FACULTY OF SCIENCE AND ENGINEERING

DEPARTMENT OF MATHEMATICS AND STATISTICS

END OF SEMESTER EXAMINATION PAPER 2015

MODULE CODE: MA4505 SEMESTER: Autumn 2015

MODULE TITLE: Chemometrics DURATION OF EXAM: 2.5 hours

LECTURER: Mr. Kevin O'Brien GRADING SCHEME: 100 marks
70% of module grade

EXTERNAL EXAMINER: Prof. J. King

INSTRUCTIONS TO CANDIDATES

Scientific calculators approved by the University of Limerick can be used.
Formula sheet and statistical tables provided at the end of the exam paper.
There are 5 questions in this exam. Students must attempt any 4 questions.

Question 1. (25 marks) Single Sample Inference Procedures and Distributional Testing

Question 1 Part A (15 Marks)

A test of a specific blood factor has been devised such that, for adults in Western Europe, the test score is normally distributed with mean 100 and standard deviation 10. A clinical research organization is carrying out research on the blood factor levels for sufferers of a particular disease.

- A study has obtained the following test scores for 14 randomly selected patients suffering from the disease in Scotland

$$\{118, 116, 114, 110, 118, 111, 124, 117, 107, 116, 125, 93, 106, 119\}$$

- A similar study has obtained the following test scores for 15 randomly selected patients suffering from the disease in Norway.

$$\{122, 135, 112, 118, 114, 116, 99, 108, 123, 111, 109, 126, 117, 115, 119\}$$

The following blocks of `R` code (i.e. blocks A to E) are based on the data for this assessment. Write a short report on your conclusion for this assessment.

Marking Scheme*: Either 2 or 3 Marks will be awarded for a correct interpretation of each code segment, for a total of 12 Marks.*
State the purpose of each code segment, and then state if it is useful and/or valid in the overall analysis.
Remember to state the null and alternative hypotheses when relevant. 3 Marks will also be award for an overall conclusion.

Block A (3 Marks)

```
> grubbs.test(X)

Grubbs test for one outlier

data:  X
G = 3.11950, U = 0.19387, p-value = 9.184e-05
..

> grubbs.test(Y)

Grubbs test for one outlier

data:  Y
G = 2.20890, U = 0.62658, p-value = 0.1164

..
```

Block B (2 Marks)

```
> shapiro.test(X)

Shapiro-Wilk normality test

data:  X
W = 0.71132, p-value = 0.0004852


> shapiro.test(Y)

Shapiro-Wilk normality test

data:  Y
W = 0.98139, p-value = 0.9781
```

Block C (2 Marks)

```
> var.test(X,Y)

F test to compare two variances

data:  X and Y
F = 0.65607, num df = 13, denom df = 14, p-value = 0.4544
alternative hypothesis: true ratio of variances is not equal to 1

95 percent confidence interval:
0.2178253 2.0219019

sample estimates:
ratio of variances
0.6560667
```

Block D

```
> wilcox.test(X,Y)

Wilcoxon rank sum test with continuity correction
```

```
data:  X and Y
W = 99, p-value = 0.8098
alternative hypothesis: true location shift is not equal to 0
```

Block E (3 Marks)

```
> t.test(X,Y,var.equal=TRUE)

Two Sample t-test

data:  X and Y
t = -0.63849, df = 27, p-value = 0.5285
alternative hypothesis: true difference in means is not equal to 0

95 percent confidence interval:
-7.744932  4.068741
sample estimates:
mean of x mean of y
114.4286  116.2667


> t.test(X,Y,var.equal=FALSE)

Welch Two Sample t-test

data:  X and Y
t = -0.64325, df = 26.499, p-value = 0.5256
alternative hypothesis: true difference in means is not equal to 0

95 percent confidence interval:
-7.706429  4.030238
sample estimates:
mean of x mean of y
114.4286  116.2667
```

Part A - One Way ANOVA (9 Marks)

Specimens of milk from dairies in three different districts are assayed for their concentrations of the radioactive isotope Strontium-90. The results, in picocuries per litre, are as shown in the table below.

District							mean $\bar{x}_i$	variance s_i^2
A	7.6	8.1	8.5	8.3	7.9	8.8	8.2	0.184
B	8.7	10.2	11.4	10.9	7.2	9.2	9.6	2.404
C	10.3	9.9	11.5	11.6	10.6	8.5	10.4	1.312
Overall							9.4	2.022

(i) (2 Marks) Showing your workings, compute the **Between Group Sum of Squares** ($SSbetween$).

(ii) (2 Marks) Showing your workings, compute the **Within Group Sum of Squares**
($SSwithin$).

(iii) (2 Mark) Showing your workings, compute the **Total Group Sum of Squares** ($SStotal$).

(iv) (1 Mark) Complete the **Degrees of Freedom** Column for the ANOVA table below.

(iv) (1 Mark) Complete the **Mean Square** Column for the ANOVA table below.

(iv) (1 Mark) Complete the **F** Column (i.e. the column for Test Statistic) for the ANOVA table below.

	DF	SS	MS	F
Between				
Within				
Total				

Part C (5 Marks)

(i.) (3 Marks) Provide a brief description for three tests from the family of Grubb's Outliers Tests. Include in your description a statement of the null and alternative hypothesis for each test

(ii.) (2 Marks) Describe any required assumptions for tests, and the limitations of these tests.

(i.) (3 Marks) Provide a brief description for three tests from the family of Grubbs' Outliers Tests. Include in your description a statement of the null and alternative hypothesis for each test, any required assumptions and the limitations of these tests.

