Faculty Experimental Sciences

SYLLABUS

Undergraduate Degree in Chemistry

Course Information

Name:
CÁLCULO NUMÉRICO Y ESTADÍSTICA
English name:
NUMERICAL ANALYSIS AND STATISTICS

Code:	Type:
757509107	BASIC (OBLIGATORY)

Hours:

	Total	In class	Out of class
Time distribution	150	60	90

ECTS:

Large group	Small groups			
	Classroom	Lab	Fieldwork	Computer Lab
4	0	0	0	2

Departments:	Knowledge areas:
INTEGRATED SCIENCES	MATHEMATICAL ANALYSIS
INTEGRATED SCIENCES	APPLIED MATHEMATICS
Year:	**Semester**
FIRST	SECOND

TEACHING STAFF

Name:	E-mail:	Telephone

ANEXO I

JARED AURENTZ	JARED.AURENTZ@DCI.UHU.ES	
Others Data (Tutoring, schedule...)		

SPECIFIC INFORMATION OF THE COURSE

1. Content description:

1.1 In English:

Numerical methods are very important for the experimental sciences since they provide techniques to approximate solutions of practical problems which have been previously formulated mathematically.

Statistics deals with extracting information from data to make inferences about the behavior of the population from which the data comes from.

1.2 In Spanish:

El Cálculo Numérico es muy importante para las Ciencias Experimentales ya que facilita métodos que aproximan las soluciones de problemas prácticos, que han sido previamente formulados matemáticamente, evaluando por otra parte los errores cometidos.

La Estadística se ocupa de extraer la información que aportan los datos de una muestra para hacer inferencias sobre el comportamiento de la población de la que esa muestra procede, lo que la convierte en un instrumento muy útil para la toma de decisiones.

2. Background:

2.1 Situation within the Degree:

Knowledge of numerical methods and statistics will be useful skills for completing

2.2 Recommendations

It is highly recommended that the student has successfully completed the mathematics course from the first semester.

3. Learning Objectives:

- Learn how to apply fundamental mathematical knowledge to organize information and initiate correctly the steps needed to solve a given a problem.
- Develop the capacity to be able to express a problem in mathematical form, identify the appropriate techniques needed to solve the problem and interpret correctly the results.
- Understand that Numerical Analysis and Statistics are essential tools for analyzing information.

4. Skills to be acquired

4.1 Specific Skills:

C21: Apply the necessary mathematical concepts in order understand and rigorously express the relationships between the variables and the physio-chemical functions.

C22: Demonstrate a basic understanding of statistics that permits one to estimate the veracity of experimental data.

C23: Develop numerical methods to approximately solve scientific problems.

P5: Interpret experimental data in terms of its significance and the underlying theory.

Q2: Ability to apply knowledge to solve qualitative and quantitative problems according to previously developed mathematical models.

4.2 General, Basic or Transversal Skills:

CB1: That the student demonstrates possession and comprehension in an area beyond secondary education that, with the help of text books, includes understanding at the forefront of their area of study.

CB2: That students know how to apply their knowledge to their work or vocation in a professional way and have the skills that are usually demonstrated through the development and defense of arguments and problem solving within their area of study.

CB3: That students have the ability to gather and interpret relevant data (usually within their area of study) to make judgments that include reflection on relevant issues of a social, scientific or ethical nature.

CB4: That students can transmit information, ideas, problems and solutions to both specialized and non-specialized audiences.

CB5: That students have developed those learning skills necessary to undertake further studies with a high degree of autonomy.

CG1: That students have developed and demonstrated learning skills and knowledge from their field of study, being able to apply them in their work, interpreting relevant data to make judgments on various kinds of topics, being able to transmit them to both a specialized and non-specialized audience.

CT2: Develop critical-thinking skills with the ability to analyze and synthesize.

CT4: Develop research skills that permit the continual reflection and advancement of knowledge.

5. Training Activities and Teaching Methods

5.1 Training Activities:

- Practical theoretical group.
- Laboratory teaching group.
- Tutored Work Group.
- Individual Activity.

