

Lesson 2.1 Analysis of 2^k Factorial Experiments

Introduction

Factorial designs are widely used in experiments involving several factors where it is necessary to study the joint effect of the factors on a response. In Stat 141 we discussed general methods for the analysis of factorial designs. However, several special cases of the general factorial design are important because they are widely used in research work and also because they form the basis of other designs of considerable practical value.

The most important of these special cases is that of k factors, each at only two levels. These levels may be quantitative, such as two values of temperature, pressure, or time; or they may be qualitative, such as two machines, two operators, the “high” (“+”) and “low” (“-”) levels of a factor, or perhaps the presence and absence of a factor. A complete replicate of such a design requires $2 \times 2 \times \cdots \times 2 = 2^k$ observations and is called a 2^k factorial experiment. In general, If the number of levels for each factor is the same, we call it as a **symmetrical** factorial experiment.

In this module, we assume that (1) the factors are fixed, (2) the designs are completely randomized, and (3) the usual normality assumptions are satisfied.

The 2^k design is particularly useful in the early stages of experimental work when many factors are likely to be investigated. It provides the smallest number of runs with which k factors can be studied in a complete factorial design. Consequently, these designs are widely used in factor screening experiments. Because there are only two levels for each factor, we assume that the response is approximately linear over the range of the factor levels chosen. In many factor screening experiments, when we are just starting to study the process or the system, this is often a reasonable assumption.

2^2 Factorial Experiment

The first design in the 2^k series is one with only two factors, say A and B, each run at two levels. This design is called a 2^2 factorial design. The levels of the factors may be arbitrarily called *low* and *high*. Geometrically, this can be displayed as a square, with the corners representing the treatment combinations.

A (low), B (low)	A_1B_1	a_0b_0	00	(1)
A (high), B (low)	A_2B_1	a_1b_0	10	a
A (low), B (high)	A_1B_2	a_0b_1	01	b
A (high), B (high)	A_2B_2	a_1b_1	11	ab

As an example, consider an investigation into the effect of the concentration of the reactant and the amount of the catalyst on the conversion (yield) in a chemical process. The objective of the experiment was to determine if adjustments to either of these two factors would increase the yield. Let the reactant concentration be factor A and let the two levels of interest be 15 and 25 percent. The catalyst is factor B, with the high level denoting the use of 2 pounds of the catalyst and the low level denoting the use of only 1 pound. The experiment is replicated three times, so there are 12 runs. The order in which the runs are made is random, so this is a completely randomized experiment. The data obtained are as follows:

A	B	Treatment Combination	Replicate			Total
			I	II	III	
-	-	A low, B low	28	25	27	80
+	-	A high, B low	36	32	32	100
-	+	A low, B high	18	19	23	60
+	+	A high, B high	31	30	29	90

In a two-level factorial design, we may define the average effect of a factor as the change in response produced by a change in the level of that factor averaged over the levels of the other factor. Also, the symbols (1) , a , b , and ab now represent the total of the response observation at all r replicates taken at the treatment combination.

Now the effect of A at the low level of B is $[a - (1)]/r$, and the effect of A at the high level of B is $[ab - b]/r$. Averaging these two quantities yields the main effect of A:

$$\begin{aligned} A &= \frac{1}{2r} \{ [ab - b] + [a - (1)] \} \\ &= \frac{1}{2r} \{ ab + a - b - (1) \} \end{aligned}$$

Similarly, the main effect of B is found from the effect of B at the low level of A ($[b - (1)]/r$) and at the high level of A ($[ab - a]/r$). Thus,

$$\begin{aligned} B &= \frac{1}{2r} \{ [ab - a] + [b - (1)] \} \\ &= \frac{1}{2r} \{ ab + b - a - (1) \} \end{aligned}$$

Finally, the interaction effect AB is defined as the average difference between the effect of A at the high level of B and the effect of A at the low level of B. Thus,

$$\begin{aligned} AB &= \frac{1}{2r} \{ [ab - b] - [a - (1)] \} \\ &= \frac{1}{2r} \{ ab - a - b + (1) \} \end{aligned}$$

Alternatively, we may define AB as the average difference between the effect of B at the high level of A and the effect of B at the low level of A

$$\begin{aligned} AB &= \frac{1}{2r} \{ [ab - a] - [b - (1)] \} \\ &= \frac{1}{2r} \{ ab - a - b + (1) \} \end{aligned}$$

Before we illustrate how the effects are calculated these formulas using the data in the example experiment, note that these formulas are consistent with our definitions of main effects and interaction effect in Stat 141.