(ii.) (3 Marks) Showing your working, use the Dixon Q Test to test the hypothesis that the lowest value of the following data set is an outlier.

$$11, 22, 23, 24, 25, 26, 29, 34$$

Question 2. (25 marks) Regression Models

Part A - Short Questions (8 Marks)

(i) (1 Mark) In the context of regression models, explain what is meant by Heteroscedascity and Homoescedascity.

(ii) (1 Mark) Explain how the *Akaike information criterion* would used to compare two models fitted for the same data.

(iii) (1 Mark) Explain why the adjusted R^2 value may differ in value from the corresponding multiple R^2 value for the same fitted model.

(iv) (1 Mark) Write a short note to compare and contrast the multiple R squared and asjusted R squared.

Standard Additions

The gold content of a concentrated sea-water sample was determined by using atomic-absorption spectrometry with the method of standard additions.

```
> summary(lm(Abso~Gold))

Call:
lm(formula = Abso ~ Gold)

Residuals:
      Min        1Q    Median        3Q       Max
-0.034662 -0.014833 -0.013924  0.004695  0.096057

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.2589060  0.0234791   11.03 4.07e-06 ***
Gold        0.0056720  0.0004668   12.15 1.95e-06 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.03852 on 8 degrees of freedom
Multiple R-squared:  0.9486,    Adjusted R-squared:  0.9422
F-statistic: 147.6 on 1 and 8 DF,  p-value: 1.949e-06
```

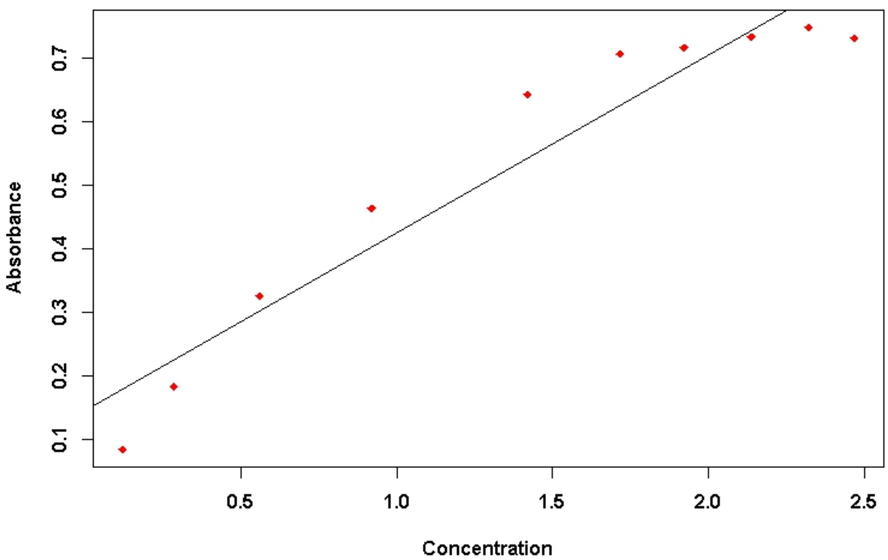
The results obtained were as follows:

Gold Addition (ng/ml)	Absorbance	
1	30.00	0.41
2	40.00	0.47
3	50.00	0.53
4	60.00	0.58
5	70.00	0.64
6	0.00	0.27
7	10.00	0.32
8	20.00	0.37
9	80.00	0.68
10	70.00	0.75

Part B - Linear Regression (8 Marks)

In an experiment to determine hydrolysable tannins in plants by absorption spectroscopy, the following results from ten samples were obtained and are tabulated below. A simple linear regression model, predicting absorbance values using concentration as the independent variable, was fitted to the data. The scatterplot is depicted below.

Sample	1	2	3	4	5
Absorbance	0.084	0.183	0.326	0.464	0.643
Concentration	0.123	0.288	0.562	0.921	1.420
Sample	6	7	8	9	10
Absorbance	0.707	0.717	0.734	0.749	0.732
Concentration	1.717	1.921	2.137	2.321	2.467



(i.) (1 marks) Is the simple linear regression model approach suitable for this study? Explain your answer with reference to the scatter-plot.

(ii.) (3 marks) Two polynomial models were also fitted to the data. Description of all three fitted models are found in the three blocks of `R` code on the following pages. The *Akaike information criterion* is listed, for each of the three fitted models. Write down the regression equations of each of the three models.

(iii.) (2 marks) Specify which one of the models you would use. Justify your answer with appropriate statistical values.

(iv.) (2 marks) Using the best fitting model, predict a value for absorbance when the concentration level is 1.2 mg/ml.

Model 1

```
> summary(Model1)
Call:
lm(formula = Absorb ~ Conc)
...
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)    0.14412    0.04721   3.053   0.0158 *
Concentration  0.28088    0.02930   9.586 1.16e-05 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.07584 on 8 degrees of freedom
Multiple R-squared: 0.9199,     Adjusted R-squared: 0.9099
F-statistic: 91.89 on 1 and 8 DF,  p-value: 1.163e-05
>
>
>AIC(Model1)
[1] -19.4343
```

Model 2

```
> summary(Model2)
Call:
lm(formula = Absorb ~ Conc + Conc.Squared)
...
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)    0.006582   0.008013   0.821    0.439
Concentration  0.642935   0.015568  41.299 1.27e-09 ***
```

```
Conc.Squared  -0.140573   0.005894 -23.851 5.79e-08 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.008939 on 7 degrees of freedom
Multiple R-squared: 0.999,      Adjusted R-squared: 0.9987
F-statistic:  3592 on 2 and 7 DF,  p-value: 2.879e-11
>
>
> AIC(Model2)
[1] -61.5338
```

