STA305/1004-Class 14

October 29, 2019

Example of a factorial design

Suppose that an investigator is interested in examining three components of a weight loss intervention. The three components are:

1. Keeping a food diary (yes/no)
2. Increasing activity (yes/no)
3. Home visit (yes/no)

Factorial designs

The investigator plans to investigate all $2x2x2 = 2^3 = 8$ combinations of experimental conditions.

The experimental conditions will be.

Expt condition	Keep food diary	Increase physical activity	Home visit	weight loss
1	No	No	No	y_1
2	No	No	Yes	y_2
3	No	Yes	No	y_3
4	No	Yes	Yes	y_4
5	Yes	No	No	y_5
6	Yes	No	Yes	y_6
7	Yes	Yes	No	y_7
8	Yes	Yes	Yes	y_8

Factorial designs at two levels

- To perform a factorial design, you select a fixed number of levels of each of a number of factors (variables) and then run experiments in all possible combinations.

Factorial designs at two levels

- The factors can be quantitative or qualitative.
- Two levels of a quantitative variable could be two different temperatures or two different concentrations.
- Qualitative factors might be two types of catalysts or the presence and absence of some entity.

Factorial design

The notation 2^3 identifies: - the number of factors (3) - the number of levels of each factor (2) - how many experimental conditions are in the design ($2^3 = 8$)

Factorial experiments can involve factors with different numbers of levels.

Factorial design

Consider a 4^2x3^2x2 design.

(a) How many factors?
(b) How many levels of each factor?
(c) How many experimental conditions (runs)?

Difference between ANOVA and Factorial Designs

In ANOVA the objective is to compare the individual experimental conditions with each other. In a factorial experiment the objective is generally to compare combinations of experimental conditions.

Let's consider the food diary study above. What is the effect of keeping a food diary?

Expt condition	Keep food diary	Increase physical activity	Home visit	weight loss
1	No	No	No	y_1
2	No	No	Yes	y_2
3	No	Yes	No	y_3
4	No	Yes	Yes	y_4
5	Yes	No	No	y_5
6	Yes	No	Yes	y_6
7	Yes	Yes	No	y_7
8	Yes	Yes	Yes	y_8

We can estimate the effect of food diary by comparing the mean of all conditions where food diary is set to NO (conditions 1-4) and mean of all conditions where food diary set to YES (conditions 5-8). This is also called the **main effect** of food diary, the adjective *main* being a reminder that this average is taken over the levels of the other factors.

Difference between ANOVA and Factorial Designs

Expt condition	Keep food diary	Increase physical activity	Home visit	weight loss
1	No	No	No	y_1
2	No	No	Yes	y_2
3	No	Yes	No	y_3
4	No	Yes	Yes	y_4
5	Yes	No	No	y_5
6	Yes	No	Yes	y_6
7	Yes	Yes	No	y_7
8	Yes	Yes	Yes	y_8

The main effect of food diary is:

$$\frac{y_1 + y_2 + y_3 + y_4}{4} - \frac{y_5 + y_6 + y_7 + y_8}{4}.$$

The main effect of physical activity is:

$$\frac{y_1 + y_2 + y_5 + y_6}{4} - \frac{y_3 + y_4 + y_7 + y_8}{4}.$$

The main effect of home visit is:

$$\frac{y_1 + y_3 + y_5 + y_7}{4} - \frac{y_2 + y_4 + y_6 + y_8}{4}.$$

Question

A chemical reaction experiment was carried out with the objective of comparing if a new catalyst B would give higher yields than the old catalyst A, but yield is also known to vary with temperature (high versus low). Two runs measured yield using catalyst A at a high tempertaure, and two runs measured yield using catalyst B at a high temperture.

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The experimental design is:

2^2 factorial design.	**A**
2×2 factorial design.	**B**
4^1 factorial design.	**C**
Paired design.	**D**
None of the above	**E**

Total Results: 0

Factorial designs at two levels

To perform a factorial design:

1. Select a fixed number of levels of each factor.
2. Run experiments in all possible combinations.

Factorial designs at two levels

- We will discuss designs where there are just two levels for each factor.
- Factors can be quantitative or qualitative.
- Two levels of quantitative variable could be two different temperatures or concentrations.
- Two levels of a quantitative variable could be two different types of catalysts or presence/absence of some entity.