5.2 Teaching Methods::

- In-person classes related to the theoretical and practical contents (problems) of the subject, using didactic resources such as transparencies, computerized presentations and videos.
- Use of the computer room to reinforce previously acquired theoretical and practical knowledge.
- Making presentations by the students of aspects related to the agenda of the subject.
- Test and resolution of theoretical-practical questions.
- Discussion of scientific articles.
- Any directed activity that helps the acquisition of knowledge, skills and abilities.
- Monitoring of other tasks assigned to them.
- Resolution of doubts.
- Self-assessment exercises on the contents of the subject.
- Use of Web pages to support the teaching of the subject.

5.3 Development and Justification:

6. Detailed Contents

BLOCK I: NUMERICAL ANALYSIS

Topic 1. *Numbering systems, machine numbers and error theory. (2 weeks). Numbering systems. The IEEE-754 standard: representation of numbers as machine numbers. error theory.*

Topic 2. *Analysis of the error in Taylor's formula. Taylor series. (1 week) Review of Taylor's formula: remainders. Error analysis. Taylor series. Applications.*

Topic 3. *Numerical resolution of equations. (1.5 weeks) Bisection method. Fixed point methods. Newton-Raphson method. Other methods.*

Topic 4. *Interpolation and adjustment of functions. (1.5 weeks) Polynomial interpolation. Interpolation using cubic splines. Function setting. The method of least squares. Other methods.*

Topic 5. *Initial value problems for ordinary differential equations. (1.5 weeks) Elementary theory of initial value problems. Euler's method. Higher order Taylor methods. Runge-Kutta method.*

BLOCK II: PROBABILITY AND STATISTICS.

Topic 6. *Descriptive statistics. (1.5 weeks) Organization of data. Distributions of a variable. Distributions of two variables. Regression and correlation.*

Topic 7. *Review of combinatorics and probability theory. (2 weeks) Ordinary combinatory and with*

repetition. Axioms of probability. Assignment of probabilities. Conditional probability. independent events. Total probability and Bayes' theorems.

Topic 8. *Probabilistic models. (2 weeks) Random variables. Probability distributions. Chebyshev's theorem. The binomial distribution and other discrete distributions. The normal distribution and other continuous distributions.*

Topic 9. *Statistical inference. (2 weeks) Spot Estimate. Interval estimation. Contrasts of Hypothesis.*

COMPUTER SCIENCE BLOCK 1

L1. Topic 1 (2 hours)

L2. Topic 2 (2 hours)

L3. Topic 3 (2 hours)

L4. Topic 4 (2 hours)

L5. Topic 5 (2 hours)

COMPUTER PRACTICES BLOCK 2

L6. Topic 6 (2 hours)

L7. Topic 7 (2 hours)

L8. Topic 8 (2 hours)

L9. Topic 9 (2 hours)

L10. Various exercises (2 hours)

7. Bibliography

7.1 Basic Bibliography:

- Richard L. Burden - Douglas J. Faires - Annette M. Burden: Numerical Analysis (10 ed) Cengage Learning (2017) ISBN: 978-607-526-411-0
- Ronald E. Walpole - Raymond H. Myers - Sharon L. Myers - Keying Ye: Probability and Statistics for Science and Engineering (9 ed) PEARSON EDUCATION, México, 2012 ISBN: 978-607-32-1417-9

7.2 Additional Bibliography:

8. Systems and Assessment Criteria

8.1 System for Assessment:

- Final Exam
- Individual Activity
- Continuous Evaluation

8.2 Assessment Criteria and Marks:

8.2.1 Examinations Convocation I

The subject is divided into two blocks: **B1** (Numerical Calculation) and **B2** (Probability and Statistics)

Each of the two blocks, **B1** and **B2**, is evaluated separately.

The evaluation of each block consists of a theoretical-practical exam (**ExB1** and **ExB2**), computer practice exam (**INF1** and **INF2**) and the qualification for attendance and participation (**AyP1** and **AyP2**).

