Research Methods

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Objectives

You should be able to

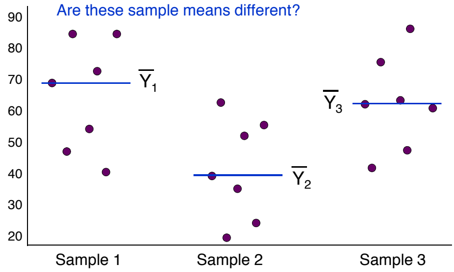
- Explain the limitations of the OFAT experiment design strategy
- Analyse main effects plots and identify interactions
- Write our response tables for 2^k experimental plans
- Compute main effects from the results of a 2^k experiment
- Build a random effects model to predict the outcome of an experiment for a particular set of factors
- Use a two-way ANOVA to compute the statistically significant factors of an experiment
- Interpret the results of two-way ANOVA

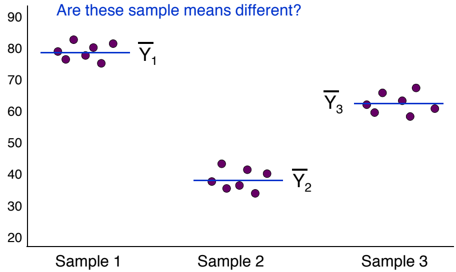
ANOVA review

Used for:

- Comparing the mean performance of more than two data sets
- Comparing Key Process Input Variables (KPIVs) on a continuous Key Process Output Variable (KPOV)
  - e.g. comparing the effect of working conditions on profit.
- Quantifying interaction between different KPIVs on a KPOV

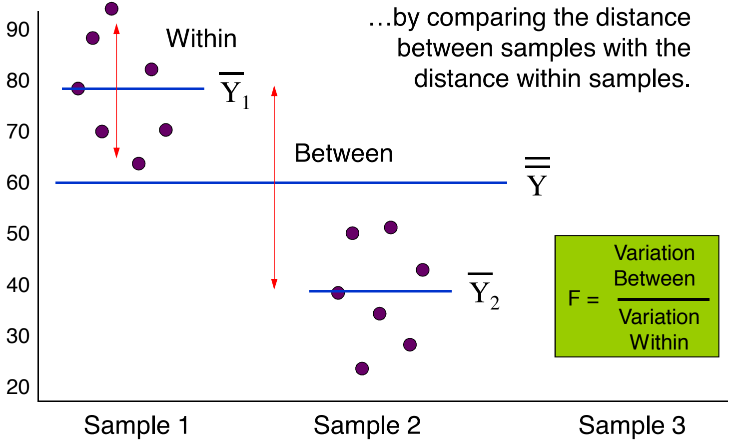
ANOVA review



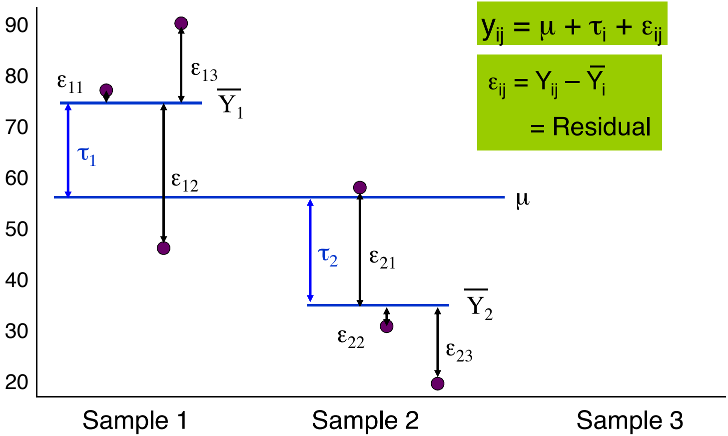


ANOVA review

…by comparing the distance between samples with the distance within samples.



Single Factor ANOVA Model



μ is the overal mean effect, τ_i is the effect of the i^{th} level, and ε_{ij} is a normal random error of mean 0 and variance σ^2 for the j^{th} replicate measurement.

The basic ANOVA question

Is the mean response at different factors levels the same?

- I.e. does the factor, x, significantly influence the mean response, y?
- H_0: $\mu_{pop1} = \mu_{pop2} = \mu_{pop3} = \mu_{pop4}$
- H_A: at least of of the means is different

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Statistical Design of Experiments

Statistical design of experiments (DoE) is a plan for the collection and analysis of data.