Using the data in the above example, we may estimate the average effects as

$$\begin{aligned} A &= \frac{1}{2r} \{ ab + a - b - (1) \} = \frac{1}{2(3)} (90 + 100 - 60 - 80) = 8.33 \\ B &= \frac{1}{2r} \{ ab + b - a - (1) \} = \frac{1}{2(3)} (90 + 60 - 100 - 80) = -5.00 \\ AB &= \frac{1}{2r} \{ ab - a - b + (1) \} = \frac{1}{2(3)} (90 - 100 - 60 + 80) = 1.67 \end{aligned}$$

The effect of A (reactant concentration) is positive; this suggests that increasing A from the low level (15%) to the high level (25%) will increase the yield. The effect of B (catalyst) is negative; this suggests that increasing the amount of catalyst added to the process will decrease the yield. The interaction effect appears to be small relative to the two main effects.

In experiments involving 2^k designs, it is always important to examine the magnitude and direction of the factor effects to determine which variables are likely to be important. The analysis of variance can generally be used to confirm this interpretation. Effect magnitude and direction should always be considered along with the ANOVA, because the ANOVA alone does not convey this information.

Note that a contrast is used in estimating the effects A, B and AB. We have

$$\begin{aligned} Contrast_A &= ab + a - b - (1) \\ Contrast_B &= ab + b - a - (1) \\ Contrast_{AB} &= ab - a - b + (1) \end{aligned}$$

In determining these contrasts, use the following:

1. To find the contrast for A: observe that $(a - 1)(b + 1) = ab + a - b - 1$,
2. To find the contrast for B: observe that $(a + 1)(b - 1) = ab + b - a - 1$, and
3. To find the contrast for AB: observe that $(a - 1)(b - 1) = ab - a - b + 1$.

The sum of squares for any contrast can be computed as the contrast squared divided by the number of observations in each total in the contrast times the sum of the squares of the contrast coefficients. Consequently, we have

$$\begin{aligned}SSA &= \frac{[ab + b - a - (1)]^2}{4r} \\SSB &= \frac{[ab + a - b - (1)]^2}{4r} \\SSAB &= \frac{[ab - a - b + (1)]^2}{4r}\end{aligned}$$

Using the same data, we have

$$\begin{aligned}SSA &= \frac{[ab + b - a - (1)]^2}{4r} = \frac{[90 + 100 - 60 - 80]^2}{4(3)} = 208.33 \\SSB &= \frac{[ab + a - b - (1)]^2}{4r} = \frac{[90 + 60 - 100 - 80]^2}{4(3)} = 75.00 \\SSAB &= \frac{[ab - a - b + (1)]^2}{4r} = \frac{[90 - 100 - 60 + 80]^2}{4(3)} = 8.33\end{aligned}$$

The total sum of squares and the sum of squares for residuals/errors are calculated in the usual way. The resulting ANOVA table is given below. [VERIFY!]

Source of variation	Sum of squares	df	Mean squares	F	p
A	208.33	1	208.33	53.15	0.0001
B	75.00	1	75.00	19.13	0.0024
AB	8.33	1	8.33	2.13	0.1826
Error	31.34	8	3.92		
Total	323.00	11			

Note that the contrast coefficients for estimating the interaction effect are just the product of the corresponding coefficients for the two main effects. The contrast coefficient is always either +1 or -1, and a table of plus and minus signs such as below can be used to determine the proper sign for each treatment combination.