In all cases it is graded from 0 to 10.

General considerations:

Class attendance is mandatory because we are in a face-to-face university.

An attendance rate in normal classes that does not exceed 80% implies a grade of 0 in the **AyP1** and/or **AyP2** section.

The attendance to the practices of Computer science is obligatory. Non-attendance will be penalized, in each block, with a reduction of two points for each unjustified absence in the final grade of **INF1** and/or **INF2**.

The qualification of EACH BLOCK will be:

Rating Block **i** (i=1,2) **CaBi** = 0.7 x **ExBi** + 0.2 x **INFi** + 0.1 x **AyPi** (i=1.2)

CALCULATION OF THE FINAL GRADE

June rating = 0.5 x **CaB1** + 0.5 x **CaB2**

A minimum note is not needed in each block. In the end, send the average.

If the final average is less than 5 but in one of the blocks it is 5 or higher, the qualification of said block is saved for September but not for subsequent calls. If it is less than 5, it is not saved.

Note: since 4 tests are needed to determine the final grade, every attempt will be made to organize them on different days so as not to overwhelm anyone. The dates of the exams, whenever possible, will be agreed with the students through their legal representatives.

8.2.2 Examinations Convocation II

There will be two different exams, one for block **B1** and another for block **B2**. Both blocks will be evaluated in the same exam, although in both cases the practical part could be done in a different session (and day), since it would be the laboratory part, which would require a special classroom. In the latter case, for both blocks, the practical part would be 20% and the theoretical-practical exam 80%. As in June, the final grade would be:

September rating= 0.5 x **CaB1** + 0.5 x **CaB2**

From that moment on, partial grades are NOT saved for subsequent calls.

8.2.3 Examinations Convocation III

As in call II, with the exception that the previous grades are NOT valid and partial grades are not saved.

8.2.4 Extraordinary Convocation

The same as Convocation III.

8.3 One-time Final Examination

8.3.1 Examinations Convocation I

The fact that a student opts for the final single assessment does NOT mean that said administrative act cannot be included in several sessions nor that said sessions must be carried out on a single day. Of course, since both laboratory tests and theoretical-practical tests are contemplated, it would be counterproductive and not very pedagogical to accumulate all the tests on the same day.

In addition, it is clear that the content required of all students must be the same as otherwise we would be facing a comparative burden. So, the theoretical-practical and laboratory tests for students who opt for this type of assessment will be **THE SAME** that the corresponding tests must overcome for students who opt for continuous assessment (and, logically, will be examined **on the same dates**).

As in the case of continuous evaluation, all tests are graded with a score from 0 to 10.

Those students who, in application of the current Regulations, opt for a single final assessment, must carry out:

- **ExB1** theoretical-practical exam.
- The **INF1** informatics practice exam.
- **ExB2** theoretical-practical exam.
- The **INF2** informatics practice exam.

The **CaBi** qualification (i=1,2) of each of the two blocks will be obtained using the formula:

CaBi=0.80 x **ExBi** + 0.2 x **INFi** (i=1.2)

CALCULO DE LA CALIFICICACIÓN FINAL

The final **CaF** qualification will be obtained by the formula:

CaF = 0.5 x **CB1** + 0.5 x **CB2**.

EN LA EVALUACIÓN ÚNICA FINAL NO SE GUARDAN NOTAS PARTIALES PARA SEPTIEMBRE.

8.3.2 Examinations Convocation II

There will be two different exams, one for block **B1** and the other for **B2**. The two blocks will be evaluated in the same exam in a si bien, in both cases the practical part could be done in a different session (and day) because it would be the laboratory part which would require a special class. In the latter case, for both blocks, the practical part is 20% and the theoretical-practical exam is 80%. As in June, the final qualification would be:

Qualification September = 0.5 x **CaB1** + 0.5 x **CaB2**

Partial notes are NOT kept for later calls.

8.3.3 Examinations Convocation III

The same as Convocation II.

8.3.4 Extraordinary Convocation

The same as Convocation II.