We will use ANOVA techniques for the design of experiments. For example we learn a technique to quickly screen the design parameter space to answer questions like: "In an experiment that depends on variables A, B, & C, how can I determine which variables are most influential on the response?" and "What is the most efficient way to design an experiment to understand the relationship between A, B, & C"

Design of Experiments

Suppose the objective is to optimise some process. You believe the process depends on the factors: Time, Temperature, and Pressure.

To find the optimum Time, Temperature, and Pressure combination, we need to test the response of the process to these variables?

One Factor At a Time (OFAT)

Assume two factors A & B, each at two levels, -1 and +1, and also assume that we want to maximise the response.

Factor A	+1	Run 2 **50**	Run 3 **47**
	-1	Run 1 **45**	Not Tested **57**
		-1	+1
		Factor B	

Assume we first check the effect of A on the response.

- Runs 1 and 2 indicate that A+, B- is better than A–,B–
    - So A is held high and we change B
- Run 3 indicates that A+B– is better than A+B+
- therefore from 3 runs we would conclude that A+,B–, maximises the response, however, we would have missed run 4, which shows that A–, B+ is best.
- Runs 1 and 2 indicate that A+, B– is better than A–,B–

Factorial Design of Experiments

Valuable for screening the effect of a large number of possible factors on the response.

- Useful at early stage of experiment to get a preliminary understanding of the relationship between factors and the response variable
- Used to model the relationship that describes the response: $y = F(x_1, x_2, x_3, ...)$
- Can provide insight into the framing of more complete experimental designs
- Extensively used in R&D of products and processes

2^k Factorial Design

2^k factorial design means that only two levels for each factor k are tested:

- one level represents the lower range of variables (coded as $-$)
- one level represents the higher range of variables(coded as $+$)
- k is the number of different factors considered (i.e for understanding the effect of time, temperature, and pressure, $k = 3$

Example: Growing crystals

Suppose you want to know which factor has the greatest effect on the size of a single crystal. You decide the investigate the following factors:

- Temperature
- Time
- pressure

We want to quantify the relationship:
$size = f(Temp, Time, Pressure)$

We can consider One Factor At a Time (OFAT) or Full Factorial Experiment (DoE).

2^k full factorial DoE

Generally:

- 2^k factorial design refers to K factors, each with 2 levels
- One full factorial design requires 2^K runs
- The design matrix for 2^K factorial is usually shown in coded units:

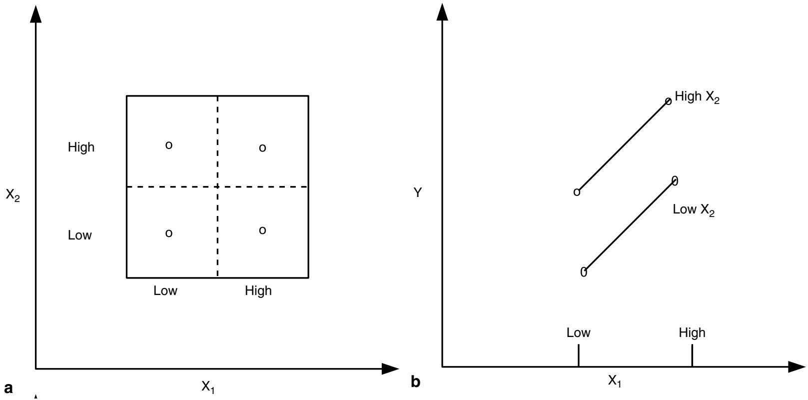
  -1: low level

  $+1$: high level

  0: center point

- Run the experiment for each possible combination of factors and levels.
  - Ensure that the "combination" or cells are run in a random order, by the same operator with the same lot of raw material and process set-up and in the same environmental conditions

Building models from factorial design



For 2^2 factorial design, x_1 and x_2 are split into high (+1) and low (-1) ranges. A line is used to assess correlations between x_1 and x_2, and the response y.

Response Tables

Response table allow measurements to be planned in a modular and logical manner. For a two factor experiment, 2^2 different experiments are required to characterise the response. For a three factor experiment $2^3 = 8$ experiments are necessary. The response table for a three (k=3) factor experiment is shown below.

