



FACULTY OF SCIENCE AND ENGINEERING
DEPARTMENT OF MATHEMATICS AND STATISTICS

END OF SEMESTER EXAMINATION PAPER 2016

MODULE CODE: MA4605

SEMESTER: Autumn 2016

MODULE TITLE: Chemometrics

DURATION OF EXAM: 2.5 hours

LECTURER: Mr. Kevin O'Brien

GRADING SCHEME: 100 marks
60% 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 are provided at the end of the exam paper.
Students must attempt any 4 questions from 5.

Questions Here

Critical Values for Dixon Q Test

N	$\alpha = 0.10$	$\alpha = 0.05$	$\alpha = 0.01$
3	0.941	0.970	0.994
4	0.765	0.829	0.926
5	0.642	0.710	0.821
6	0.560	0.625	0.740
7	0.507	0.568	0.680
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	0.410	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

$$MS_A = c \times S_r^2$$

$$MS_B = r \times S_c^2$$

Control Limits for Control Charts

$$\bar{\bar{x}} \pm 3 \frac{\bar{s}}{c_4 \sqrt{n}}$$

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

$$[\bar{R}D_3, \bar{R}D_4]$$

Process Capability Indices

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

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

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

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

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

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

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