Model 3

```
> summary(Model3)

Call:
lm(formula = Absorb ~ Conc+ Conc.Squared + Conc.Cubed)
...
...
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept)    0.013712   0.011629   1.179   0.2830
Concentration  0.608682   0.042825  14.213 7.58e-06 ***
Conc.Squared  -0.108186   0.038088  -2.840   0.0296 *
Conc.Cubed    -0.008196   0.009518  -0.861   0.4223
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.009109 on 6 degrees of freedom
Multiple R-squared: 0.9991,     Adjusted R-squared: 0.9987
F-statistic:  2306 on 3 and 6 DF,  p-value: 1.422e-09
>
>
> AIC(Model3)
[1] -60.69903
```

Part C - Robust Regression (7 Marks)

In certain circumstances, Robust Regression may be used in preference to Ordinary Least Squares Regression. Answer the following questions relating to Robust Regression.

(i.) (1 Mark) Describe what these circumstances might be.

(ii.) (1 Mark) State one difference between OLS and Robust regression techniques, in terms of computing regression equations.

(iii.) (2 Marks) Explain the process of Huber Weighting for Residuals, stating the algorithm used to compute weightings.

(iv.) (3 Marks) Suppose that Huber Weighting, with a tuning constanct of $k = 13.45$, was applied to the observations tabulated below. What would be the outcome of the procedure for each case.

Observation i	Residual e_i
11	-9.07
14	14.54
18	22.91

Part C Influence (10 Marks)

(i.) (1 Marks) Explain the term "Influence" in the context of linear regression models. Support your answer with sketches.

(ii.) (1 Marks) Explain the term "Cook's Distance" in the context of linear regression models.

(iii.) (2 Marks) The following plot is the *Residual vs Fitted* plot, the first of `R`'s diagnostic plots for linear models. Briefly describe how to interpet this plot. What is your conclusion?

(iv.) (2 Marks) Explain the term "Heteroscedascity" in the context of linear regression models. Support your answer with sketches.

(v.) (1 Mark) The Outliers Test Test was carried out to test for Heteroscedascity. The output is depicted below. State your conclusion to the following procedure.

```
> outlierTest(ModelQ2)
rstudent unadjusted p-value Bonferonni p
3 1203.539         2.5441e-22   2.7985e-21
```

(vi.) (2 Marks) The Durbin Watson Test was carried out to test for Autocorrelation. Briefly describe autocorrelation. You may support your answer with sketches.

(vii.) (1 Mark) State your conclusion to the following procedure.

```
> durbinWatsonTest(ModelQ2)
lag Autocorrelation D-W Statistic p-value
1     -0.08428163      2.143578   0.806
Alternative hypothesis: rho != 0
```

Question 3 Part D (12 Marks)

The mercury level of several tests of sea-water from costal areas was determined by atomic-absorption spectrometry. The results obtained are as follows

Conc	0	10	20	30	40	50	60	70	80	90	100
Abso	0.321	0.834	1.254	1.773	2.237	2.741	3.196	3.678	4.217	4.774	5.261

The analysis of the relationship between concentration and absorbance is obtained in R and presented below.

```
x<-seq(0,100,by=10)
y<- c(0.321, 0.834, 1.254, 1.773, 2.237, 2.741, 3.196, 3.678,
4.217, 4.774, 5.261)
model<- lm(y~x)
summary(model)

Call:
lm(formula = y ~ x)
```

```
Coefficients:
Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.2933636  0.0234754   12.50 5.45e-07
x           0.0491982  0.0003968  123.98 7.34e-16
---

Residual standard error: 0.04162 on 9 degrees of freedom
Multiple R-squared: 0.9994,     Adjusted R-squared: 0.9993
F-statistic: 1.537e+04 on 1 and 9 DF,  p-value: 7.337e-16

confint(model)
                 2.5 %     97.5 %
(Intercept) 0.24025851 0.34646876
x           0.04830054 0.05009582
```

(i) (2 marks) Determine and interpret the slope and the intercept of the regression line.

(ii) (2 marks) State the 95% confidence interval for the slope and the intercept coefficients. Interpret this intervals with respect to any relevant hypothesis tests

(iii) (2 marks) Explain in which way is the prediction intervals different from the confidence intervals for fitted values in linear regression?

(iv) (2 Marks) The following piece of `R` code gives us a statistical metric. What is this metric? What is it used for? How should it be interpreted.

```
> AIC(model)
[1] -34.93389
```

Part B Regression ANOVA (6 Marks)

Suppose we have a regression model, described by the following equation

$$\hat{y} = 28.81 + 6.45x_1 + 7.82x_2$$

We are given the following pieces of information.

- The standard deviation of the response variance y is 10 units.
- There are 53 observations.

- The *Coefficient of Determination* (also known as the *Multiple R-Squared*) is 0.75.

Complete the *Analysis of Variance* Table for a linear regression model. The required values are indicated by question marks.

	DF	Sum Sq	Mean Sq	F value	Pr(>F)
Regression	?	?	?	?	$< 2.2e^{-16}$
Error	?	?	?		
Total	?	?			

Question 3. (25 marks) Experimental Design

(f) (4 marks) What is the purpose of a post hoc test?

(f) (4 marks) What are the key components that need to be identified when designing an experiment?

(f) (4 marks) What is a completely randomised design?

