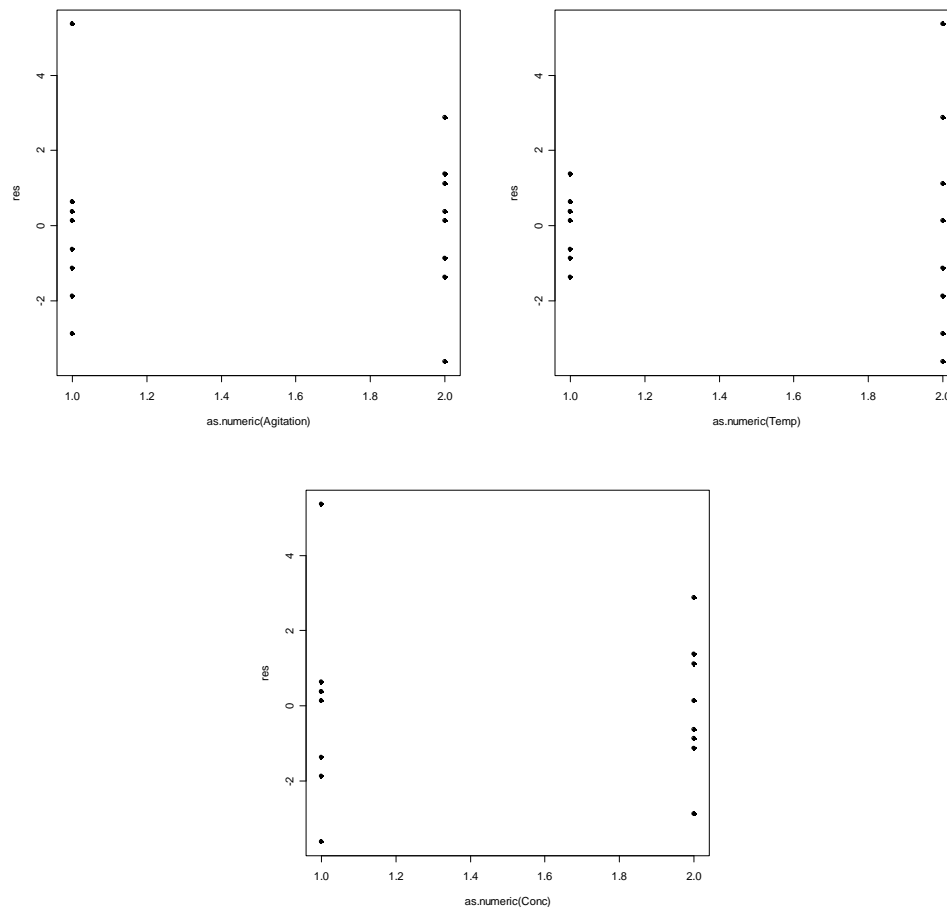
$Tukey.p
[1] 0.3929634

$Devn.SS
[1] 64.48224

> res <- resid.errors(Frf5Reac.Fit.aov)
> fit <- fitted.errors(Frf5Reac.Fit.aov)
> plot(fit, res, pch=16)
> qqnorm(res, pch=16)
> qqline(res)
> attach(Frf5Reac.dat)
> plot(as.numeric(Feed), res, pch=16)
> plot(as.numeric(Catal), res, pch=16)
> plot(as.numeric(Agitation), res, pch=16)
> plot(as.numeric(Temp), res, pch=16)
> plot(as.numeric(Conc), res, pch=16)

```





The diagnostic checking indicates there is a problem with a large residual and perhaps a problem with different variances between the two temperatures.

Finding the aliasing patterns

Fortunately, we can use the calculus, described in section VIII.C, for multiplying columns together to obtain the aliasing pattern.

Definition VIII.15: A set of columns designating an elementwise product of a set of columns is called a **word**. ■

Definition VIII.16: The **generator(s)** of a fractional 2^k experiment are the relationship(s) between factors that are used to obtain the design. The **generating relations** express these as words equal to **I**. ■

Definition VIII.17: The **defining relations** of a fractional 2^k experiment is the set of all words equal to the identity column **I**. It includes the generating relations and all possible products of these relations. ■

The defining relation(s) are the key to the design since multiplying them on both sides of the equals sign by particular column combinations yields the relationships between the columns.

Example VIII.9 A half-fraction of a 2^5 factorial experiment (continued)

The 2^{5-1} design was constructed by setting $\mathbf{5} = \mathbf{1234}$. That is, this relation is the generator of the design. Multiplying both sides by $\mathbf{5}$ we obtain $\mathbf{55} = \mathbf{12345}$ or $\mathbf{I} = \mathbf{12345}$. This identity can be confirmed by multiplying together the columns in the table of coefficients for the design. The half fraction is defined by a single generating relation $\mathbf{I} = \mathbf{12345}$ so that the relation $\mathbf{I} = \mathbf{12345}$ also provides the defining relation of the design. (For more highly fractionated designs more than one defining relation is needed.)

To find out which column combination is aliased with $\mathbf{45}$, multiply the defining relation on both sides by $\mathbf{45}$: $\mathbf{45I} = \mathbf{4512345} = \mathbf{123}$ which is precisely the relation given in the above table. The other aliasing relations can be found similarly.