	Level of Factors			
Trial	A	B	C	Response
1	−	−	−	y_1
2	+	−	−	y_2
3	−	+	−	y_3
4	+	+	−	y_4
5	−	−	+	y_5
6	+	−	+	y_6
7	−	+	+	y_7
8	+	+	+	y_8

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Main Effects

The main effect of a particular factor is determined by calculating the average value of all the high range (+) terms and subtracting the average of all the low range (–) terms. For example the main effect of factor C is calculated as follows:

$$ME_C = \bar{C}^+ - \bar{C}^- == \frac{y_5 + y_6 + y_7 + y_8}{4} - \frac{y_1 + y_2 + y_3 + y_4}{4}$$

Interactions

Some factors may interact. For example factors A & B may each give a low response, but interact together to give a high response. This effect needs to be considered. Again we can use response tables to modulize the measurements in a logical manner.
The sign coding for the interactions is determined by multiplying the signs of each of the two corresponding factors.

	Level of Factors			Interactions				
Trial	A	B	C	AB	AC	BC	ABC	Response
1	−	−	−	+	+	+	−	y_1
2	+	−	−	−	−	+	+	y_2
3	−	+	−	−	+	−	+	y_3
4	+	+	−	+	−	−	−	y_4
5	−	−	+	+	−	−	+	y_5
6	+	−	+	−	+	−	−	y_6
7	−	+	+	−	−	+	−	y_7
8	+	+	+	+	+	+	+	y_8

Calculating interaction effect

The interaction effect of, say, BC can be determined by the average of the B effect when C is held constant at + 1 minus the B effect when C is held constant at –1. Thus:

$$IE_{BC} = \frac{\text{sum of terms that result in +ve BC}}{4} - \frac{\text{sum of terms that result in -ve BC}}{4} \tag{1}$$

$$IE_{BC} = \frac{\bar{B}^- C^- + \bar{B}^+ C^+}{4} - \frac{\bar{B}^+ C^- + \bar{B}^- + C^+}{4} \tag{2}$$

$$IE_{BC} = \frac{y_1 + y_2 + y_7 + y_8}{4} - \frac{y_3 + y_4 + y_5 + y_6}{4} \tag{3}$$

2^3 Interactions response table

Trial	Resp.	A_+	A_-	B_+	B_-	C_+	C_-	AB_+	AB_-	AC_+	AC_-	BC_+	BC_-
1	y_1		y_1		y_1		y_1	y_1		y_1		y_1	
2	y_2	y_2			y_2		y_2		y_2		y_2	y_2	
3	y_3		y_3	y_3			y_3		y_3	y_3			y_3
4	y_4	y_4		y_4			y_4	y_4			y_4		y_4
5	y_5		y_5		y_5	y_5		y_5			y_5		y_5
6	y_6	y_6			y_6	y_6			y_6	y_6			y_6
7	y_7		y_7	y_7		y_7			y_7		y_7	y_7	
8	y_8	y_8		y_8		y_8		y_8		y_8		y_8	
Sum													
No.	8	4	4	4	4	4	4	4	4	4	4	4	4
Avg		$\bar{A}_+$	$\bar{A}_-$	$\bar{B}_+$	$\bar{B}_-$	$\bar{C}_+$	$\bar{C}_-$	$\overline{AB}_+$	$\overline{AB}_-$	$\overline{AC}_+$	$\overline{AC}_-$	$\overline{BC}_+$	$\overline{BC}_-$
Effect		$\bar{A}_+ - \bar{A}_-$		$\bar{B}_+ - \bar{B}_-$		$\bar{C}_+ - \bar{C}_-$		$\overline{AB}_+ - \overline{AB}_-$		$\overline{AC}_+ - \overline{AC}_-$		$\overline{BC}_+ - \overline{BC}_-$	

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

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Modeling response

The Main effects and interaction effects can be summed to provide an empirical predictive model:

$$\hat{y} = \underbrace{b_0 + b_1 A + b_2 B + b_3 C}_{\text{Main effects}} + \underbrace{b_{12} AB + b_{13} AC + b_{23} BC + b_{123} ABC}_{\text{Interaction terms}}$$

b_0 is the grand average of all measurements.
The simple interpretation of the model parameters is that b_i measures the unit influence of A, B, or C on y (i.e., denotes the slope wrt A,B, or C. Note that this is strictly true only when the variables are really independent or uncorrelated.