(f) (4 marks) What is a randomised block design?

(f) (4 marks) What is an "a x b" factorial experimental design?

(f) (4 marks) What is the difference between a between-treatments estimate and a withintreatments estimate?

(f) (4 marks) What distinguishes a factorial experiment from a completely randomised experiment or a randomised block experiment?

(f) (4 marks) What is the purpose of a post hoc test?

(g) (4 marks) What is an "$a \times b$" factorial experimental design?

(f) (4 marks) How would you fit a quadratic regression model to bivariate data and why?

Question 2 - Two Way ANOVA (6 Marks)

Suppose you want to determine whether the brand of cleaning product used and the temperature affects the amount of dirt removed from your machinery.
You are also interested in determining if there is an interaction between the two variables.
You buy two different brand of detergent ("*Super*" and "*Best*") and choose three different temperature levels ("*Cold?*, "*Warm*", and "*Hot*"). There are four measurements per treatment group.

	Cold	Warm	Hot
Super	4,5,6,5	7,9,8,12	10,12,11,9
Best	6,6,4,4	13,15,12,12	12,13,10,13

- Detergent is Factor A.
- Temperature is Factor B.
- The variance of the response variable is 12.2011.

Source	DF	SS	MS	F
A	?	22.04	?	?
B	?	?	102.37	?
A:B	?	16.08	?	?
Resid	?	?	?	
Total	?	?		

Water Nitrate (One Way ANOVA MA4605)

Four investigators, A, B, C and D, performed six determination of nitrate in water using the same procedure. The results in μM were:

A	B	C	D
6.7	6.3	6.8	6.9
6.8	6.2	6.9	7.1
6.5	6.1	7.1	6.3
6.8	6.3	6.9	6.2
6.9	6.5	7.2	6.1
7.1	6.4	7.1	6.4

We are also given the summmary statistics for each of the three investigators, as well as for the samples combined.

	Sample Mean	Sample Variance
A	6.8	0.040
B	6.3	0.020
C	7	0.024
D	6.5	0.164
Overall	6.65	0.1295

An analysis of variance procedure is used to determine if there is a significant difference between the mean of the determinations made by the three investigators.

The following questions will result in the completion of the ANOVA Table on the next page. The $p-$value is already provided.

(i.) (3 Marks) Compute the Between Groups Sum of Squares. (Show your workings.)

(ii.) (3 Marks) Compute the Within Groups Sum of Squares.(Show your workings.)

(iii.) (2 Marks) Compute the Total Sum of Squares. (Show your workings).

(iv.) (1 Mark) State the degrees of freedom for the ANOVA Tables

(v.) (1 Mark) Compute the Mean Square values.

(vi.) (1 Marks) Compute the test Statistic for this procedure (i.e. the F-value.)

(vii.) (3 Marks) This analysis is used to assess if there is any difference between the mean determinations made by the three investigators. What is your conclusion? Clearly state the null and alternative hypothesis.

Source	DF	SS	MS	F	p-value
Between	?	?	?	?	0.000454
Within	?	?	?		
Total	?	?			

Question 3 Part B (4 Marks) - check ANOVA Assumptions

The `R` code and graphical procedures, below and on the following page, are relevant to checking whether the underlying assumptions are met for an ANOVA model.

(i.) (2 marks) State two testable assumptions required for ANOVA procedures? (You may refer to the code output below.)

(ii.) (2 marks) Assess the validity of these assumptions for an ANOVA model based on the following code outputs.

```
> #Shapiro-Wilk normality test
> shapiro.test(resid(model))

Shapiro-Wilk normality test

data:  resid(model)
W = 0.96108, p-value = 0.4604
```

```
> bartlett.test(investigator~group)

Bartlett test of homogeneity of variances

data:  investigator by group
Bartlett's K-squared = 7.1354, df = 3, p-value = 0.0677
```

Question 3 Part C (7 Marks) Two Way ANOVA No Replicates

A supermarket buys a particular product from five suppliers (V,W,X,Y and Z), and conducts regular tasting tests by three expert panels. Various characteristics are scored and an analysis of the totals of these scores is made.

	V	W	X	Y	Z
Panel 1	22	25	23	23	24
Panel 2	21	16	16	19	16
Panel 3	23	22	19	23	22

You are also given the following information:

- $S_r^2 = 8.9733$
- $S_c^2 = 1.0777$
- The variance of scores in the table above is $\text{Var}(y) = 9.0666$

The following questions will result in the completion of the ANOVA Table on the bottom of this page. The $p-$values for both tests are already provided.

(i.) (4 Marks) Complete the Sum of Squares column. (Show your workings.)

(ii.) (1 Mark) State the degrees of freedom for the ANOVA Table.

(iii.) (2 Marks) Based on the p-values, provided, what is your conclusion? Clearly state the null and alternative hypotheses for both tests.

Source	DF	SS	MS	F	p-value
Factor A	?	?	?	?	0.00205 **
Factor B	?	?	?	?	0.43290
Error	?	?	?		
Total	?	?			

One-Way ANOVA F-test

Question 2 - Two Way ANOVA with Replicates(6 Marks)

Suppose you want to determine whether the brand of cleaning product used and the temperature affects the amount of dirt removed from your machinery.
You are also interested in determining if there is an interaction between the two variables.

You buy two different brand of detergent ("*Super*" and "*Best*") and choose three different temperature levels ("*Cold*, "*Warm*", and "*Hot*"). There are four measurements per treatment group.