Pilot plant investigation - example of factorial design

A pilot plant invsetiagtion employed a 2^3 factorial design (Box, Hunter, and Hunter (2005)) with

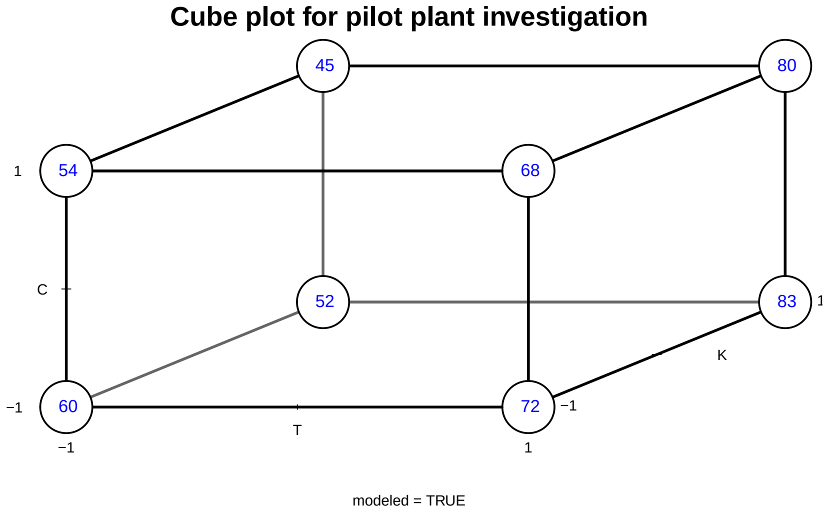
Factors	level 1	level 2
Temperature	$160\mathrm{C}^{\circ}$(-1)	$180\mathrm{C}^{\circ}(+1)$
Concentration	20% (-1)	40% (+1)
Catalyst	A (-1)	B(+1)

run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

- Each data value recorded is for the response yield y averaged over two duplicate runs.

Cube plots

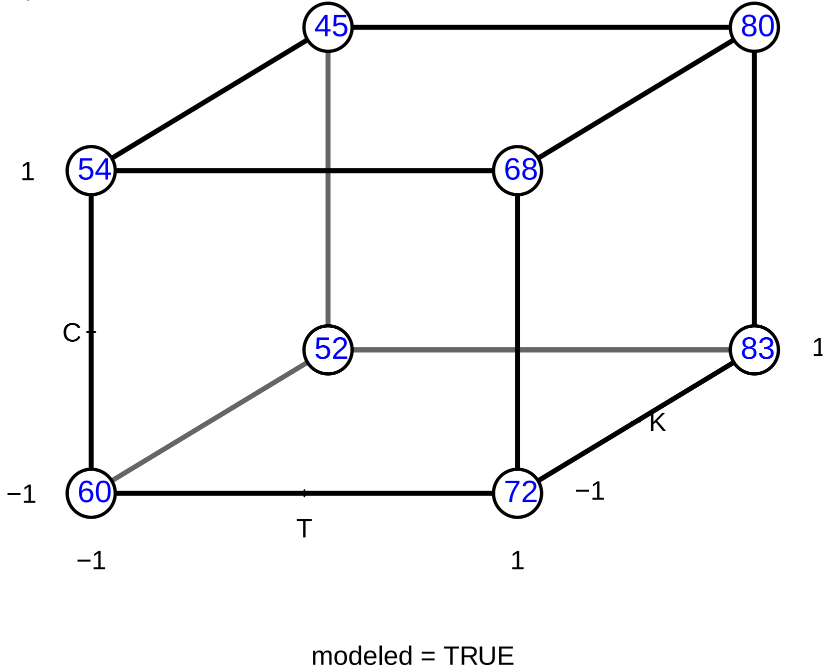
```
library("FrF2")
bhh54 <- lm(y~T*C*K,data=tab0502)
cubePlot(bhh54,"T","K","C",main="Cube plot for pilot plant investigation", size
```