b) More on construction and use of half-fractions

The complimentary half-fraction

Definition VIII.18: The **complimentary half-fraction** is obtained by reversing the sign of the generating relation. ■

In practice, either half-fraction may be used.

Example VIII.9 A half-fraction of a 2^5 factorial experiment (continued)

As already mentioned the design we have been discussing was constructed using the generator $\mathbf{5} = \mathbf{1234}$; that is, we formed the fifth column by multiplying together the other 4 columns. The complimentary half fraction is generated by putting $\mathbf{5} = -\mathbf{1234}$; that is, taking minus the product of the first 4 columns. The half fraction corresponding to the runs not marked with an asterisk in the complete experiment is obtained. The defining relation for this design may be written as $\mathbf{I} = -\mathbf{12345}$.

The complimentary half fraction would give:

$$l_1 \rightarrow \mathbf{1 - 2345}$$

$$l_2 \rightarrow \mathbf{2 - 1345} \text{ etc.}$$

Sequential experimentation

An experimenter contemplating the investigation of 5 factors, may be willing to run all 32 runs required for a 2^5 . It is almost always better to run a half-fraction first and analyze them. If necessary, the other half-fraction can always be run later to complete the full design. Frequently, however, the first half-fraction will allow progress to the next stage of experimental investigation.

c) The concept of design resolution

Definition VIII.19: The **resolution R** of a fractional design is the number of columns in the smallest word in the defining relations. ■

Thus a 2^{5-1} half fraction with defining relation $I = \pm 12345$ has resolution V and is referred to as a 2_{V}^{5-1} design. A 2^{3-1} with defining relation $I = \pm 123$ has resolution III and is referred to as a 2_{III}^{5-1} design.

Theorem VIII.2: The half-fraction of a 2^k experiment with highest resolution is the one for which the generator is $k = 123 \dots (k-1)$ and so the generating and defining relation is $I = 123 \dots k$.

Proof: it is clear that the largest word possible has been used for the generating relationship. ■

The half-fraction is the one that it was suggested as best in rule VIII.1.

Rule VIII.2: A design of resolution R is one in which i -factor effects ($i \leq R/2$) may be aliased with effects containing $R - i$ factors or more. ■

Example VIII.9 A half-fraction of a 2^5 factorial experiment (continued)

The 2^{5-1} design we have been discussing is a resolution V design and so all i -factor interactions are aliased with $V-i$ interactions. Hence, all one-factor interactions are aliased with four-factor interactions and all two-factor interactions are aliased with three-factor interactions. ■

For the various sized fractions of a 2^k :

1. a design of resolution III does not alias main effects with one another, but does alias main effects with two factor interactions;
2. a design of resolution IV does not alias main effects and two-factor interactions, but does alias two factor interactions with one another;
3. a design of resolution V does not alias main effects and two-factor with one another, but does alias two factor interactions with three-factor interactions.

Embedded factorials

One of the very important aspects of resolution is that a fractional factorial design of resolution R contains complete factorials (possibly replicated) in every set of $R-1$ factors. Suppose then that an experimenter has a number of candidate factors but believes that all but $R-1$ of them (specific identity unknown) may have no detectable effects. If she employs a fractional factorial design of resolution R she will have a complete factorial design in the effective factors.

Example VIII.9 A half-fraction of a 2^5 factorial experiment (continued)

The 2_{IV}^{5-1} design is a complete factorial in any four of the five factors. Thus, if we can identify a factor that is having no effect, the experiment can be interpreted as a complete factorial. In the analysis discussed above factors **1** (Feed) and **3** (Agitation) are without effect, so that the experiment can be viewed as a replicated 2^3 factorial experiment.

Results from a 2_{IV}^{5-1} factorial design viewed as a 2^3 — chemical experiment

Factor	–	+
1 feed rate (l/min)	10	15
2 catalyst (%)	1	2
3 agitation rate (rpm)	100	120
4 temperature (°C)	140	180
5 concentration (%)	3	6

Run	Factor			% reacted
	2	4	5	
2	–	–	–	53
5	–	–	–	53
17	–	–	+	56
22	–	–	+	55
9	–	+	–	69
14	–	+	–	60
26	–	+	+	45
29	–	+	+	49
3	+	–	–	63
8	+	–	–	61
20	+	–	+	65
23	+	–	+	67
12	+	+	–	93
15	+	+	–	95
27	+	+	+	78
32	+	+	+	82

d) Resolution III designs (also called main effect plans)

In a resolution III design, the main effects are aliased with two-factor interactions. It is possible to construct resolution III designs for investigating up to $k = n - 1$ factors, where n is a multiple of 4. A particularly important subset of these designs are those for which n is a power of 2. In particular, designs for investigating up to 3 factors in 4 runs, up to 7 factors in 8 runs and up to 15 factors in 16 runs.

Definition VIII.20: A fractional design is said to be a **saturated design** if the number of factors $k = n - 1$; that is, all contrasts are associated with main effects. ■

Saturated designs are at the heart of the Taguchi quality control methods which have been attributed as being the basis of Japanese industrial supremacy. They have used these designs in developing products to determine which factors in an industrial manufacturing process affect product quality. In using these designs they are assuming that all two-factor interactions are negligible. Because of this they are not so useful in agriculture.

Resolution III designs for which n is a power of 2.