	Cold	Warm	Hot
Super	4,5,6,5	7,9,8,12	10,12,11,9
Best	6,6,4,4	13,15,12,12	12,13,10,13

- Detergent is Factor A.
- Temperature is Factor B.
- The variance of the response variable is 12.2011.

Exercises For the Table above, replace the questions marks with the correct values in each of the following columns. (The number of marks for each column is indicated here:)

(i) (2 Marks) Degrees of freedom

(ii) (2 Mark) Sums of Squares column

(iii) (1 Mark) Mean Square Values

(iv) (1 Mark)F-Values

Source	DF	SS	MS	F
A				
B				
A:B				
Resid				
Total				

Question 3 Part C (7 Marks)

Six analysts each made seven determinations of the paracetamol content of the same batch of tablets. The results are shown below. There are 42 determinations in total.

Analyst	Content						
A	84.32	84.61	84.64	84.62	84.51	84.63	84.51
B	84.24	84.13	84.00	84.02	84.25	84.41	84.30
C	84.29	84.28	84.40	84.63	84.40	84.68	84.36
D	84.14	84.48	84.27	84.22	84.22	84.02	84.33
E	84.50	83.91	84.11	83.99	83.88	84.49	84.06
F	84.70	84.36	84.61	84.15	84.17	84.11	83.81

The following `R` output has been produced as a result of analysis of these data:

```
Analysis of Variance Table

Df   Sum Sq   Mean Sq   F value    Pr(>F)
Analyst        5   0.8611   0.17222     4.236   0.00394 **
Residuals     36   1.4635   0.04065
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
```

Response: Y	Df	Sum Sq	Mean Sq	F value	$Pr(> F)$
Analyst	?	?	?	?	0.00394 **
Residuals	?	?	0.04065		
Total	?	2.3246			

(i.) (6 Marks) Complete the ANOVA table in your answer sheet, replacing the "?" entries with the correct values.
(You are not required to carry out a hypothesis test.)

Question 2 Part C (7 Marks)

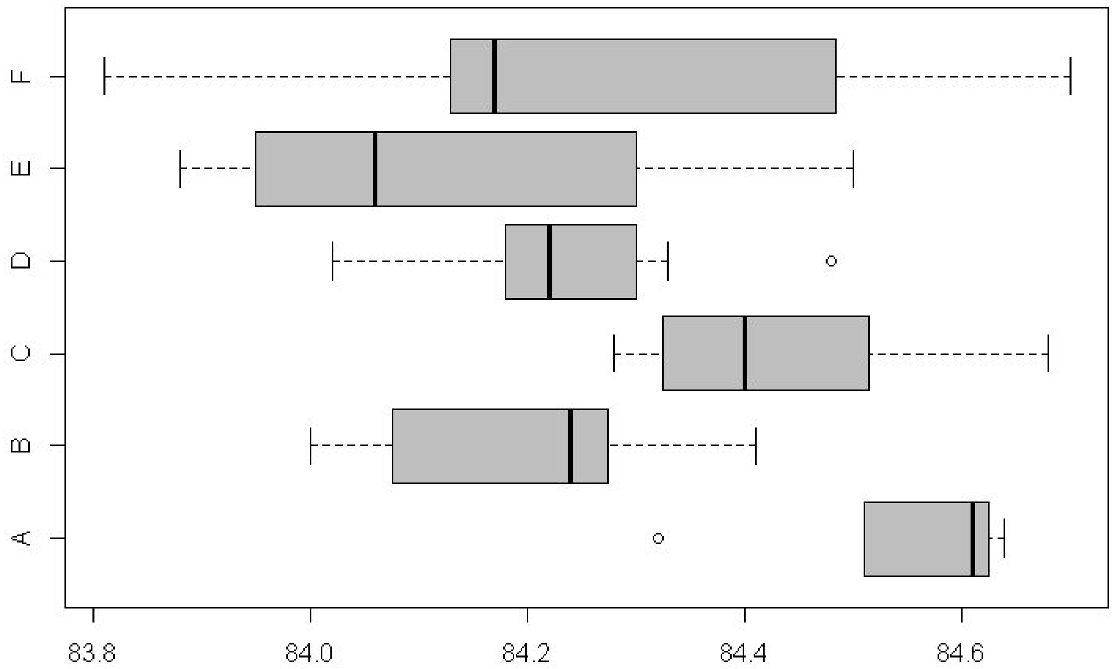
The R code and graphical procedures, below and on the following page, are relevant to checking whether the underlying assumptions are met for the ANOVA model in part (b).