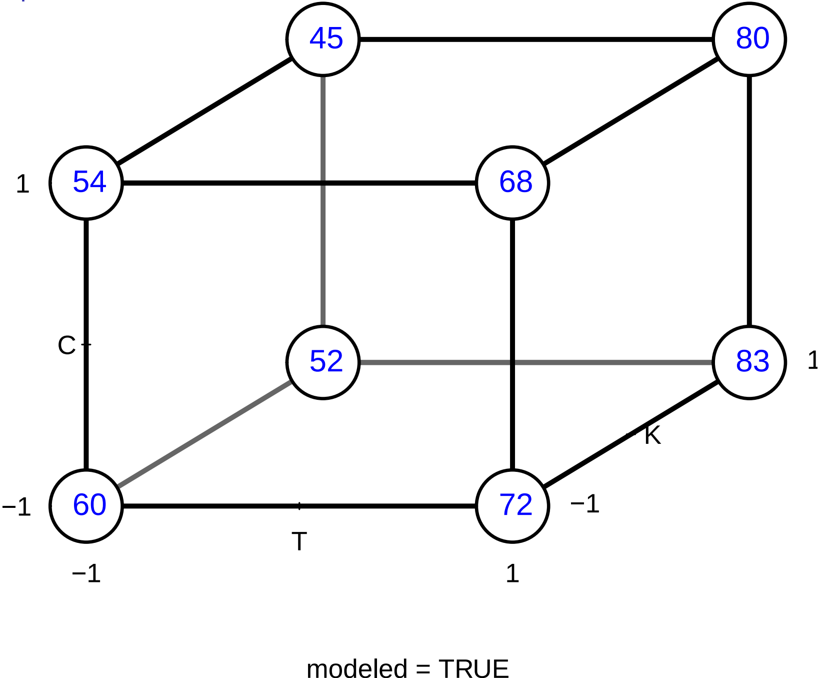
Cube plots

- 8 run design produces 12 comparisons
- Each edge of cube only one factor changed while other 2 held constant.
- Therefore experimenter that believes in only changing one factor at a time is satisfied.

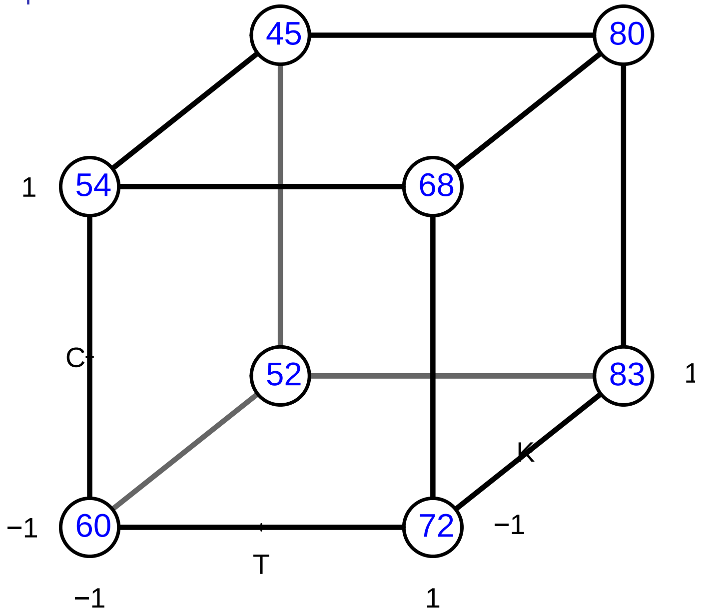
Cube plots



Cube plots



Cube plots



Cube plots

- 8 run design produces 12 comparisons
- Each edge of cube only one factor changed while other 2 held constant.
- Therefore experimenter that believes in only changing one factor at a time is satisfied.

Cube plots

Using the cube plot below the main effects for T, C, K (respectively) are approximately:

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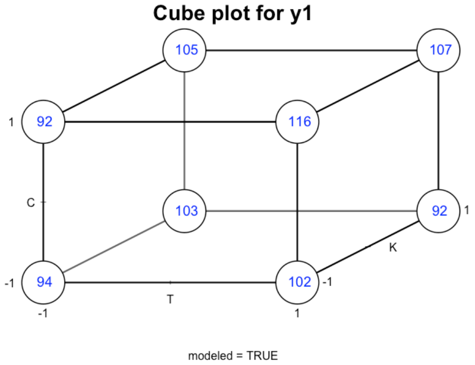
T=2.88; C=3.63; K=0.38	**A**
T=5.75; C=7.25; K=0.75	**B**
T=11.5; C=14.5; K=1.5	**C**