Case problem 10.1

Crystal growth 2^2 full factorial DoE

The size of a crystal is collected for different pressures and temperatures as follows:

	Pressure 1	Pressure 2
Temp 1	20	30
Temp 2	40	52

i. Write down the design matrix using coded levels of factor

ii. Calculate the main effect for each factor

iii. Write out the interaction table

Case problem 1 Solution

The size data collected is the following:

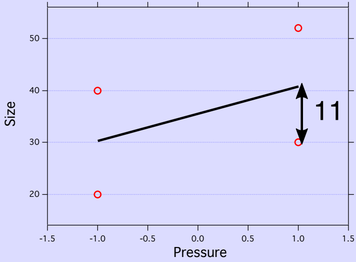
	Pressure 1	Pressure 2
Temp 1	20	30
Temp 2	40	52

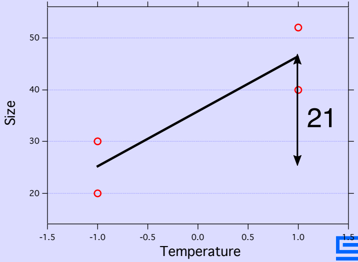
The design matrix using coded levels of factors is:

Temp	Pressure	Size
-1	-1	20
1	-1	40
-1	1	30
1	1	52

Crystal growth 2^2 full factorial DoE

Temp	Pressure	Size
-1	-1	20
1	-1	40
-1	1	30
1	1	52





Crystal growth 2^2: Main Effect

Main Effect of a factor: the average change in the output variable produced by a change in the levels of a factor.

The change in size across Pressures (the Main Effect for Pressure) is defined as:

$$ME_{Press} = \frac{30+52}{2} - \frac{40+20}{2} = 11$$

As the pressure increases from -1 to 1, the size increases by 11.

The change in size across Temperatures (the Main Effect for Temp) is defined as:

$$ME_{Temp} = \frac{40+52}{2} - \frac{30+20}{2} = 21$$

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Crystal growth 2^2: Main Effect Table

To determine the main effect across factor:

- Add up the response values when the factor level is -1
- Add up the response values when the factor level is +1
- Subtract the -1 sum from the +1 sum
- Divide by 2 (find the average) to determine the EFFECT

	Temp	Pressure	Size
	-1	-1	20
	1	-1	40
	-1	1	30
	1	1	52
Total –	50	60	
Total +	92	82	
Difference	42	22	
Effect	21	11	

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2^2 Interaction

Sometimes we find that when fixing one factor, the effect between the levels of another factor is not the same as it's overall main effect.

In this case we have an **interaction** between factors.

Temp	Pressure	Size
-1	-1	20
1	-1	40
-1	1	30
1	1	52

$\Delta Y_{P\text{-}1}(\text{Temp})=20$

$\Delta Y_{P\text{-}2}(\text{Temp})=22$

Calculating the interaction

The Temp x Press interaction effect = 1

The interaction is calculated by:

- The average difference between:
  - The effect of Temperature on size at the high level of Pressure $52 - 30 = 22$, i.e. when $P = P^+$, the Temperature goes up and the yield goes up 22 points
  - The effect of Temperature on yield at low level of Pressure $40 - 20 = 20$, i.e. when $P = P^-$, the Temperature goes up the yield goes up 20 points

$$IE_{Press \times Temp} = \frac{(52 - 30) - (40 - 20)}{2} = 1$$

Determining the EFFECT of an interaction

- Find the level by multiplying the factor terms
- Add up the response values when the factor level is -1
- Add up the response values when the factor level is +1
- Subtract the -1 sum from the +1 sum
- Divide by 2 (find the average) to determine the **EFFECT**

	Temp	Pressure	Interaction	Size
	-1	-1	1	20
	1	-1	-1	40
	-1	1	-1	30
	1	1	1	52
Total –	50	60	70	
Total +	92	82	72	
Difference	42	22	2	
Effect	21	11	1	

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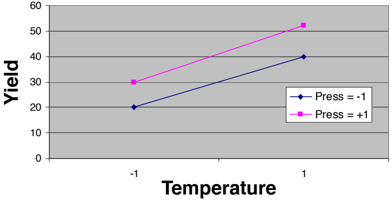
Interaction graphs

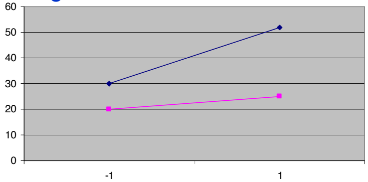
- We can graph interactions

Temp	Pressure	Yield
-1	-1	20
1	-1	40
-1	1	30
1	1	52

- Parallel lines indicate no interaction



- Non-parallel lines indicate strong interaction



Two factor ANOVA and DoE

ANOVA lets us test whether the contribution of a particular factor or interaction significantly influences the response.