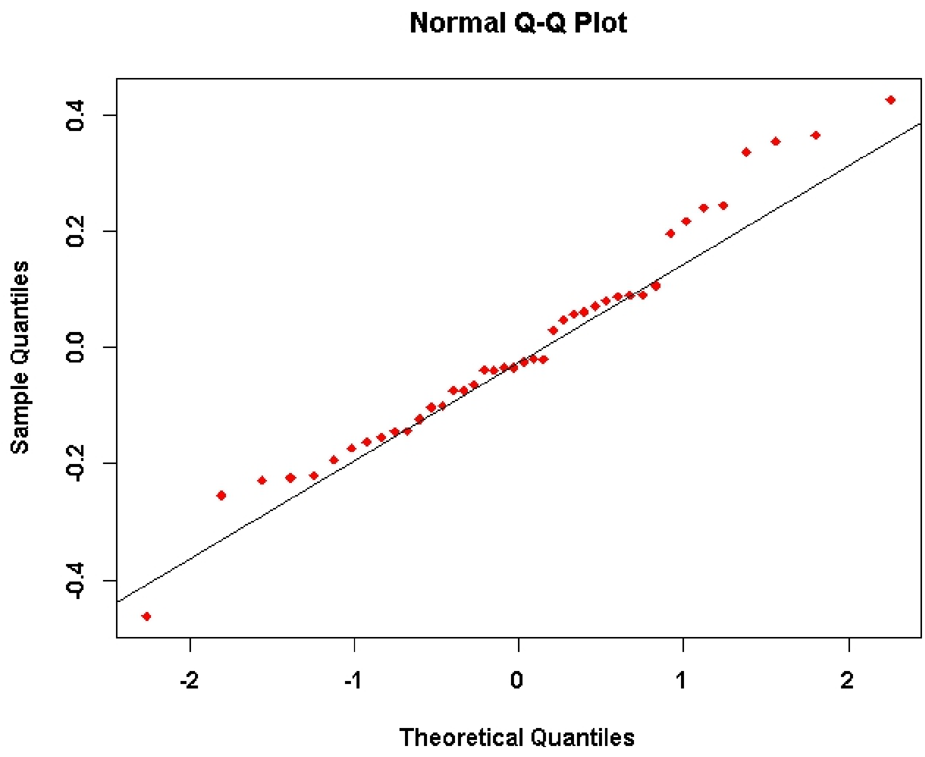
(i.) (3 marks) What are the assumptions underlying ANOVA?

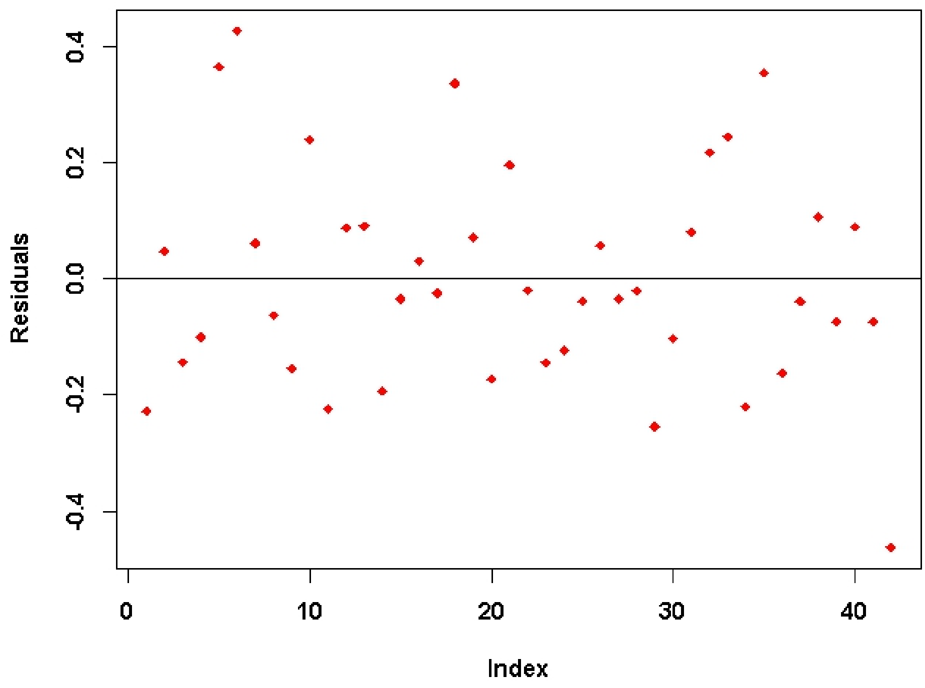
(ii.) (4 marks) Assess the validity of these assumptions for the ANOVA model in Part B.

```
Shapiro-Wilk normality test

data:  Residuals
W = 0.9719, p-value = 0.3819
```

```
Bartlett test of homogeneity of variances

data:  Experiment
Bartlett's K-squared = 105.9585, df = 1, p-value < 2.2e-16
```




Normal Q-Q Plot
Sample Quantiles
Theoretical Quantiles
-0.4
-0.2
0.0
0.2
0.4
-2
-1
0
1
2


Residuals
Index
-0.4
-0.2
0.0
0.2
0.4
0
10
20
30
40

Question 3. Two Way ANOVA Procedures (25 marks)

Question 3 Part A (6 Marks)

A supermarket buys a particular product from four suppliers, A, B, C, D, and regular tasting tests by expert panels are carried out as the product is sold in their food halls. Various characteristics are scored and an analysis of the totals of these scores is made. Four tasters a, b, c, d obtained these results at four sessions 1-4.

		A	B	C	D
Taster a b c d		21	17	18	20
		20	22	23	19
		20	24	22	19
		22	21	22	26

(a) In the context of the above example, distinguish between the treatment and the blocking variables involved. Give reasons.

(b) The above data are an example of a particular experimental design. What is the general name given to this type of experimental design? Name one serious limitation of this type of experimental design.

(c) Complete the ANOVA table substituting the symbols ? with their correct values.

(d) Interpret the results.

(e) What is the key property of the experimental design above which allows factor effects to be estimated independently of one another. Show how this property presents itself in the above design.

Battery - Partial Completion ANOVA (MA4605)

An engineer is designing a battery for use in a device that will be subjected to some extreme variations in temperature.

The only design parameter that he can select at this point is the plate material for the battery, and he has three possible choices. When the device is manufactured and is shipped to the field, the engineer has no control over the temperature extremes that the device will encounter, and he knows from experience that temperature will probably affect the effective battery life.