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

The column headings the table are the main effects (A and B), the AB interaction, and I, which represents the total or average of the entire experiment. Notice that the column corresponding to I has only plus signs. The row lables are the treatment combinations. To find the contrast for estimating any effect, simply multiply the signs in the appropriate column of the table by the corresponding treatment combination and add. For example, to estimate A, the contrast is $(1) + a - b + ab$. Note that the contrasts for the effects A, B, and AB are orthogonal. Thus, the 2^2 (and all 2^k designs) is an orthogonal design. The ± 1 coding for the low and high levels of the factors is often called the **orthogonal** coding or the **effects** coding.

Treatment	Totals	I	A	B	AB
(1)	80	+	-	-	+
a	100	+	+	-	-
b	60	+	-	+	-
ab	90	+	+	+	+
Contrast		50	-30	10	
Effects		8.33	-5.00	1.67	
SS		208.33	75.00	8.33	

In general for any 2^k factorial experiment, the divisors for calculating the effects and sums of squares are, respectively,

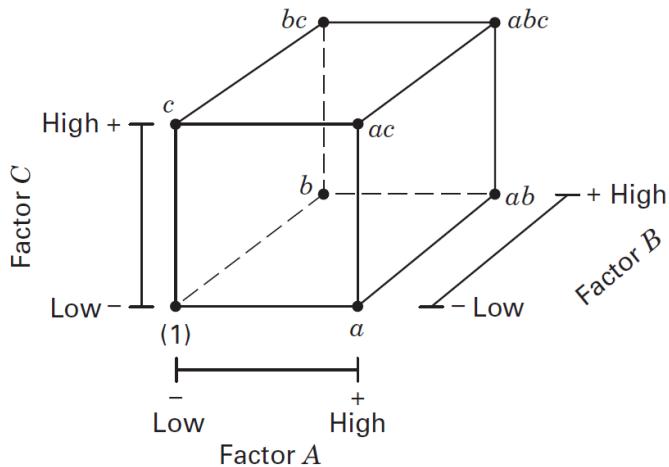
$$r \times 2^{k-1}$$

and

$$r \times 2^k.$$

2^3 Factorial Experiment

Suppose that three factors, A, B, and C, each at two levels, are of interest. The design is called a 2^3 factorial design, and the eight treatment combinations can now be displayed geometrically as a cube.



An experiment was conducted to determine if the yield of a chemical process is affected by temperature (medium, high), pressure (260 psi, 270 psi), and reactant concentration (15%, 25%). The data is given below.

Temperature	Pressure	Concentration	Rep 1	Rep 2	Total
Medium	260	15%	83	86	169
		25%	85	87	172
	270	15%	90	88	178
		25%	91	90	181
High	260	15%	91	93	184
		25%	90	91	181
	270	15%	92	94	186
		25%	91	94	185

Tasks:

1. Construct the table of the algebraic signs of the effects for this experiment.
2. Calculate the contrasts, effects and sums of squares.
3. Construct the ANOVA table.

A Single Replicate of the 2^k Design

For even a moderate number of factors, the total number of treatment combinations in a 2^k factorial experiment is large. For example, a 2^5 design has 32 treatment combinations, a 2^6 design has 64 treatment combinations, and so on. Because resources are usually limited, the number of replicates that the experimenter can employ may be restricted. Frequently, available resources only allow a single replicate of the design to be run, unless the experimenter is willing to omit some of the original factors.

The single-replicate strategy is often used in screening experiments when there are relatively many factors under consideration. Because we can never be entirely certain in such cases that the experimental error is small, a good practice in these types of experiments is to spread out the factor levels aggressively.

A single replicate of a 2^k experiment is sometimes called an **unreplicated** factorial. With only one replicate, there is no internal estimate of error (or “pure error”). One approach to the analysis of an unreplicated factorial is to assume that certain high-order interactions are negligible and combine their mean squares to estimate the error. This is an appeal to the **sparsity** of effects principle; that is, most systems are dominated by some of the main effects and low-order interactions, and most high-order interactions are negligible.

