Universida_{de}Vigo

IDENTIFYING DATA
Numerical methods in chemistry

Subject	Numerical methods in chemistry			
Code	V11G200V01402			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	2nd
Teaching language	Galician			
Department				
Coordinator	Besada Morais, Manuel			
Lecturers	Besada Morais, Manuel			
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General description	"Machine translation into english of the original teaching guide" This matter is the mathemetical practical version of application to observed data and of numerical solution of numerous problems that have difficult, or impossible, analytical solution. It will allow to the student to obtain skills to handle big amounts of numerical information and consolidate the handle of a scientific calculator of big power.			

Competencies

Code	
A3	Students have the ability to gather and interpret relevant data (usually within their field of study) to inform judgments that include reflection on relevant social, scientific or ethical issues
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C22	Process and perform computational calculations with chemical information and chemical data
C29	Demonstrate skills for numerical calculations and interpretation of experimental data, with special emphasis on precision and accuracy
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions

Learning outcomes

Expected results from this subject	Training and Learning Results		
Use the numerical and symbolic packages of **MATLAB.		C22 C29	D5
Control distinct bases of numbering and *enterarse of the existence of errors committed in the approximations	A3	C29	D6 D9 D13 D14

Look for approximations of roots of equations of a variable and systems of equations.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14
Use *polynomials that adjust to several points of the plane.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14
Derive and integrate numerically, relate these numerical and analytical concepts and understand the because of his need.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14
Handle adjust of data to distinct types of curves of previous election by means of computer packages.	A3 A5	C19 C22 C29	D3 D4 D5 D6 D7 D9 D12 D13 D14

Contents

Topic	
Subject 1. *Introduction the analysis **numerica.	Systems of numbering Need of the numerical methods. *Fontes And analysis of the error. Available *software.
Subject 2. Approximation of roots of equations of a variable.	*Condicionamiento Of the calculation of roots. Methods of separation of roots- Method of the *bisection. Method of Newton-**Raphson. *Theorem of the point did.
Subject 3. *Numerical interpolation.	The general problem of *interpolation. *Interpolation of *Lagrange. Error of *interpolation and excellent election of *nodes. *Interpolation **polinomial.
Subject 4. It adjust of curves.	It adjust of data. Straight of regression by square minima. Approximation of functions by square minima. *Interpolation **polinomial to *pieces.
Subject 5. *Derivación And numerical integration.	Diagrams of *derivación numerical *based in *interpolation. Formulas of *derivación *finite. Error of *derivación. Formulas of integration with *polynomial *interpolation. Error of integration. Formulas of *quadratures.
Subject 6. Numerical resolution of systems of equations.	Direct methods of resolution of linear systems: *Gauss. Classical *iterative methods. Methods of descent: Máximo descend and *gradient *conjugado. Resolution of systems no linear.

Planning

	Class hours	Hours outside the classroom	Total hours	
Master Session	13	26	39	
Practice in computer rooms	26	52	78	
Multiple choice tests	4	12	16	
Troubleshooting and / or exercises	2	8	10	
Jobs and projects	0	7	7	

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies

	Description
Master Session	Exhibition of the theoretical bases and orientation by part of the *profesorado on the contents of the matter
Practice in computer rooms	Development in the classrooms of computing of the exercises that propose in the theoretical classrooms using the scientific calculator **MATLAB.

Personalized attention

Methodologies	Description
Practice in computer rooms	The students will work of autonomous way with the permanent supervision of the professor

Assessment

	Description	Qualification	Training and Learning Results	
Practice in computer rooms	At the end of the sessions in the classrooms of computing, the student will resolve some exercises of the even type that the ones of the realised in the classroom.	25	C19 C22 C29	D6
Multiple choice tests	During the course will realise **alomenos three partial proofs short type test and practical type that will explain a 25 by one hundred in the final qualification. Besides, in a final proof, will realise another tests type test of **tódala matter that *contabilizará another 10 by one hundred in the final qualification.	35	C19 C22 C29	D6
Troubleshooting and / or exercises	When finalising the course **realizaráse a practical proof resolving some practical exercises in the classroom of computing	30	C19 C22 C29	D6
Jobs and projects	**Participacion With *aprovechamiento in all the activities proposed by the *profesorado, are these to realise inside or out of the classroom.	10	C19 C22 C29	D6

Other comments on the Evaluation

The students that do not surpass the *materiaen the common announcement and pretend to do it in the *convocatoriaextraordinaria, will keep the qualifications obtained during the course in each *unode the previous sections, except the qualifications of the practical proofs of computing, that will be able to be recovered, and *lasdos proofs realised at the end of course that will be evaluated in the *examencorrespondiente. In this case, the student has to put in contact with the professor with sufficient *antelación to agree the work to realise before the final proofs.The participation of the student in any of the acts of evaluation of the matter will involve the condition of &*quot;presented&*quot; and, therefore, the allocation of a qualification. They consider acts of evaluation the assistance to the practices of computing (four or more), the realisation of some proof or the delivery of a minimum of 25% of the problems or exercises commissioned by the professor.

Sources of information

Chapra, S.C.; Canale, R.P., **Métodos numéricos para ingenieros**, 2010,
Besada, M., **MATLAB: todo un mundo**, 2007,
Mathews, J.H.; Fink, K.D., **Métodos numéricos con MATLAB**, 2000,
Nakamura, S., **Análisis numérico y visualización gráfica con MATLAB**, 1997,

Recommendations

Subjects that it is recommended to have taken before

Mathematics: Mathematics I/V11G200V01104
Mathematics: Mathematics II/V11G200V01203