Two factor ANOVA and DoE

- Imagine the outcome of an experiment depends on two factors: A and B
- There are a levels of A and b levels of B
- n replicate measurements are made on each factor at each level. Thus a total of nab measurements are made for all possible treatments
- Each measurement can be labelled Y_{ijk} where i denotes the level of A, j denotes the level of B and k denotes the replicate number
- These nab measurements should be made in **random order**, thus creating a *randomised experimental design*.

These observations can then be described by a linear statistical model:

$$Y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk} \tag{4}$$

where μ is the overall mean effect, τ_i is the effect of the i^{th} level of factor A, β_j is the effect of the j^{th} level of factor B, $(\tau\beta)_{ij}$ is the effect of the interaction between A and B, and ϵ_{ijk} is a random error component with a Normal distribution having a mean 0 and variance σ^2.

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Two factor ANOVA and DoE

The data shown below is collected from a two factor experiment. The averages correspond to either the rows or columns of measurements.

		Factor B		Average
		Level 1	Level 2	
Factor A	Level 1	10,14	18,14	14
	Level 2	23,21	16,20	20
	Level 3	31,27	21,25	26
Average		21	19	20

Table 1: Example of a two factor ANOVA dataset

Here, each treatment is replicated twice ($n = 2$). There are three levels for Factor A, ($a = 3$). There are two levels for Factor B, ($b = 2$). So using the the Y_{ijk} notation, $Y_{321} = 21$.

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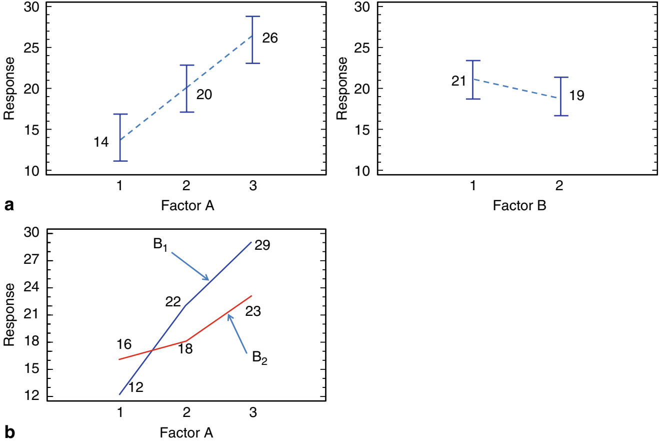
Two factor ANOVA and DoE

The main effect plots are shown below (a), and (b) shows the interaction plot.
Notice that there appears to be an interfaction (non-parallel lines), but is the interaction significant?



Two factor ANOVA and DoE

We studied single factor ANOVA in week 8. As before, ANOVA decomposes the variability in the data into component and comparing them in this decomposition. Thus the total variability is:

$$SST = SSA + SSB + SS(AB) + SSE \tag{5}$$

Where SSA quantifies the variability of factor A due to factor B changing (i.e. the rows in table 1), and SSB quantifies the variability of factor B due to factor A changing (i.e. the columns of table 1).

The total sum of squares can also be calculated from the variance of the whole data set:

$$\begin{aligned} SST &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk} - < y >)^2 && (6)\\ &= S^2(abn-1) && (7)\\ & && (8)\end{aligned}$$

Two factor ANOVA and DoE

The variability of Factor A due to the level of B changing is:

$$SSA = b.n. \sum_{i=1}^{a} \left(\bar{A}_i - < y >\right)^2 \tag{9}$$

The variability of Factor B due to the level of A changing is:

$$SSB = a.n. \sum_{j=1}^{b} \left(\bar{B}_j - < y >\right)^2 \tag{10}$$

The sum of squares error (within-group variability) is :

$$SSE = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n} \left(y_{ijn} - \bar{y_{ij}}\right)^2 \tag{11}$$

Here, the SSE measures the total variability for within each treatment.

