MACHAKOS UNIVERSITY

University Examinations for 2021/2022 Academic Year

SCHOOL OF PURE AND APPLIED SCIENCES

DEPARTMENT OF PHYSICAL SCIENCES

SECOND YEAR SECOND SEMESTER EXAMINATION FOR

BACHELOR OF SCIENCE (ANALYTICAL CHEMISTRY)

BACHELOR OF EDUCATION (SCIENCE)

SAN 204: CHEMOMETRICS

DATE: 14/12/2021 **TIME: 2.00-4.00 PM**

Instructions:

1. **Answer question 1 (Compulsory) in Section A and ANY other 2 questions in Section B.**
2. **Candidates are advised not to write on the question paper.**
3. **Candidates must hand in their answer booklets to the invigilator while in the examination room**

   NOTE: Find the STATISTICAL TABLES at the end of this booklet

SECTION A (COMPULSORY)

QUESTION ONE (30 MARKS)

a) Define the following terms;

i) Limit of detection

ii) Systematic error

iii) Null hypothesis

iv) Statistical test

v) Outlier

vi) Significance test (6 marks)

b) The following results were obtained in the determination of Fe^{3+} in water samples at 5 % confidence level. 54.1 ppm 50.7 ppm 49.1 ppm 49.0 ppm 51.1 ppm

Is there a need to reject or accept the outlier using the following tests?

i) Q-test (4 marks)

ii) Grubbs test (4 marks)

c) Describe the various stages involved in data analysis. (6 marks)

d) The following figures refer to the concentration of albumin, in gL-1, in the blood sera of 16 healthy adults: 37, 39, 37, 42, 39, 45, 42, 39, 44, 40, 39, 45, 47, 47, 43, 41

The first eight figures are for men and the second eight for women. Test whether the mean concentrations for men and women differ significantly. (6 marks)

e) Briefly describe the **TWO** types of data commonly encountered in scientific world. (4 marks)

SECTION B: ANSWER ANY TWO QUESTIONS

QUESTION TWO (20 MARKS)

a) Describe the types of errors encountered in most evaluation of results. (8 marks)

b) Distinguish between accuracy and precision? (3 marks)

c) Discuss the steps involved in the testing of hypothesis for the means of a given population. (5 marks)

d) The number of binding sites per molecule in a sample of monoclonal antibody is determined four times, with results of 1.95, 1.95, 1.92 and 1.97. Comment on the precision and accuracy of these results. (4 marks)

QUESTION THREE (20 MARKS)

a) State the various methods used to predict data correlation. (4 marks)

b) Using sketches compare a sample data that is perfectly negative correlation to no correlation. (3 marks)

c) Differentiate between a Type I and II error. (3 marks)

d) In statistical analysis, when is the F-test considered for use? (2 marks)

e) A new method X for the determination of the chemical oxygen demand of wastewater was compared with the standard method Y. The following results were obtained for a sewage effluent sample: Both samples had 8 values, thus degree of freedom is 7 at 5 % significance level.

Methods	Average (mol/L)	Standard deviations (mol/L)
X	0.467	0.0229
Y	0.503	0.0182

Is the precision of method B significantly greater than that of the method A? (5 marks)

f) State any **THREE** statistical softwares for data analysis commonly used. (3 marks)

QUESTION FOUR (20 MAKRS)

a) Calculate the following descriptive statistics for the data 8.02; 7.84; 7.98; 7.95; 8.01; 8.07; 7.89 on water hardness (mmol L^{-1}) given as follows:

i) arithmetic mean

ii) median

iii) standard deviation

iv) variance

v) range (10 marks)

b) The morphine levels (%) of seven batches of seized heroin were determined, with the following results: 15.1, 21.2, 18.5, 25.3, 19.2, 16.0, and 17.8. Calculate the;

i) 95 % and

ii) 99 % confidence limits for these measurements. (6 marks)

c) Briefly state the factors that affect Type II error. (4 marks)

Tables

Table A.5 Critical values of G ($P = 0.05$) for a two-sided test

Sample size	Critical value
3	1.155
4	1.481
5	1.715
6	1.887
7	2.020
8	2.126
9	2.215
10	2.290

Taken from Barnett, V. and Lewis, T., 1984, *Outliers in Statistical Data*, 2nd edn, John Wiley & Sons Limited.

Table A.6 Critical values of Q ($P = 0.05$) for a two-sided test

Sample size	Critical value
4	0.829
5	0.710
6	0.625
7	0.568

Adapted with permission from Statistical treatment for rejection of deviant values: critical values of Dixon's "Q" parameter and related subrange ratios at the 95% confidence level, *Analytical Chemistry*, 63(2), pp. 139–46 (Rorabacher, D.B. 1991), American Chemical Society. Copyright 1991 American Chemical Society.