



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: 60 marks

ASSESSORS: Dr. M.F. Brezzo

C.F. Ryback

60% of module grade

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

Question 1. Inference Procedures and Distributional Testing

Question 2. Regression Techniques

Question 3. ANOVA Procedures and Experimental Design

Question 4. Statistical Process Control and Process Capability

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

Process Capability Indices

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

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

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

2³ Design: Interaction Effects

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

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

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

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

Factorial Design: Sums of Squares

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

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

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