Interaction effects - two factor interactions

run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

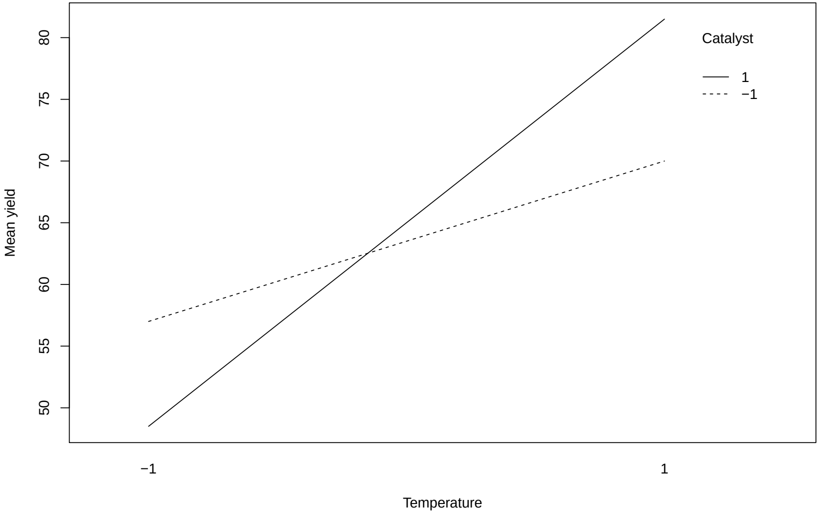
- When the catalyst K is A the temperature effect is: $\frac{68+72}{2} - \frac{60+54}{2} = 70 - 57 = 13.$
- When the catalyst K is B the temperature effect is: $\frac{83+80}{2} - \frac{52+45}{2} = 81.5 - 48.5 = 33.$
- The average difference between these two average differences is called the **interaction** between temperature and catalyst denoted by TK. This is the interaction between the two factors temperature and catalyst - the two factor interaction between temperature and catalyst.

$$TK = \frac{33 - 13}{2} = 10$$

.

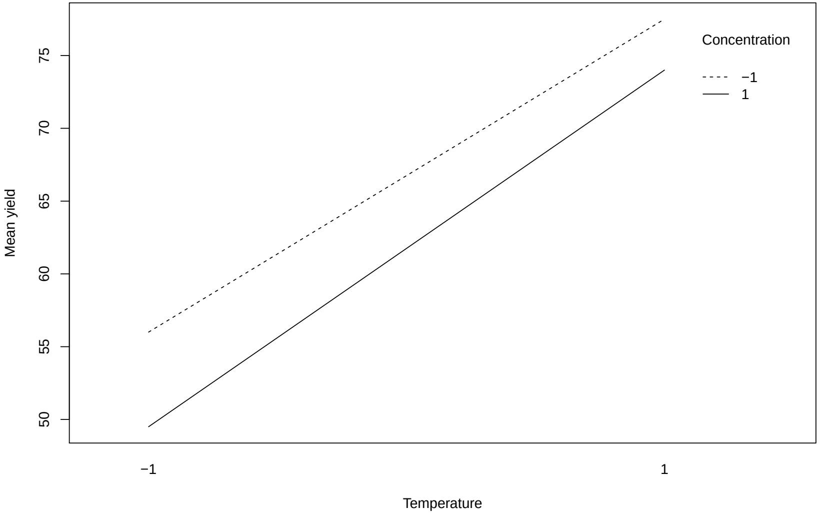
Interaction plots - Temperature by catalyst

```r
interaction.plot(tab0502$T,tab0502$K,tab0502$y, type="l",
                 trace.label="Catalyst",xlab = "Temperature",
                 ylab="Mean yield")
```



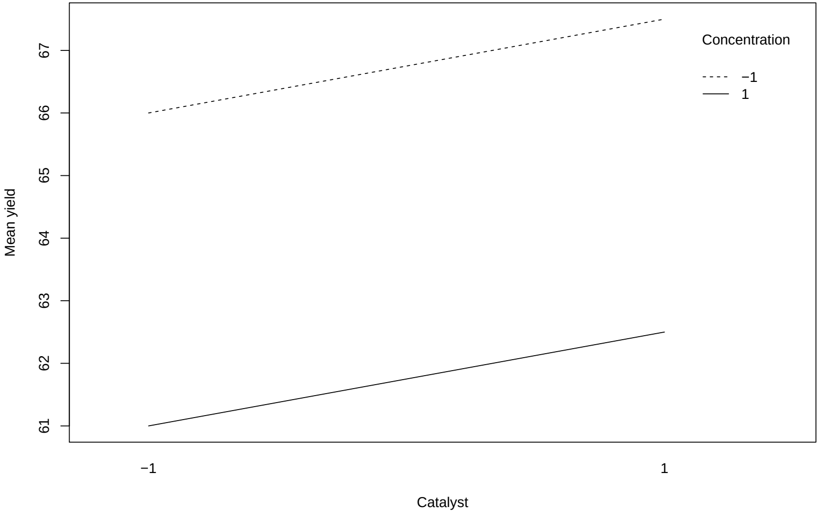
Interaction plots - Concentration by temperature

```
interaction.plot(tab0502$T,tab0502$C,tab0502$y, type="l",
                 xlab="Temperature",trace.label="Concentration",
                 ylab="Mean yield")
```



Interaction plots - Concentration by catalyst

```
interaction.plot(tab0502$K,tab0502$C,tab0502$y, type="l",
                 xlab="Catalyst",trace.label="Concentration",
                 ylab="Mean yield")
```



