FACULTY OF SCIENCE AND ENGINEERING

DEPARTMENT OF MATHEMATICS AND STATISTICS

END OF SEMESTER EXAMINATION PAPER 2015

MODULE CODE: MA4605 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

ASSESSORS: Dr. C.F. Ryback

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.
Students must attempt all 4 questions. There are options within each of the 4 questions.

Question 1

What is going here?

- Testing that Data is normally distributed (may appear elsewhere)
- Transformation of Data (Tukey's Ladder)
- Outliers and Boxplots (Grubbs Test, Dixon Q-test)
- Interpreting Output for Inference Procedures
- F-test for Equality of Variance
- One Way ANOVA Tests for Multiple Means (may appear elsewhere) (HAND)
- Non-Parametric Procedures (e.g. Wilcoxon test, Kolmogorov Smirnov Test)

Question 2

What is going here?

- Simple and Multiple Linear Regression
- Regression ANOVA (HAND)
- Model Fit Metrics such as AIC, and both R Squared
- Residuals - Heteroscedascity, Interpreting Diagnostic Plots, Cook's Distances
- Robust Regression, Huber Weighting
- Method Comparison, Deming Regression
- Limits of Detection, Standard Addtions Method

Question 3

What is going here?

- One Way Anova Tests for Multiple Means (HAND)
- Two Way ANOVA Testing (HAND)
- Checking Model Assumptions (Bartlett Test)
- Introduction to Experimental Design (Theory Questions)
- Factorial Design

Question 4

What is going here?

- Statistical Process Control
- Control Charts : Rules and Interpretation
- Process Capability Indices (HAND)
- Testing for Univariate Normality (may appear in Q1)
- Skewness and Kurtosis
- Multivariate Normality : DAgostino Test

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

Critical Values for Chi Square Test

n	$\alpha = 0.10$	$\alpha = 0.05$	$\alpha = 0.01$	$\alpha = 0.001$
1	2.705	3.841	6.634	10.827
2	4.605	5.991	7.378	9.21
3	6.251	7.815	9.348	11.345
4	7.779	9.488	11.143	13.277
5	9.236	11.07	12.833	15.086
6	10.645	12.592	14.449	16.812
7	12.017	14.067	16.013	18.475
8	13.362	15.507	17.535	20.09
9	14.684	16.919	19.023	21.666
10	15.987	18.307	20.483	23.209

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

Process Capability Indices

$$\hat{C}_p = \frac{\text{USL} - \text{LSL}}{6s}$$

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

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

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

$$\text{Effect} = \frac{(\text{Contrast})}{n2^{k-1}}$$

$$\text{Sums of Squares} = \frac{(\text{Contrast})^2}{n2^k}$$