Rule VIII.3: 2_{III}^{k-p} designs in which $n = 2^{k-p}$ are constructed as follows:

1. Write down a complete design in $k - p$ factors.
2. Compute the column of signs for additional factors by associating the factors with the interaction columns of the factors in the complete design. ■

We will now investigate the use of resolution III designs. In particular, their use in sequential experimentation will be illustrated.

Example VIII.10 A bike experiment

Consider the following 2_{III}^{7-4} experiment designed to investigate the effects of 7 factors on the time it takes a particular person to cycle up a hill. That is, it is a one sixteenth fraction of a 2^7 experiment involving $2^3 = 8$ runs. The design is constructed by writing down a full factorial design for the three variables **1**, **2** and **3**; the additional variables **4**, **5**, **6** and **7** are associated with all the interaction columns **12**, **13**, **23** and **123**, respectively. Hence, the generating relations of the design are $I = 124$, $I = 135$, $I = 236$, $I = 1237$. The design is shown in the following table:

A 2_{III}^{7-4} Experiment for Studying Bicycle Times

Factor		-	+
1	Seat	up	down
2	Dynamo	off	on
3	Handlebars	up	down
4	Gear	low	medium
5	Raincoat	on	off
6	Breakfast	yes	no
7	Tyres	hard	soft

Run	1	2	3	4	5	6	7	Time
1	-	-	-	+	+	+	-	69
2	+	-	-	-	-	+	+	52
3	-	+	-	-	+	-	+	60
4	+	+	-	+	-	-	-	83
5	-	-	+	+	-	-	+	71
6	+	-	+	-	+	-	-	50
7	-	+	+	-	-	+	-	59
8	+	+	+	+	+	+	+	88

Notice that all contrasts are associated with a main effect and so this design is saturated.

The experimental structure for this experiment is:

Structure	Formula
unrandomized	8 Runs
randomized	2 Seat+2 Dynamo+2 Handbars+2 Gear +2 Raincoat+2 Brekkie+2 Tyres

The pluses indicate that the factors have to be assumed to be independent.

The R output for the analysis is:

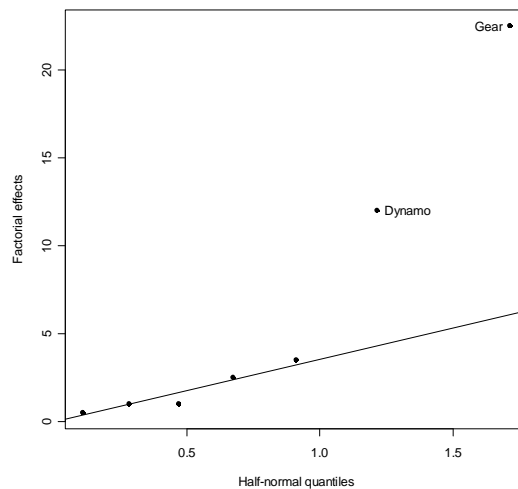
```
> #
> # set up data.frame
> #
> mp <- c("-", "+")
> fnames <- list(Seat = mp, Dynamo = mp, Handbars = mp)
> Frf7Bike.Treats <- fac.gen(generate = fnames, order="yates")
> attach(Frf7Bike.Treats)
> Frf7Bike.Treats$Gear <- factor(mpone(Seat)*mpone(Dynamo), labels = mp)
> Frf7Bike.Treats$Raincoat <- factor(mpone(Seat)*mpone(Handbars), labels = mp)
> Frf7Bike.Treats$Brekkie <- factor(mpone(Dynamo)*mpone(Handbars), labels = mp)
> Frf7Bike.Treats$Tyres <- factor(mpone(Seat)*mpone(Dynamo)*mpone(Handbars),
+                               labels = mp)
> detach(Frf7Bike.Treats)
> Frf7Bike.dat <- data.frame(Runs = factor(1:8), Frf7Bike.Treats)
> Frf7Bike.dat$Time <- as.vector(c(69, 52, 60, 83, 71, 50, 59, 88))
> Frf7Bike.dat
  Runs Seat Dynamo Handbars Gear Raincoat Brekkie Tyres Time
```

```

1  1  -   -   -   +   +   +   -   69
2  2  +   -   -   -   -   -   +   52
3  3  -   +   -   -   -   +   -   60
4  4  +   +   -   -   +   -   -   83
5  5  -   -   +   +   -   -   +   71
6  6  +   -   +   -   +   -   -   50
7  7  -   +   +   -   -   +   -   59
8  8  +   +   +   +   +   +   +   88
> #
> # analyse
> #
> Frf7Bike.aov <- aov(Time ~ (Seat + Dynamo + Handbars + Gear + Raincoat + Brekkie
+                               Tyres)^2 + Error(Runs), Frf7Bike.dat)
> summary(Frf7Bike.aov)

Error: Runs
      Df Sum Sq Mean Sq
Seat    1  24.5    24.5
Dynamo  1 288.0   288.0
Handbars 1   2.0    2.0
Gear    1 1012.5 1012.5
Raincoat 1   0.5    0.5
Brekkie  1   2.0    2.0
Tyres   1  12.5   12.5
> qqeffects(Frf7Bike.aov, error.term = "Runs", data=Frf7Bike.dat)
Effect(s) labelled: Dynamo Gear
> round(yates.effects(Frf7Bike.aov, error.term="Runs", data=Frf7Bike.dat), 2)
      Seat  Dynamo Handbars  Gear Raincoat  Brekkie  Tyres
      3.5    12.0     1.0   22.5     0.5     1.0    2.5

```



The estimated effects and the abbreviated aliasing pattern (ignoring interactions with three or more factors) for this experiment are as follows:

Estimated Effects and Abbreviated Aliasing Pattern

Seat	$l_1 = 3.5$	→	1 + 24 + 35 + 67
Dynamo	$l_2 = 12.0$	→	2 + 14 + 36 + 57
Handlebars	$l_3 = 1.0$	→	3 + 15 + 26 + 47
Gear	$l_4 = 22.5$	→	4 + 12 + 56 + 37
Raincoat	$l_5 = 0.5$	→	5 + 13 + 46 + 27
Breakfast	$l_6 = 1.0$	→	6 + 23 + 45 + 17
Tyres	$l_7 = 2.5$	→	7 + 34 + 25 + 16
	$(l_1 = 66.5)$	→	average)

Suppose that previous experience suggests the standard deviation for repeated runs up the hill is about 3 seconds. Then, as each effect is the difference of two averages based on 4 observations, the standard error of the effects is about $3\sqrt{\frac{1}{4} + \frac{1}{4}} = 2.1$. Evidently, only two contrasts are distinguishable from uncontrolled variation: l_2 and l_4 .

