UCLouvain

lbirc2106

2019

Chemometrics

In view of the health context linked to the spread of the coronavirus, the methods of organisation and evaluation of the learning units could be adapted in different situations; these possible new methods have been - or will be - communicated by the teachers to the students.

3 credits	22.5 h + 15.0 h	Q1

Teacher(s)	Govaerts Bernadette ;
Language :	French
Place of the course	Louvain-la-Neuve
Main themes	1 . Statistics for measurement methods: reminders of Metrology (error types, quantification of error uncertainty, error propagation'), variance components estimation by ANOVA, control charts, simple linear calibration. 2 . Experimental design in product and process development: Methodology , multiple regression and multiple response optimization , factorial designs and derivatives, screening designs, response surface designs , mixture designs and optimal designs 3 . Multivariate statistical methods in chemistry: principal component analysis , partial least squares (PLS) , clustering, discriminant analysis and its application to multivariate calibration in analytical chemistry 4 . Applications with the JMP software
Aims	Contribution à l'activité du référentiel 1.1, 1.2, 1.4, 2.1, 2.2, 2.3, 3.4, 3.5, 3.6 At the end of the course students will be able to : - Explain the interest of statistical tools in the work of the chemical engineer - Explain the purpose and usage of each statistical tool seen in the course. select the one adapted to a given situation and calculate related parameters. - Demonstrate their understanding of main course concepts by solving methodological exercises 1 - Use JMP software to apply the methods presented in the course. - Interpret the results of a statistical analysis in the context of a case study in chemistry or life science. For specific tools - Use statistical tools to quantify the precision of a measurement method - Organise an experiment with the design of experiment methodology from the design selection to the statistical analysis - Summarize / visualize large data sets (eg from spectral analytical methods) using multivariate statistical tools - - - - *The contribution of this Teaching Unit to the development and command of the skills and learning outcomes of the programme(s) can be accessed at the end of this sheet, in the section entitled "Programmes/courses offering this Teaching Unit".*
Evaluation methods	**Due to the COVID-19 crisis, the information in this section is particularly likely to change.** Written exam (16pts/20) containing • Methodological exercices to verify the intergration of course main concepts. • Questions on the selection and application of methods adapted to given practical situations. • Interpretation of JMP software outputs. The exam is organised in the computing lab (Word and JMP available) Home-work and projects count also for 4pts/20

Teaching methods	**Due to the COVID-19 crisis, the information in this section is particularly likely to change.** Lectures (22.5h) • Methods presentation on the basis of real-life situations. • Formal but intuitive discussion of theoretical concepts and formulae for most methods. • Interpretation of software outputs and use of the JMP software in class. • Interactive lectures: students are encouraged to participate during the course. Computer labs (15h) • Case studies on JMP, methodological exercises, and JMP Output interpretation. Homework and projects • The student is invited to prepare each week an exercise, a quiz or a small project in order to apply and integrate course content.
Content	1 . Statistics for measurement methods : reminders of Metrology vocabulary, measure uncertainty quantification (for simple or combined measures), variance components estimation by ANOVA, simple linear calibration. 2 . Experimental design in product and process development : Methodology , multiple regression and multiple response optimization , factorial designs and derivatives, screening designs, response surface designs , mixture designs and optimal designs 3 . Multivariate statistical methods in chemistry : principal component analysis , partial least squares (PLS) , clustering,... and its application to multivariate calibration in analytical chemistry 4 . Applications with the JMP software
Inline resources	All course documents are on Moodle: https://moodleucl.uclouvain.be/mod/page/view.php?id=511035
Other infos	Accessibility to a public who does not speak the language of instruction • No, the lectures and course material are in French Equivalent activities • No course strictly equivalent at UCL • LSTAT2320 course on experimental designs is partly equivalent.
Faculty or entity in charge	AGRO

Programmes containing this learning unit (UE)

Program title	Acronym	Credits	Prerequisite	Aims
Master [120] in Biomedical Engineering	GBIO2M	3		
Master [120] in Chemistry and Bioindustries	BIRC2M	3		
Master [120] in Mathematical Engineering	MAP2M	3		
Master [120] in Chemistry	CHIM2M	3		
Certificat d'université : Statistique et sciences des données (15/30 crédits)	STAT2FC	3		