However, temperature can be controlled in the product development laboratory for the purposes of a test. The engineer decides to test all three place materials at three temperature levels 15, 70, and 125 degrees.

Four batteries are tested at each combination of plate material and temperature, and all 36 tests are run in random order.

The following partial ANOVA table resulted:

Analysis of Variance for Battery Life Data

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square
Material types	2	10,683.72	5,341.86
Temperature	2	39,118.72	19,559.36
Interaction	4	9,613.78	2,403.44
Error	27	18,230.75	675.21
Total	35	77,646.97	

(i.) Carry out appropriate tests stating clearly the null hypotheses and conclusions.

(ii.) Would the engineer be satisfied with his design of the experiment? Explain your answer.

Question 4. (25 marks) Factorial Design

In an investigation into the extraction of nitrate-nitrogen from air dried soil, three quantitative variables were investigated at two levels. These were the amount of oxidised activated charcoal (A) added to the extracting solution to remove organic interferences, the strength of CaSO4 extracting solution (C), and the time the soil was shaken with the solution (T). The aim of the investigation was to optimise the extraction procedure. The levels of the variables are given here:

		-	+
Activated charcoal (g)	A	0.5	1
CaSO4 (%)	C	0.1	0.2
Time (minutes)	T	30	60

The results are given below and are the amounts recovered (expressed as the percentage of known nitrate concentration).

A	C	T	y		
-1	-1	-1	33.95	33.46	34.32
1	-1	-1	33.76	33.93	33.18
-1	1	-1	34.32	35.05	34.75
1	1	-1	32.90	32.89	33.25
-1	-1	1	24.88	24.33	25.46
1	-1	1	38.67	40.23	39.14
-1	1	1	24.57	23.93	25.49
1	1	1	39.20	40.03	38.43

(i.) (7 Marks) Calculate the contrasts.

(ii.) (3 Marks) Calculate the effects.

(iii.) (3 Marks) Calculate the sum of squares for the ANOVA Table.

(iv.) (4 Marks) Using the computed sums of squares values, complete the ANOVA table (see the `R` code below).

(v.) (4 Marks) Comment on the tests for significant for the main effects and interactions. State clearly your conclusions.

(vi.) (4 Marks) Write down a regression equation that can be used predicting amounts based on the results of this experiment.

	DF	Sum Sq	Mean Sq	F value	Pr(>F)
A	...	...	...	...	$7.39e^{-15}$ ***
B	...	...	...	...	0.960
C	...	...	...	...	$3.92e^{-06}$ ***
A:B	...	...	...	...	0.257
A:C	...	...	...	...	$6.25e^{-16}$ ***
B:C	...	...	...	...	0.322
A:B:C	...	...	...	...	0.203
Residuals	...	...			
Total	...	1172.985			

Question 5. (25 marks) Statistical Process Control

Question 5 Part A (6 Marks)

A normally distributed quality characteristic is monitored through the use of control charts. These charts have the following parameters. All charts are in control.

	LCL	Centre Line	UCL
$\bar{X}$-Chart	542	550	558
R-Chart	0	8.236	16.504

i (2 marks) What sample size is being used for this analysis?

ii. (2 marks) Estimate the standard deviation of this process.

iii. (2 marks) Compute the control limits for the process standard deviation chart (i.e. the s-chart).

Question 5 Part B (7 Marks)

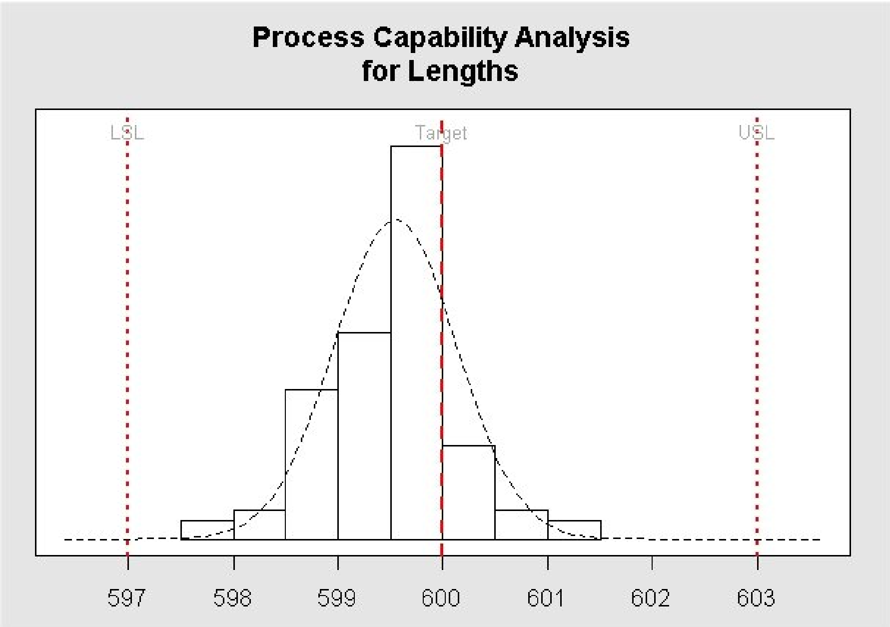
An automobile assembly plant concerned about quality improvement measured sets of five camshafts on twenty occasions throughout the day. The specifications for the process state that the design specification limits at 600±3mm.

(i.) (4 Marks) Determine the *Process Capability Indices* C_p and C_{pk}, commenting on the respective values. Use the `R` code output on the following page.

(ii.) (2 Mark) Explain why there would be a discrepancy between C_p and C_{pk}. Illustrate your answer with sketches.