The interpretation of the experiment would appear to be that only factors **2** (dynamo) and **4** (gear) affect the time and they do this independently. Having the dynamo on adds about 12 seconds and using medium gear rather than low adds about 22 seconds.

However, there is some ambiguity in these conclusions. It may be, for example, that l_4 is large, not because of a large main effect **4**, but because one or more of the interactions **12**, **56** and **37** are large. A further experiment would concentrate on factor **4** to confirm that there is a large main effect for this factor.

Also, note that, being a resolution III design, it will contain complete 2^2 factorial experiments replicated twice in every pair of factors. Thus, it contains a complete factorial in factors **2** and **4**.

Other 2_{III}^{7-4} fractions

The design we have used is only one particular 1/16 fraction of a full 2^7 design. How can the other one-sixteenth fractions be generated? The first design was generated by setting

$$\mathbf{4 = 12, 5 = 13, 6 = 23, 7 = 123}$$

but, for example, we could equally have used

$$\mathbf{4 = -12, 5 = 13, 6 = 23, 7 = 123.}$$

The fraction that would be generated in this case is:

A second 2_{III}^{7-4} experiment for studying bicycle times

Factor		–	+					
1	Seat	up	down					
2	Dynamo	off	on					
3	Handlebars	up	down					
4	Gear	low	medium					
5	Raincoat	on	off					
6	Breakfast	yes	no					
7	Tyres	hard	soft					

Run	1	2	3	4	5	6	7	Time
				–12	13	23	123	
1	–	–	–	–	+	+	–	47
2	+	–	–	+	–	+	+	74
3	–	+	–	+	+	–	+	84
4	+	+	–	–	–	–	–	62
5	–	–	+	–	–	–	+	53
6	+	–	+	+	+	–	–	78
7	–	+	+	+	–	+	–	87
8	+	+	+	–	+	+	+	60

This fraction has been obtained by reversing the signs of column **4** and this produces a completely new set of factor combinations, none having been included in the first experiment. Of course, the experimental structure remains the same.

However, the aliasing pattern has also been altered. It can be obtained from the original by reversing the sign of any interaction term involving **4** and the terms aliased with **4**. Thus, it is now:

Estimated Effects and Abbreviated Aliasing Pattern

Seat	$\ell'_1 = 0.8 \rightarrow 1 - 24 + 35 + 67$
Dynamo	$\ell'_2 = 10.2 \rightarrow 2 - 14 + 36 + 57$
Handlebars	$\ell'_3 = 2.7 \rightarrow 3 + 15 + 26 - 47$
Gear	$\ell'_4 = 25.2 \rightarrow 4 - 12 - 56 - 37$
Raincoat	$\ell'_5 = -1.7 \rightarrow 5 + 13 - 46 + 27$
Breakfast	$\ell'_6 = 2.2 \rightarrow 6 + 23 - 45 + 17$
Tyres	$\ell'_7 = -0.7 \rightarrow 7 - 34 + 25 + 16$

There are 16 different ways of allocating signs to the four generators:

$$\mathbf{4 = \pm 12, 5 = \pm 13, 6 = \pm 23, 7 = \pm 123}$$

Thus, switching the signs of columns **4**, **5**, **6**, and **7** will produce the 16 fractions that make up the complete factorial and the corresponding sign switching for the aliasing pattern produces the appropriate aliasing pattern.