When analyzing data from unreplicated factorial designs, occasionally real high-order interactions occur. The use of an error mean square obtained by pooling high-order interactions is inappropriate in these cases. A method of analysis attributed to Daniel (1959) provides a simple way to overcome this problem. Daniel suggests examining a normal probability plot of the estimates of the effects. The effects that are negligible are normally distributed, with mean zero and variance σ^2 and will tend to fall along a straight line on this plot, whereas significant effects will have nonzero means and will not lie along the straight line. Thus, the preliminary model will be specified to contain those effects that are apparently nonzero, based on the normal probability plot. The apparently negligible effects are combined as an estimate of error.

The smallest design for which the procedure is recommended is 2^4 . It is also suggested that only non-significant higher-order interactions must be combined to form the MSE. But if for example in a 2^5 design with a single replicate AB and AC are significant, then ABC interaction must be retained in the final model.

To illustrate the suggestion of Daniel (1959), consider the following experiment.

A chemical product is produced in a pressure vessel. A factorial experiment is carried out in the pilot plant to study the factors thought to influence the filtration rate of this product. The four factors are temperature (A), pressure (B), concentration of formaldehyde (C), and stirring rate (D). Each factor is present at two levels. The design matrix and the response data obtained from a single replicate of the 2^4 experiment are shown below.

Pilot Plant Filtration Rate Experiment

Run Number	Factor				Run Label	Filtration Rate (gal/h)
	A	B	C	D		
1	-	-	-	-	(1)	45
2	+	-	-	-	a	71
3	-	+	-	-	b	48
4	+	+	-	-	ab	65
5	-	-	+	-	c	68
6	+	-	+	-	ac	60
7	-	+	+	-	bc	80
8	+	+	+	-	abc	65
9	-	-	-	+	d	43
10	+	-	-	+	ad	100
11	-	+	-	+	bd	45
12	+	+	-	+	abd	104
13	-	-	+	+	cd	75
14	+	-	+	+	acd	86
15	-	+	+	+	bcd	70
16	+	+	+	+	abcd	96

You can verify that the contrasts, effects, and sums of squares for this data (computed using the method discussed previously in class) are given below.

Terms	Contrasts	Effects	SS
A	173	21.625	1870.5625
B	25	3.125	39.0625
C	79	9.875	390.0625
D	117	14.625	855.5625
AB	1	0.125	0.0625
AC	-145	-18.125	1314.0625
BC	19	2.375	22.5625
AD	133	16.625	1105.5625
BD	-3	-0.375	0.5625
CD	-9	-1.125	5.0625
ABC	15	1.875	14.0625
ABD	33	4.125	68.0625
ACD	-13	-1.625	10.5625
BCD	-21	-2.625	27.5625
ABCD	11	1.375	7.5625

The *DanielPLOT()* in the **FrF2** package can be used to show the plot of the effects to determine which of these are negligible and will be combined to form the MSE.

```

library(tidyverse)
library(FrF2)

#generates the design matrix
design <- expand.grid(A = c(-1, 1),
                      B = c(-1, 1),
                      C = c(-1, 1),
                      D = c(-1, 1))

rate <- c(45, 71, 48, 65, 68, 60, 80, 65, 43, 100, 45, 104, 75, 86, 70, 96)

#Add the response column
df <- design %>%
  mutate(Y = rate)

#prints the design matrix with the response
df

##      A  B  C  D   Y
## 1  -1 -1 -1 -1  45
## 2   1 -1 -1 -1  71
## 3  -1  1 -1 -1  48
## 4   1  1 -1 -1  65
## 5  -1 -1  1 -1  68
## 6   1 -1  1 -1  60
## 7  -1  1  1 -1  80
## 8   1  1  1 -1  65
## 9  -1 -1 -1  1  43
## 10  1 -1 -1  1 100
## 11 -1  1 -1  1  45
## 12  1  1 -1  1 104
## 13 -1 -1  1  1  75
## 14  1 -1  1  1  86
## 15 -1  1  1  1  70
## 16  1  1  1  1  96

#fits the model using lm() function
model <- lm(Y ~ A*B*C*D, data = df)

#prints the estimates
summary(model)

##