Sum of Squares AB Interaction

SS(AB) is deduced from equation 5 as all other quantities are calculable.
i.e.

$$SSAB = SST - SSA - SSB - SSE$$

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Mean Squares

By dividing the sum of squares by the the degrees of freedom, then the mean squares can be calculated:

$MSA = \frac{SSA}{a-1}$, $MSB = \frac{SSB}{b-1}$, $MS_{AB} = \frac{SSAB}{(a-1)(b-1)}$, $MSE = \frac{SSE}{ab(n-1)}$

Then the F-test can be performed for each factor to see if it *significantly* influences the experiment:

$$F = \frac{MSA}{MSE},\ F = \frac{MSB}{MSE},\ F = \frac{MSAB}{MSE}$$

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Expected Values

It can be shown that the **expected values** of the mean squares are:

$$\langle MSA \rangle = \langle \frac{SSA}{a-1} \rangle = \sigma^2 + \frac{bn \sum_{i=1}^{a} \tau_i^2}{a-1} \tag{12}$$

$$\langle MSB \rangle = \langle \frac{SSB}{b-1} \rangle = \sigma^2 + \frac{an \sum_{j=1}^{b} \beta_j^2}{b-1} \tag{13}$$

$$\langle MSAB \rangle = \langle \frac{SSAB}{(a-1)(b-1)} \rangle = \sigma^2 + \frac{n \sum_{i=1}^{a} \sum_{j=1}^{b} (\tau\beta)_{ij}^2}{(a-1)(b-1)} \tag{14}$$

$$\langle MSE \rangle = \langle \frac{SSE}{ab(n-1)} \rangle = \sigma^2 \tag{15}$$

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Summary of two factor ANOVA symbols and labels

y = observation under k^{th} replication when A is at level i and B is at level j
a = number of levels of factor A
b = number of levels of factor B
n = number of replications per cell
$\bar{y}_{ij}$ =average for each cell (i.e., across replications)
$< y >$ = grand average
i=1, ... a is the index for levels of factor A
j=1, . . . b is the index for levels of factor B
k = 1, ... n is the index for replicate.

Random Effects Model

Used to predict the response for a set of factors that are susceptible to random variation. The model starts with the grand average and adds individual effects of the factors, interaction terms and noise.

$$\boxed{y_{ij} =< y > +\alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ij}} \tag{16}$$

- α_i the main effect for factor a at level i $= \bar{A}_i - < y >$, and $\sum_{i=1}^{a} \alpha_i = 0$
- β_j the main effect for factor b at level j $= \bar{B}_i - < y >$, and $\sum_{j=1}^{b} \beta_j = 0$
- $\alpha\beta_{ij}$ the interaction of (ab) at level ij $=$ $\bar{y}_{ij} - (< y > +\alpha_i + \beta_j)$, and $\sum_{j=1}^{b} \sum_{i=1}^{a} (\alpha_i \beta_j) = 0$
- ϵ_{ij} Uncorrelated error with a mean of zero and σ^2=MSE

Two factor ANOVA Summary

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	DoF for p-value
Factor A	SSA	a-1	MSA=SSA/(a-1)	MSA/MSE	a-1, ab(n-1)
Factor B	SSB	b-1	MSB=SSB/(b-1)	MSB/MSE	b-1, ab(n-1)
AB Interaction	SSAB	(a-1)(b-1)	MSAB=SSAB/(a-1)(b-1)	MSAB/MSE	(a-1)(b-1), ab(n-1)
Error	SSE	ab(n-1)	MSE=SSE/[ab(n-1)]	-	-
Total	SST	abn-1	-	-	-

Table 2: ANOVA table for two factor analysis

Case Problem 10.2

Two factor ANOVA

- Using the data below, determine whether the main effect of factor A, main effect of factor B, and the interaction effect of AB are statistically significant at $\alpha = 0.05$.
- Identify a linear statistical model to describe the dependence on the two factors.