Three factor interactions

run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

The temperature by concentration interaction when the catalyst is B (at it's +1 level) is:

$$\text{Interaction TC} = \frac{(y_8 - y_7) - (y_6 - y_5)}{2} = \frac{(80 - 45) - (83 - 52)}{2} = 2.$$

The temperature by concentration interaction when the catalyst is A (at it's -1 level) is:

$$\text{Interaction TC} = \frac{(y_4 - y_3) - (y_2 - y_1)}{2} = \frac{(68 - 54) - (72 - 60)}{2} = 1.$$

$$\text{TCK} = \frac{2 - 1}{2} = \frac{1}{2}.$$

Three factor interaction

- Interactions are symmetric in all factors.
- It could have been defined as half the difference between the temperature-by-catalyst interactions at each of the two concentrations.
- Mostly rely on statistical software such as R.

Replicate runs

- Each of the 8 responses in the table is the average of two (genuinely) replicated runs.
- Genuinely replicated run means that variation between runs made at same experimental conditions is a reflection of the total run-to-run variability.

run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

Replicate runs

- Randomization of the run order for all 16 runs ensures the replication is genuine.
- `run1` is order of the first run and `run2` is order of the second run.

run1	run2	T	C	K	y1	y2	diff
6	13	-1	-1	-1	59	61	-2
2	4	1	-1	-1	74	70	4
1	16	-1	1	-1	50	58	-8
5	10	1	1	-1	69	67	2
8	12	-1	-1	1	50	54	-4
9	14	1	-1	1	81	85	-4
3	11	-1	1	1	46	44	2
7	15	1	1	1	79	81	-2

Replicate runs

- Replication not always feasible or easy.
- For the pilot plant experiment a run involved: cleaning the reactor; inserting the appropriate catalyst charge; and running the apparatus at a given concentration for 3 hours, and sampling output every 15 minutes.
- A genuine run involved taking all of these steps all over again!

Replicate runs

- There are usually better ways to employ 16 independent runs than by fully replicating a 2^3 factorial.
- Other designs can study four or five factors with a 16 run two-level design.

Estimate of error variance of the effects from replicated runs

run1	run2	T	C	K	y1	y2	diff
6	13	-1	-1	-1	59	61	-2
2	4	1	-1	-1	74	70	4
1	16	-1	1	-1	50	58	-8
5	10	1	1	-1	69	67	2
8	12	-1	-1	1	50	54	-4
9	14	1	-1	1	81	85	-4
3	11	-1	1	1	46	44	2
7	15	1	1	1	79	81	-2

$$s_i^2 = \frac{(y_{i1} - y_{i2})^2}{2},$$

- y_{i1} is the first outcome from *ith* run.
- $\text{diff}_i = (y_{i1} - y_{i2})$.
- A pooled estimate of σ^2 is

$$s^2 = \frac{\sum_{i=1}^{8} s_i^2}{8} = \frac{64}{8} = 8.$$

- The variance of an effect is:

$$Var(\text{effect}) = \left(\frac{1}{8} + \frac{1}{8}\right) s^2 = 8/4 = 2$$

Interpretation of results

- Which effects are real and which can be explained by chance?
- A rough rule of thumb: any effect that is 2-3 times their standard error are not easily explained by chance alone.

Interpretation of results

- Assume that the observations are independent and normally distributed then

$$\text{effect}/se\left(\text{effect}\right) \sim t_8.$$

- A 95% confidence interval can be calculated as:

$$\text{effect} \pm t_{8,.05/2} \times se\left(\text{effect}\right).$$

where $t_{8,.05/2}$ is the 97.5th percentile of the t_8. This is obtained in R via the `qt()` function.

```
qt(p = 1-.025,df = 8)
```

```
## [1] 2.306004
```

- In the pilot plant study

$$\text{effect} \pm 2.3 \times 1.4 = \text{effect} \pm 3.2.$$

Interpretation of results

- The main effect of a factor should be individually interpreted only if there is no evidence that the factor interacts with other factors.
- Which effects should be considered jointly and which independently?

Effects	95% Confidence Interval
T	(19.8, 26.2)
C	(-8.2, -1.8)
K	(-1.7, 4.7)
TC	(-1.7, 4.7)
TK	(6.8, 13.2)
CK	(-3.2, 3.2)
TCK	(-2.7, 3.7)

Interpretation of results

- The effect of changing concentration over the ranges studied is to reduce yield by about 5 units. This is irrespective of the tested level of other variables.
- The effects of temperature and catalyst cannot be interpreted separately because of the large TK interaction. With catalyst A the temperature effect is 13 units and with catalyst B it is 33 units.