Combining two fractions

Suppose that the results of the two 2_{III}^{7-4} fractional experiments were combined. As it will now be possible to estimate interactions, the relationship between the factors must be altered to be crossed. The experimental structure is:

Structure	Formula
unrandomized	16 Runs
randomized	2 Seat*2 Dynamo*2 Handbars*2 Gear *2 Raincoat*2 Brekkie*2 Tyres

The R output for the analysis is:

```
> #
> # second fraction
> #
> Frf7Bike2.dat <- Frf7Bike.dat
> attach(Frf7Bike2.dat)
> Frf7Bike2.dat$Gear <- factor(-mpone(Seat)*mpone(Dynamo), labels = mp)
> detach(Frf7Bike2.dat)
> Frf7Bike2.dat$Time <- as.vector(c(47, 74, 84, 62, 53, 78, 87,60))
> #
> # combine fractions
> #
> Frf7Bike.Both.dat <- rbind(Frf7Bike.dat,Frf7Bike2.dat)
> Frf7Bike.Both.dat <- data.frame(Block = factor(rep(1:2, each=8)),
+                               Frf7Bike.Both.dat)
> Frf7Bike.Both.dat
  Block Runs Seat Dynamo Handbars Gear Raincoat Brekkie Tyres Time
1     1     1   -     -         -     +         +         +     -    69
2     1     2   +     -         -     -         -         +     +    52
3     1     3   -     +         -     -         +         -     -    60
4     1     4   +     +         -     +         -         -     -    83
5     1     5   -     -         +     +         -         -     +    71
6     1     6   +     -         +     -         +         -     -    50
7     1     7   -     +         +     -         -         +     -    59
8     1     8   +     +         +     +         +         +     +    88
9     2     1   -     -         -     -         +         +     -    47
10    2     2   +     -         -     +         -         +     +    74
11    2     3   -     +         -     +         +         -     +    84
12    2     4   +     +         -     -         -         -     -    62
13    2     5   -     -         +     -         -         -     +    53
14    2     6   +     -         +     +         +         -     -    78
15    2     7   -     +         +     +         -         +     -    87
16    2     8   +     +         +     -         +         +     +    60
> #
> # analyse
> #
> Frf7Bike.Both.aov <- aov(Time ~ Block + (Seat + Dynamo + Handbars + Gear +
+                               Raincoat + Brekkie + Tyres)^2 + Error(Block/Runs), Frf7Bike.Both.dat)
```

```

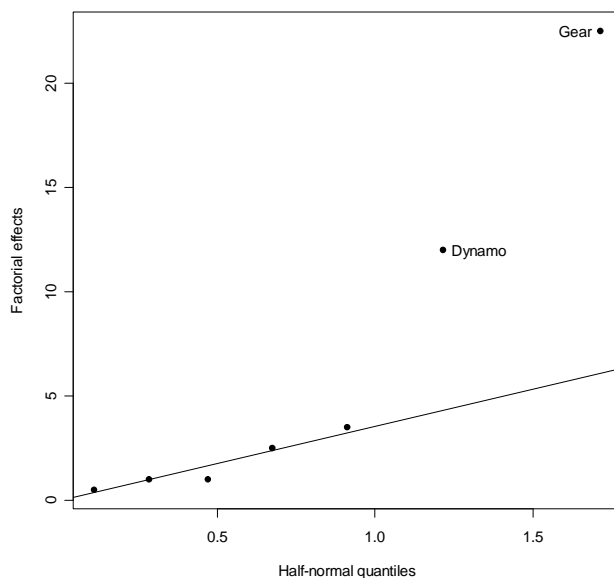
> summary(Frf7Bike.Both.aov)

Error: Block
      Df Sum Sq Mean Sq
Block  1 10.562  10.562

Error: Block:Runs
      Df  Sum Sq Mean Sq
Seat   1   18.06   18.06
Dynamo 1  495.06  495.06
Handbars 1  14.06   14.06
Gear    1 2280.06 2280.06
Raincoat 1    1.56    1.56
Brekkie 1    1.56    1.56
Tyres   1    3.06    3.06
Seat:Dynamo 1    7.56    7.56
Seat:Gear 1    3.06    3.06
Dynamo:Gear 1    7.56    7.56
Handbars:Gear 1  10.56   10.56
Gear:Raincoat 1  10.56   10.56
Gear:Brekkie 1    5.06    5.06
Gear:Tyres 1    3.06    3.06
> qqyeffects(Frf7Bike.Both.aov, error.term = "Block:Runs",
+            data=Fr7Bike.Both.dat)
Effect(s) labelled: Dynamo Gear
> round(yates.effects(Frf7Bike.Both.aov, error.term="Block:Runs",
+                    data=Fr7Bike.Both.dat), 2)
      Seat      Dynamo      Handbars      Gear      Raincoat
      2.12      11.12      1.87      23.88      -0.62
      Brekkie      Tyres      Seat:Dynamo      Seat:Gear      Dynamo:Gear
      -0.62      0.87      -1.38      0.87      1.37
Handbars:Gear Gear:Raincoat Gear:Brekkie Gear:Tyres
      1.62      1.63      1.13      -0.88

```

Notice the use of $\wedge 2$ in the model formula to restrict the analysis to main effects and two-factor interactions.



