LUNDS UNIVERSITET
Lunds Tekniska Högskola

Course syllabus

Kemometri - försöksplanering och multivariat analys
Chemometrics - Design of Experiments and Multivariate Analysis

KLGN10, 7,5 credits, A (Second Cycle)

Valid for: 2023/24
Faculty: Faculty of Engineering, LTH
Decided by: PLED B/K
Date of Decision: 2023-04-18

General Information

Elective for: B5-l, B5-mb, K5-m, K5-l, MBIO2, N4, MLAK2
Language of instruction: The course will be given in English on demand

Aim

Build on the knowledge in design of experiments in order to be able to plan and perform more complicated experiments, as well as analyse data in several dimensions.

Learning outcomes

Knowledge and understanding
For a passing grade the student must

- Be able to explain and use basic methods in factorial design.
- Be able to explain and use basic methods in cluster analysis, discriminant analysis, principal components, and partial least squares.
- Be able to evaluate and discuss results obtained using multivariate statistical methods.

Competences and skills
For a passing grade the student must

- Plan a factorial design experiment.
- Suggest which multivariate statistical methods should be used on a given problem.
- Analyse multi-dimensional data using computer software and critically assess the result.
- Report the solutions of multivariate statistical problems in written reports and orally at

seminars.
- Independently analyse and discuss a given problem at advanced level using multivariate statistical methods and design strategies.

Contents

Complete and reduced factorial designs. Response surface analysis. Cluster analysis, discriminant analysis, principal component analysis (PCA), and partial least squares (PLS).

Examination details

Grading scale: TH - (U,3,4,5) - (Fail, Three, Four, Five)
Assessment: Written project reports as well as compulsory and active participation in the seminars.

The examiner, in consultation with Disability Support Services, may deviate from the regular form of examination in order to provide a permanently disabled student with a form of examination equivalent to that of a student without a disability.

Admission

Admission requirements:

- FMA420 Linear Algebra or FMA421 Linear Algebra with Scientific Computation or FMA656 Mathematics, Linear Algebra or FMAA20 Linear Algebra with Introduction to Computer Tools or FMAB20 Linear Algebra
- FMS086 Mathematical Statistics or FMSF20 Mathematical Statistics, Basic Course or FMSF30 Mathematical Statistics or FMSF45 Mathematical Statistics, Basic Course or FMSF50 Mathematical Statistics, Basic Course or FMSF55 Mathematical Statistics, Basic Course or FMSF70 Mathematical Statistics or FMSF75 Mathematical Statistics, Basic Course

Assumed prior knowledge: Basic skills in MATLAB programming, including using MATLAB with linear algebra and basic statistics. Note that this is an important pre-requisite. Lacking these skills will make it difficult to pass the course.
The number of participants is limited to: 40
Selection: Completed university credits within the programme. Priority is given to students enrolled on programmes that include the course in their curriculum.
The course overlaps following course/s: FMS210

Reading list

- Brereton, RG: Chemometrics, Data driven extraction for science. Wiley, 2018.

Contact and other information

Course coordinator: Stephen Burleigh, stephen.burleigh@food.lth.se
Course homepage: https://www.ple.lth.se/en/