		Factor B		Average
		Level 1	Level 2	
Factor A	Level 1	10,14	18,14	14
	Level 2	23,21	16,20	20
	Level 3	31,27	21,25	26
Average		21	19	20

Case Problem 2 solution

$$
\begin{aligned}
SSA &= b.n. \sum_{i=1}^{a} (\bar{A}_i - < y >)^2 \\
&= 2 \times 2 \times \left((14-20)^2 + (20-20)^2 + (26-20)^2) \right) \\
&= 288
\end{aligned}
$$

$$
\begin{aligned}
SSB &= a.n. \sum_{i=1}^{b} (\bar{B}_i - < y >)^2 \\
&= 3 \times 2 \times \left((21-20)^2 + (19-20)^2 \right) \\
&= 12
\end{aligned}
$$

$$
\begin{aligned}
SSE &= \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n} (y_{ijk} - \bar{y_{ij}})^2 \\
&= (10-12)^2 + (14-12)^2 + (18-16)^2 + (14-16)^2 \\
&+ (23-22)^2 + (21-22)^2 + (16-18)^2 + (20-18)^2 \\
&+ (31-29)^2 + (27-29)^2 + (21-23)^2 + (25-23)^2 \\
&= 42
\end{aligned}
$$

Case Problem 2 solution

$$SST = S^2(abn-1)$$

Or

$$\begin{aligned}
SST &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk} - < y >)^2 \\
&= (10-20)^2 + (14-20)^2 + (18-20)^2 + (14-20)^2 \\
&+ (23-20)^2 + (21-20)^2 + (16-20)^2 + (20-20)^2 \\
&+ (31-20)^2 + (27-20)^2 + (21-20)^2 + (25-20)^2 \\
&= 398 \\
&= SSA + SSB + SSAB + SSE \\
SSAB &= 398 - 42 - 298 = 58
\end{aligned}$$

CP2 Solution: Mean Square Errors

$$MSA = \frac{SSA}{a-1} = \frac{288}{3-1} = 144$$

$$MSB = \frac{SSB}{b-1} = \frac{12}{2-1} = 12$$

$$MS(AB) = \frac{SSAB}{(a-1)(b-1)} = \frac{56}{2} = 28$$

$$MSE = \frac{SSE}{a \times b \times (r-1)} = \frac{42}{2 \times 3 \times (2-1)} = 7$$

CP2 Solution: F-test

$$F_A = \frac{MSA}{MSE} = \frac{144}{7} = 20.6 \qquad \text{df=1,6}$$
$$F_B = \frac{MSB}{MSE} = \frac{12}{7} = 1.7 \qquad \text{df=2,6}$$
$$F_{AB} = \frac{MS(AB)}{MSE} = \frac{28}{7} = 4.0 \qquad \text{df=2,6} \tag{17}$$

The critical F-values for significance level of $\alpha = 0.05$ are:

$$F_c(2,6) = 5.14$$
$$F_c(1,6) = 5.99 \tag{18}$$

Therefore only Factor A is significant.

CP2 Solution: Response Model

$$\alpha_1 = 14 - 20 = -6$$
$$\alpha_2 = 20 - 20 = 0$$
$$\alpha_3 = 26 - 20 = 6$$
$$\beta_1 = 21 - 20 = 1$$
$$\beta_2 = 19 - 20 = -1$$

Calculating the AB Interaction term

A	B	Effect, $\bar{y}_{ij}$	$\alpha\beta = \bar{y}_{ij} - (\langle y \rangle + \alpha_i + \beta_j)$
1	1	(10+14)/2=12	12-(20-6+1)=-3
2	1	(23+21)/2=22	22-(20+0+1)=1
3	1	(31+27)/2=29	29-(20+6+1)=2
1	1	(18+14)/2=16	16-(20-6-1)=3
1	2	(16+20)/2=18	18-(20+0-1)=-1
1	3	(21+25)/2=23	23-(20+6-1)=-2

So the model becomes:
$\hat{y}_{ij} = 20 + \{-6, 0, 6\}_i + \{1, -1\}_j + \{-3, 1, 2, 3, -1, -2\}_{ij}$
E.g. when i=1, j=1, $\hat{y}_{1,1} = 12$, which compares well with the table.

Summary

We have learnt...

- how to use ANOVA to look at multiple factors with multiple levels
- how to use factorial methods to throughly and efficiently explore the significance of the experimental factors on the experiment result
- how form an empirical model to predict the outcome of an experiment for a particular set of inputs

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