The combined analysis can be obtained by taking half sums and differences of all effects:

Estimated Effects and Abbreviated Aliasing Pattern

Seat	$\frac{1}{2}(\ell_1 + \ell'_1) = \frac{1}{2}(3.5 + 0.8)$	= 2.2	→	1 + 35 + 67
Dynamo	$\frac{1}{2}(\ell_2 + \ell'_2) = \frac{1}{2}(12.0 + 10.2)$	= 11.1	→	2 + 36 + 57
Handlebars	$\frac{1}{2}(\ell_3 + \ell'_3) = \frac{1}{2}(1.0 + 2.7)$	= 1.9	→	3 + 15 + 26
Gear	$\frac{1}{2}(\ell_4 + \ell'_4) = \frac{1}{2}(22.5 + 25.2)$	= 23.9	→	4
Raincoat	$\frac{1}{2}(\ell_5 + \ell'_5) = \frac{1}{2}(0.5 + (-1.7))$	= -0.6	→	5 + 13 + 27
Breakfast	$\frac{1}{2}(\ell_6 + \ell'_6) = \frac{1}{2}(1.0 + 2.2)$	= 1.8	→	6 + 23 + 17
Tyres	$\frac{1}{2}(\ell_7 + \ell'_7) = \frac{1}{2}(2.5 + (-0.7))$	= 0.9	→	7 + 25 + 16
	$\frac{1}{2}(\ell_1 - \ell'_1) = \frac{1}{2}(3.5 - 0.8)$	= 1.3	→	24
	$\frac{1}{2}(\ell_2 - \ell'_2) = \frac{1}{2}(12.0 - 10.2)$	= 0.9	→	14
	$\frac{1}{2}(\ell_3 - \ell'_3) = \frac{1}{2}(1.0 - 2.7)$	= -0.9	→	47
	$\frac{1}{2}(\ell_4 - \ell'_4) = \frac{1}{2}(22.5 - 25.2)$	= -1.4	→	12 + 56 + 37
	$\frac{1}{2}(\ell_5 - \ell'_5) = \frac{1}{2}(0.5 - (-1.7))$	= 1.1	→	46
	$\frac{1}{2}(\ell_6 - \ell'_6) = \frac{1}{2}(1.0 - 2.2)$	= -0.6	→	45
	$\frac{1}{2}(\ell_7 - \ell'_7) = \frac{1}{2}(2.5 - (-0.7))$	= 1.6	→	34

Note that the aliasing pattern of the combined design has been obtained by taking sums and differences of the patterns from the individual experiments.

It is evident from the table that what has been achieved in the combined design is to de-alias main effect **4** and all its two-factor interactions with the other factors. If one were contemplating doing extra runs it would seem, in view of the large effect of **4** in the first experiment, that the best strategy would be to perform the runs corresponding to this second fraction. Thus, the use of fractional factorials sequentially is a very useful application of them.

It is also possible to add a fraction to the original that would de-alias all main effects, leaving two-factor interactions aliased in groups of three.

Plackett and Burman Designs

Definition VIII.21: Plackett and Burman designs are two-level fractional factorial designs for studying $k = n - 1$ factors in n runs where n is a multiple of 4. ■

If n is a power of 2, these are identical to those previously presented. However, the Plackett and Burman designs for $n = 12, 20, 24, 28$ and 30 are sometimes of interest.

Example VIII.11: Plackett and Burman design for 11 factors in 12 runs

Run	Factor										
	1	2	3	4	5	6	7	8	9	A	B
1	+	-	+	-	-	-	+	+	+	-	+
2	+	+	-	+	-	-	-	+	+	+	-
3	-	+	+	-	+	-	-	-	+	+	+
4	+	-	+	+	-	+	-	-	-	+	+
5	+	+	-	+	+	-	+	-	-	-	+
6	+	+	+	-	+	+	-	+	-	-	-
7	-	+	+	+	-	+	+	-	+	-	-
8	-	-	+	+	+	-	+	+	-	+	-
9	-	-	-	+	+	+	-	+	+	-	+
10	+	-	-	-	+	+	+	-	+	+	-
11	-	+	-	-	-	+	+	+	-	+	+
12	-	-	-	-	-	-	-	-	-	-	-

The manner in which two-factor interactions alias main effects for most Plackett and Burman designs is complicated.

e) Table of fractional factorial designs

The following table is an extract from Table 12.15 on p. 410 of Box, Hunter and Hunter. In each cell, the type of factorial is given in the top lefthand corner. In the bottom righthand corner, either the number of times the full factorial design must be repeated or the generators for the fractional design are provided.

To use this table, examine the appropriate column if the number of factors to be investigated is fixed; examine the appropriate row if the number of runs is fixed. Note also that designs along the same leftright diagonal have the same degree of replication or fractionation.

