FACULTAD DE CIENCIAS QUÍMICAS

APPLIED STATISTICS AND NUMERICAL METHODS

COURSE GUIDE

BSc Chemistry

Academic Year 2026-2027

UNIVERSIDAD COMPLUTENSE MADRID



I.- IDENTIFICATION

COURSE NAME:	**Applied Statistics and Numerical Methods**
CREDITS (CTS):	**6**
CHARACTER:	**Mandatory**
SUBJECT:	**Statistics**
MODULE:	**Basic**
DEGREE:	**Bachelor in Chemistry**
SEMESTER/TERM TAUGHT:	**Second term (first year)**
DEPARTAMENT:	**Department of Mathematical Analysis and Applied Mathematics**

LECTURES IN CHARGE:

Course Coordinator	**Lecturer:**	**EDUARDO GARCÍA-TORAÑO ANDRÉS**
	Department:	Mathematical Analysis and Applied Mathematics
	Office:	**302C-2**
	e-mail:	eduarg14@ ucm.es

Group E		
Theory Seminars Tutorials	**Lecturer:**	**ROMAN SMIRNOV**
	Department:	Mathematical Analysis and Applied Mathematics
	Office:	**302-H**
	e-mail:	rsmirnov@mat.ucm.es

II.- OBJETIVES

GENERAL OBJETIVES

For the majority of the students this lecture is the first contact with statistics and numerical analysis and that is why the organisation of this lecture has to take it into account without giving up the rigour in the mathematical concepts.

The main goal of this lecture is to teach the students how to deal with experimental data from the point of view of statistics and how to solve various mathematical problems numerically. The students are supposed to have acquired the relevant and necessary tools to obtain these goals in the course entitled *mathematics* which they attended in the first term.

SPECIFIC OBJETIVES

- To acquire elementary techniques to manage data sets.
- To learn techniques about data fitting for empirical laws using least squares methods.
- To learn how to deal with tables of different statistical distributions.
- To learn how to apply statistical interference.
- To introduce the one way ANOVA.
- To learn methods to solve problems numerically which arise in Chemistry.
- To learn to use software programs suited to deal with data analysis.

III.- Previous knowledge and recommendations

Previous knowledge:

Basic knowledge of the courses «Mathematics I» and «Mathematics II» as described in the official program of the Spanish «Bachillerato». Of special relevance are the parts which correspond to statistics.

Recommendations:

In case the students do not possess the required prerequisites, it is strongly recommended to acquire them before the start of this lecture.

IV.- Contents

Brief description:

Descriptive Statistics. Random variables, discrete and continuous. Statistical interference. Estimates of parameters. Confidence Intervals. Statistical hypothesis testing. ANOVA. Numerical methods.

Syllabus:

1. Numerical methods.

   - Error analysis, truncation error.
   - Interpolation based on Newton's polynomial
   - Numerical differentiation, finite difference formula. First order methods: backward, centred, forward divided differences). Second order methods: centred divided differences.
   - Numerical integration, trapezoidal rule, Newton–Cotes formulas, composite trapezoidal rule.
   - ODE: Initial value problem, single step methods, Euler method.

2. Descriptive statistics

   - Population and samples.
   - Frequencies, mean, variance, covariance and standard deviation.
   - Regression analysis.

3. Basic concepts of probability theory

   - Events, sample space. Combinatorics.
   - Law of large numbers.
   - Basic properties of probability. Conditional probability, Bayes Theorem.

4. Random variables and probability distributions.

   - Discrete random variables, distribution functions, expected value, and variance
   - Continuous random variable and probability density function.
   - Binomial, Poisson and Normal distribution.
   - Multiple random variables: mean and variance of the sum of two variables. Covariance, expected value, and variance of the sum of independent variables.
   - Central limit theorem.

5. Statistical interference:

   - Student and Fisher distribution.
   - Estimator based on the mean and the variance.
   - Confidence interval for the mean, variance, and the proportion.
   - Statistical hypothesis testing, concerning the mean and the variance.
   - Statistical hypothesis testing for two samples, ANOVA.

V.- Competences

- **General:**
  - **CG6:** To analyse and to solve qualitative and quantitative problems.
  - **CG7:** To recognise and to analyse new problems develop strategies for their resolution.
- **Specific:**
  - **CE28-EC1:** To calculate the fundamental parameters of descriptive statistics.
  - **CE28-EC2:** To approximate point clouds by functions.
  - **CE28-EC3:** To recognise and to manage different random variables, their corresponding distributions, and tables.
  - **CE28-EC4:** To estimate statistic parameters and to carry out statistical hypothesis testing.
  - **CE29-EC1:** To find approximate solutions to some problems by numerical analysis.
- **Generic:**
  - **CT3:** To demonstrate critical thinking and self-criticism.
  - **CT7:** To use software packages to analyse experimental data.
  - **CT11:** To develop skills to perform self directed work.

VI.- Learning outcomes

Having passed the course, the students should be able to:

- Use basic techniques to approximate functions (Taylor series, interpolation)
- Apply numerical integration to solve integrals.
- Approximate derivatives by numerical differentiation.
- Approximate solutions to ordinary differential equations by Euler's method.
- Use a software program (spreadsheet) which allows to manipulate frequencies tables and to calculate measures that are commonly used to describe an experimental data set.
- Analyse two-dimensional sample points with one independent variable and one dependent variable by simple linear regression.
- Use basic concepts of descriptive statistics to describe and characterise populations and samples.
- Apply the concepts of probability to real life scientific problems.
- Analyse statistically a set of experimental data and deduce conclusions about the populations.
- Calculate confidence intervals for different statistic parameters of the corresponding random variables.
- Use hypothesis testing as a base for decisions.
- Master the concepts of one way ANOVA to analyse various samples.