(iii.) (1 Mark) Comment on the graphical output of the *Process Capability Analysis*, also presented on the next page.

```
Process Capability Analysis

Call:
process.capability(object = obj,
spec.limits = c(597, 603))
Number of obs = 100          Target = 600
Center = 599.548         LSL = 597
StdDev = 0.5846948       USL = 603

Capability indices:
Value   2.5%  97.5%
Cp     ...
Cp_l   ...
Cp_u   ...
Cp_k   ...
Cpm    1.353  1.134  1.572
Exp<LSL 0%   Obs<LSL 0%
```



Question 5 Part A (12 Marks)

The **Nelson Rules** are a set of eight decision rules for detecting "out-of-control" or non-random conditions on control charts. These rules are applied to a control chart on which the magnitude of some variable is plotted against time. The rules are based on the mean value and the standard deviation of the samples.

(i) (4×2 Marks) Discuss any four of these rules, and how they would be used to detect "out of control" processes. Support your answer with sketch.

In your answer, you may make reference to the following properties of the Normal Distribution. Consider the random variable X distributed as

$$X \sim \mathcal{N}(\mu, \sigma^2)$$

where μ is the mean and σ^2 is the variance of an random variable X.

- $\Pr(\mu - 1\sigma \leq X \leq \mu + 1\sigma) = 0.6827$
- $\Pr(\mu - 2\sigma \leq X \leq \mu + 2\sigma) = 0.9545$
- $\Pr(\mu - 3\sigma \leq X \leq \mu + 3\sigma) = 0.9973$

Formulas and Tables

Critical Values for Dixon Q Test

N	$\alpha = 0.10$	$\alpha = 0.05$	$\alpha = 0.01$
3	0.941	0.97	0.994
4	0.765	0.829	0.926
5	0.642	0.71	0.821
6	0.56	0.625	0.74
7	0.507	0.568	0.68
8	0.468	0.526	0.634
9	0.437	0.493	0.598
10	0.412	0.466	0.568
11	0.392	0.444	0.542
12	0.376	0.426	0.522
13	0.361	0.41	0.503
14	0.349	0.396	0.488
15	0.338	0.384	0.475
16	0.329	0.374	0.463

Two Way ANOVA

$$MS_A = c \times S_r^2 \qquad MS_B = r \times S_c^2$$

Control Limits for Control Charts

$$\bar{s} \pm 3\frac{c_5\bar{s}}{c_4}$$

$$\bar{\bar{x}} \pm 3\frac{\bar{s}}{c_4\sqrt{n}} \qquad [\bar{R}D_3, \bar{R}D_4]$$

2^3 Design: Interaction Effects

$$AB = \frac{1}{4n}\left[abc - bc + ab - b - ac + c - a + (1)\right]$$

$$AC = \frac{1}{4n}\left[(1) - a + b - ab - c + ac - bc + abc\right]$$

$$BC = \frac{1}{4n}\left[(1) + a - b - ab - c - ac + bc + abc\right]$$

$$ABC = \frac{1}{4n}\left[abc - bc - ac + c - ab + b + a - (1)\right]$$

Factorial Design: Sums of Squares

$$\text{Effect} = \frac{\text{Contrast}}{4n}$$

$$\text{Sums of Squares} = \frac{(\text{Contrast})^2}{8n}$$

Process Capability Indices

$$\hat{C}_p = \frac{\text{USL} - \text{LSL}}{6s} \qquad \hat{C}_{pm} = \frac{\text{USL} - \text{LSL}}{6\sqrt{s^2 + (\bar{x} - T)^2}}$$

$$\hat{C}_{pk} = \min\left[\frac{\text{USL} - \bar{x}}{3s}, \frac{\bar{x} - \text{LSL}}{3s}\right]$$

Factors for Control Charts

Sample Size (n)	c4	c5	d2	d3	D3	D4
2	0.7979	0.6028	1.128	0.853	0	3.267
3	0.8862	0.4633	1.693	0.888	0	2.574
4	0.9213	0.3889	2.059	0.88	0	2.282
5	0.9400	0.3412	2.326	0.864	0	2.114
6	0.9515	0.3076	2.534	0.848	0	2.004
7	0.9594	0.282	2.704	0.833	0.076	1.924
8	0.9650	0.2622	2.847	0.82	0.136	1.864
9	0.9693	0.2459	2.970	0.808	0.184	1.816
10	0.9727	0.2321	3.078	0.797	0.223	1.777
11	0.9754	0.2204	3.173	0.787	0.256	1.744
12	0.9776	0.2105	3.258	0.778	0.283	1.717
13	0.9794	0.2019	3.336	0.770	0.307	1.693
14	0.9810	0.1940	3.407	0.763	0.328	1.672
15	0.9823	0.1873	3.472	0.756	0.347	1.653
16	0.9835	0.1809	3.532	0.750	0.363	1.637
17	0.9845	0.1754	3.588	0.744	0.378	1.622
18	0.9854	0.1703	3.64	0.739	0.391	1.608
19	0.9862	0.1656	3.689	0.734	0.403	1.597
20	0.9869	0.1613	3.735	0.729	0.415	1.585
21	0.9876	0.1570	3.778	0.724	0.425	1.575
22	0.9882	0.1532	3.819	0.720	0.434	1.566
23	0.9887	0.1499	3.858	0.716	0.443	1.557
24	0.9892	0.1466	3.895	0.712	0.451	1.548
25	0.9896	0.1438	3.931	0.708	0.459	1.541