		Number of factors					
		3	4	5	6	7	8
Number of runs	4	2_{III}^{3-1} $\pm 3=12$					
	8	2^3	2_{IV}^{4-1} $\pm 4=123$	2_{III}^{5-2} $\pm 4=12$ $\pm 5=13$	2_{III}^{6-3} $\pm 4=12$ $\pm 5=13$ $\pm 6=23$	2_{III}^{7-4} $\pm 4=12$ $\pm 5=13$ $\pm 6=23$ $\pm 7=123$	
	16	2^3 2 times	2^4	2_V^{5-1} $\pm 5=1234$	2_{IV}^{6-2} $\pm 5=123$ $\pm 6=234$	2_{IV}^{7-3} $\pm 5=123$ $\pm 6=234$ $\pm 7=134$	2_{IV}^{8-4} $\pm 5=234$ $\pm 6=134$ $\pm 7=123$ $\pm 8=124$
	32	2^3 4 times	2^4 2 times	2^5	2_{VI}^{6-1} $\pm 6=12345$	2_{IV}^{7-2} $\pm 6=1234$ $\pm 7=1245$	2_{IV}^{8-3} $\pm 6=123$ $\pm 7=124$ $\pm 8=2345$
	64	2^3 8 times	2^4 4 times	2^5 2 times	2^6	2_{VII}^{7-1} $\pm 7=123456$	2_V^{8-2} $\pm 7=1234$ $\pm 8=1256$
	128	2^3 16 times	2^4 8 times	2^5 4 times	2^6 2 times	2^7	2_{VIII}^{8-1} $\pm 8=123456$ 7

VIII.E Summary

In this chapter we have:

- described how to design 2^k replicated, unreplicated, confounded and fractional factorial experiments;
- shown how the analysis is considerably simplified for 2^k factorial experiments; it is recommended that replicated experiments be analysed using the analysis of variance and that unreplicated experiments be analysed using normal probability plots of Yates effects;
- explained how replicating the treatment combinations is not necessary when there are many factors in an experiment because not all factors are likely to affect the response and many interactions are likely to be zero;
- outlined a calculus that can be used to identify which contrasts are aliased or confounded;
- for fractional factorial experiments:
 - discussed the concepts of generators, generating relations, defining relations and resolution;
 - considered the utility of Resolution III or main effects plans for screening experiments;
 - shown how to use fractions in sequential experimentation;

- shown how to obtain a randomized layout and the analysis of variance in R;
- discussed procedures for checking the adequacy of the proposed models;
- described how to obtain the fitted equation and use it to obtain predicted values for recommended treatment combinations.

VIII.F Exercises

VIII.1A factorial experiment was carried out on a pilot plant scale. A product was being purified by a form of steam distillation process. The five factors, each at 2 levels, were Concentration of material (A), Rate of distillation (B), Volume of solution (C), Stirring rate (D), and Solvent-to-water ratio (E). The residual acidity of material from one run on each of the 32 experimental treatment combinations was determined. The results (in coded form which does not affect the analysis) are given in the following table:

		A ₀				A ₁			
		D ₀		D ₁		D ₀		D ₁	
		E ₀	E ₁	E ₀	E ₁	E ₀	E ₁	E ₀	E ₁
B ₀	C ₀	9	3	11	8	10	9	13	7
	C ₁	3	5	7	7	5	6	10	7
	C ₀	8	4	9	8	6	6	16	6
B ₁	C ₁	6	4	7	5	10	10	13	6

What are the features of this experiment?

1. Observational unit _____
2. Response variable _____
3. Unrandomized factors _____
4. Randomized factors _____
5. Type of study _____

What is the experimental structure for this experiment?

Structure	Formula
unrandomized	
randomized	

Analyze the data using R, including diagnostic checking. What levels of the factors would you recommend be used to minimize the residual acidity? What residual acidity would be achieved with this (these) combination(s) of the factors?

VIII.2A A new rifle was being tested for performance to decide some characteristics of the weapon. The testing programme involved a four-factor factorial experiment consisting of 8 tests run over two days as only 8 tests could be run on a single day. It was decided to confound the four-factor interaction with the day difference.

The four factors to be investigated were the propellant charge, the weight of the projectile, the propellant web and two different weapons of the type being evaluated. The velocity of the projectiles was measured and the results were as follows:

Day	Test	Charge Weight	Projectile Weight	Propellant Web	Weapon	Velocity
1	1	1	1	1	1	197
	2	2	2	1	1	250
	3	1	2	2	1	115
	4	2	1	2	1	200
	5	1	2	1	2	153
	6	2	1	1	2	245
	7	1	1	2	2	126
	8	2	2	2	2	154
2	1	1	2	1	1	168
	2	2	1	1	1	251
	3	1	1	2	1	139
	4	2	2	2	1	166
	5	1	1	1	2	175
	6	2	2	1	2	241
	7	1	2	2	2	84
	8	2	1	2	2	197

What are the features of this experiment?

1. Observational unit _____
2. Response variable _____
3. Unrandomized factors _____
4. Randomized factors _____
5. Type of study _____

What is the experimental structure for this experiment?

Structure	Formula
unrandomized	
randomized	

What are the expected mean squares for the lines in the analysis of variance table based on all unrandomized factors being random and all randomized factors being fixed?

Source	df	E[MSQ]
<hr/>		
<hr/>		
Total		

Analyze the data using R, including diagnostic checking. What levels of the factors would you recommend be used to maximize the velocity? What velocity would be achieved with this (these) combination(s) of the factors?