VII. – Working hours, distributed by activity

This lecture, about applied statistics and numerical analysis, takes place in the second term and consists of 6 credits, that means, according to the criteria ECTS, 150 hours a year, which are distributed as follows:

Activity	Attendance (hours)	Self-study (hours)	Credits
Lectures	28	52	3,2
Seminars	18	22	1,6
Tutorials	3	4,5	0,3
Preparation of exams	5	17,5	0,9
Total	**54**	**96**	**6**

VIII.- Methodology

At the start of the course, during the first (**face to face**) class, the student will be informed by the Lecturer the content of this course.

Exercises will be published on the virtual campus in order to encourage the students to try to solve them individually.

The so called **seminars** are face to face lectures, dedicated to the resolution of the exercises.

A manual has been elaborated, which enables the student to learn a relevant software package for solving the problems presented during the course. This manual is supported by instructions and examples provided by the lecturer. It might be possible to have one of the lectures dedicated to that software and its corresponding manual in the computer laboratory.

IX.- Bibliography

Basic:

- Álvarez Contreras, S. J.: *"Estadística aplicada. Teoría y problemas"*, (available only in Spanish) / C.L.A.G.S.A., 2000.
- Mathews, J. H.; Fink K. D. *"Numerical Analysis with Matlab"*, Ed. Prentice-Hall. 2000.

Complementary:

- Steiner, E.: *"The Chemistry Maths Book"*, Oxford University Press, USA; 2 Revised edition edition (7 April 2008).
- Spiegel, M. R.: *"Statistics",* McGraw Hill, 1991.
- Faires, J. D.; Burden, R.: *"Numerical analysis"*, Thomson, 2004.

X.- Assessment procedure

30 percent of the mark will come from two short exams during the course and 70 percent from a 3 hour end of semester exam.

- **Short Exams:** **30%**

Two 1 hour exams will be hold during the course. Each of them will contribute 15 percent to the final mark.

The evaluation concerns subjects CG6, CG7, CE28, CE29, CT3, CT7 y CT11.

- **Final Exam:** **70%**

The **final exam** will last 3 hours and will contribute 70 percent to the final mark.

The evaluation concerns subjects CG6, CG7, CE28, CE29, CT3 y CT11

- **Resit examinations in July:** **100%**

If a student fails the exams, the student has the right to attend by a resit exam, which will last for three hours, concerns all the subjects of the course and will take place in July. This exam corresponds to 100 percent of the final mark.

The evaluation concerns subjects CG6, CG7, CE28, CE29, CT3, CT7 y CT11**.**

The students will be informed about the results of the two 1 hour exams in due time which would allow the students to prepare this exam and also to organise his other studies accordingly. In any case, the students will be informed about their qualification in a period which should not exceed 20 days after the exam. In the case of the second short exam, this period might be shorter due to the time constraints of the lectures, but in any case, the marks should be published at least 7 days before the final exam.

In order to pass the course, the student must have participated in at least 70% of the classroom activities.

Activities Schedule

Unit	Activity	Hours	Groups	Start	End
1. Numerical Analysis	Lectures	4	1	1st Week	2nd Week
	Exercises	3	1		
2. Descriptive statistics. Least square approximation.	Lectures	4	1	3rd Week	4th Week
	Exercises	3	1		
3. Basic concepts of probability	Lectures	4	1	5th Week	6th Week
	Exercises	3	1		
4. Random variables and probability distributions	Lectures	6	1	7th Week	9th Week
	Exercises	4,5	1		
5. Statistical interference	Lectures	10	1	10th Week	14th Week
	Exercises	4,5	1		
	Tutorial/supervised Activities	3	1	10th, 12th and 14th Weeks	
	Written Exams	4	1	Determined by the School	

* The supervised tutorials/activities are subject to possible modification depending on the complete organisation of the course.

Summary of the activities								
Lecture activities	**Associated Competences**	**Lecturer Activity**	**Student Activity**	**Assessment procedure**	**P**	**NP**	**Total**	**C**
Lectures	CG6, CG7, CE28, CE29 CT3, CT11	Presentation of theoretical concepts.	Listing, understanding, planning questions. Note taking, for clarifying doubts.	Short and long exams.	28	96		70% + 30%
Face to face classes for exercises		Application of the theory to problem solving. Preparation of a manual to solve problems with software packages.	Presenting solution to exercises. Question and doubt raising. Presentations on the blackboard. Use of software packages to solve problems	Short and long exams.	18			
Tutorials	CE28, CE29 CT7	Helping the students to direct their study with explanations and bibliographical recommendations. Formulation and proposal of guided work.	Inquiries to the teacher regarding conceptual and methodological difficulties encountered when studying the subject.	Mandatory attendance on assigned days.	3			
Exams	CG6, CG7, CE28, CE29, CT3, CT7, CT11	Design, control and evaluation of the exam. Grading student.	Training and examination.	Marking the exam.	5			
P : In class; NP: Self-studies C: evaluation								