```

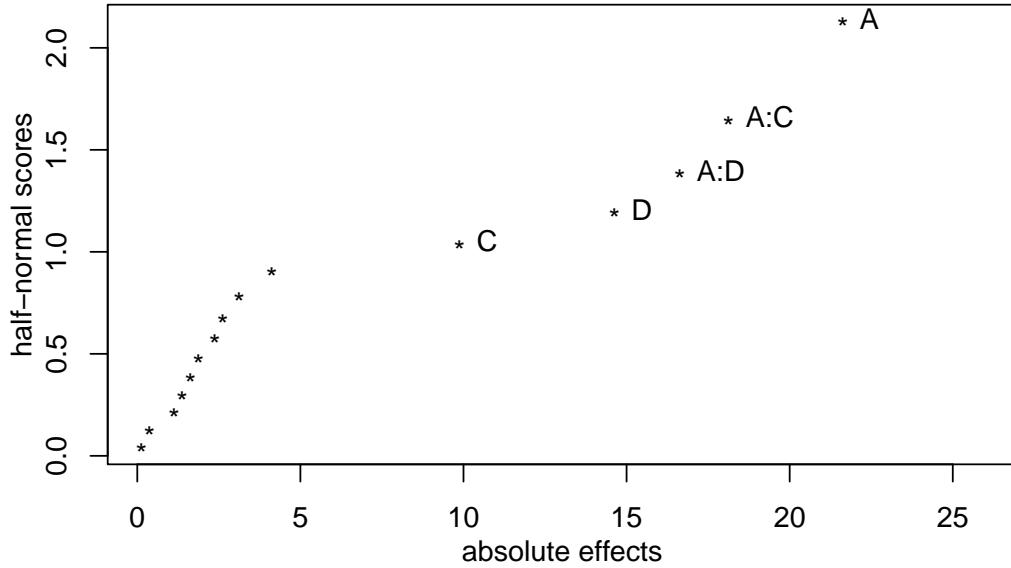
```

## Call:
## lm.default(formula = Y ~ A * B * C * D, data = df)
##
## Residuals:
## ALL 16 residuals are 0: no residual degrees of freedom!
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 70.0625     NaN      NaN      NaN
## A           10.8125    NaN      NaN      NaN
## B           1.5625     NaN      NaN      NaN
## C           4.9375    NaN      NaN      NaN
## D           7.3125    NaN      NaN      NaN
## A:B         0.0625    NaN      NaN      NaN
## A:C        -9.0625    NaN      NaN      NaN
## B:C         1.1875    NaN      NaN      NaN
## A:D         8.3125    NaN      NaN      NaN
## B:D        -0.1875    NaN      NaN      NaN
## C:D        -0.5625    NaN      NaN      NaN
## A:B:C       0.9375    NaN      NaN      NaN
## A:B:D       2.0625    NaN      NaN      NaN
## A:C:D      -0.8125    NaN      NaN      NaN
## B:C:D      -1.3125    NaN      NaN      NaN
## A:B:C:D    0.6875    NaN      NaN      NaN
##
## Residual standard error: NaN on 0 degrees of freedom
## Multiple R-squared:      1, Adjusted R-squared:      NaN
## F-statistic:   NaN on 15 and 0 DF,  p-value: NA

```

```

#generates the normal probability plot of the effects
DanielPlot(model, half = TRUE, main = "")
```



Based on the plot the significant effects are A, C, D, AD, and AC. The final ANOVA table is given below.

```
anova(lm(Y ~ A*C*D, data = df))
```

```
## Analysis of Variance Table
##
## Response: Y
##             Df  Sum Sq Mean Sq F value    Pr(>F)
## A          1 1870.56 1870.56 83.3677 1.667e-05 ***
## C          1   390.06   390.06 17.3844 0.0031244 **
## D          1   855.56   855.56 38.1309 0.0002666 ***
## A:C        1 1314.06 1314.06 58.5655 6.001e-05 ***
## A:D        1 1105.56 1105.56 49.2730 0.0001105 ***
## C:D        1     5.06     5.06  0.2256 0.6474830
## A:C:D     1    10.56    10.56  0.4708 0.5120321
## Residuals 8   179.50   22.44
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```