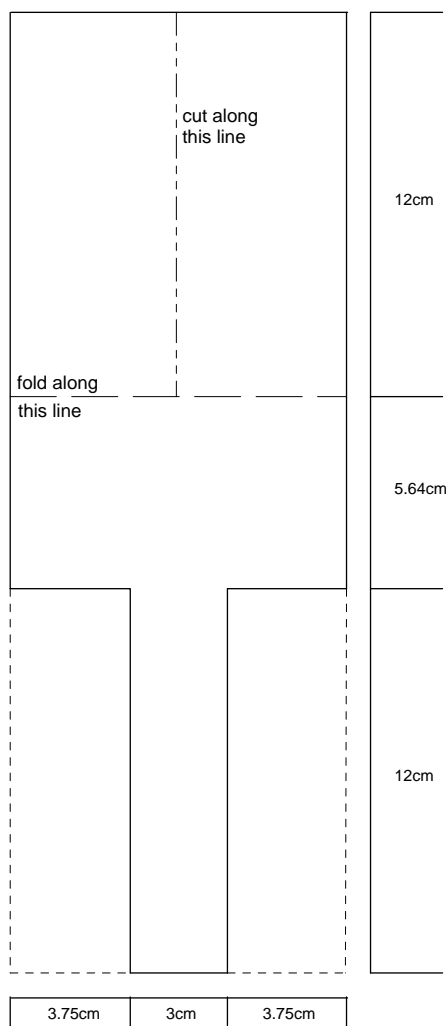
VIII.3A processing experiment is to be run to investigate the effects of 6 factors, each at two levels, on the total yield of peanut oil from batches of peanuts. To save on resources the experimenter decides to use a quarter of the complete set of treatment combinations. Use the table given in subsection e) of section X.D, *Fractional factorial design at two levels*, to identify a suitable design.

- What is the resolution of this design?
- What are the implications of the design's resolution?
- What are the generators and defining relations for the design?
- What is its aliasing pattern?
- What treatment combinations should the experimenter include in the experiment?

VIII.4An experimenter wants to investigate 5 factors at 2 levels but has only enough resources for 8 runs. Use R to obtain a randomized layout for the experimenter using a seed of 124.

VIII.5 The Light Helicopter Corporation wishes to investigate ways in which the flight time of their helicopters can be increased. The standard design for the helicopters they produce is shown below.

The standard design



Improving the design

Engineers from their company have got together and had a brainstorming session to identify modifications to the design that might increase the flight time. They suggested that the following factors be investigated.

Factors		-	+
Paper type	(P)	light	heavy
Wing length	(W)	7.5cm	12cm
Body length	(L)	7.5cm	12cm
Body width	(B)	3cm	5cm
Paper clip	(C)	no	yes
Fold	(F)	no	yes
Taped body	(T)	no	yes
Taped wing	(M)	no	yes

The aliasing pattern (ignoring three- and more-factor interactions) for this experiment is as follows:

$l_1 \rightarrow$ average	$l_0 \rightarrow$ average
$l_2 \rightarrow$ 1	$l_P \rightarrow$ P
$l_3 \rightarrow$ 2	$l_W \rightarrow$ W
$l_4 \rightarrow$ 12 + 37 + 48 + 56	$l_{PW} \rightarrow$ PW + LT + BM + CF
$l_5 \rightarrow$ 3	$l_L \rightarrow$ L
$l_6 \rightarrow$ 13 + 27 + 46 + 58	$l_{PL} \rightarrow$ PL + WT + BF + CM
$l_7 \rightarrow$ 23 + 17 + 45 + 68	$l_{WL} \rightarrow$ WL + PT + BC + FM
$l_8 \rightarrow$ 7	$l_T \rightarrow$ T
$l_9 \rightarrow$ 4	$l_B \rightarrow$ B
$l_{10} \rightarrow$ 14 + 28 + 36 + 57	$l_{PB} \rightarrow$ PB + WM + LF + CT
$l_{11} \rightarrow$ 24 + 18 + 35 + 67	$l_{WB} \rightarrow$ WB + PM + LC + FT
$l_{12} \rightarrow$ 8	$l_M \rightarrow$ M
$l_{13} \rightarrow$ 34 + 16 + 25 + 78	$l_{LB} \rightarrow$ LB + PF + WC + TM
$l_{14} \rightarrow$ 6	$l_F \rightarrow$ F
$l_{15} \rightarrow$ 5	$l_C \rightarrow$ C
$l_{16} \rightarrow$ 15 + 26 + 38 + 47	$l_{PF} \rightarrow$ PC + WF + LM + BT

The experiment will be run in the class.

Analysis of results

What is the experimental structure for this experiment?

Structure	Formula
unrandomized	
randomized	

Use R to analyse the results of the experiment and to perform appropriate diagnostic checking. What treatment combinations would give the longest flight time and what would you predict would be the flight time for these treatment combinations? The treatment combinations are available from the *Computing files* page of the web site in the file *Frf8Heli.Desgn.sdd*.

Note that the aliasing pattern (ignoring three- and more-factor interactions) is as follows:

l_1	-> average
l_2	-> 1
l_3	-> 2
l_4	-> 12 + 35 + 46 + 78
l_5	-> 3
l_6	-> 13 + 25 + 47 + 68
l_7	-> 23 + 15 + 48 + 67
l_8	-> 5
l_9	-> 4
l_{10}	-> 14 + 26 + 37 + 58
l_{11}	-> 24 + 16 + 38 + 57
l_{12}	-> 6
l_{13}	-> 34 + 17 + 28 + 56
l_{14}	-> 7
l_{15}	-> 8
l_{16}	-> 45 + 36 + 27 + 18

What is the experimental structure for this experiment?

Structure	Formula
unrandomized	16 Simulations
randomized	2 A*2 B*2 C*2 D*2 E*2 F*2 G*2 H

On the basis of previous simulation studies it could be assumed that the standard deviation of an estimated effect was 0.35.

Analyze this data using R. Perform appropriate diagnostic checking.