Universidade Federal do Rio Grande do Sul
Instituto de Química
Graduate Program in Chemistry (Grade 7/CAPES)
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COURSE SYLLABUS

1. Identification
Code and title: QUP 176 – Special Topics in Chemometrics
Professors: Adriano de Araújo Gomes and Marco Flôres Ferrão
Level: Master and Doctorate
Credit hours: 2
Revised: June_2020

2. Summary
Linear and statistical algebra: concepts. Multiway data: generation and organization. Fundamentals and application of multiway calibration/classification. Tucker, Parallel Factors Analysis (PARAFAC and PARAFAC2) Methods. Multivariate curves Resolution (MCR). Independent component analysis (ICA). Methods based on residual multilinearization (U-PLS, N-PLS). Data fusion. Figures of merit in calibration and classification.

3. Objective
To understand and apply the different techniques of multivariate /multiway data treatment in classification and calibration problems related to diverse areas such as chemistry, materials, pharmaceutical, forensic, environmental, among others. To recognize the advantages and limitations of each technique.

4. Contents
- Chemometrics: a brief introduction;
- Linear and statistical algebra concepts;
- Data generation and organization;
- Basics and applications of multiway calibration;
- Tucker Methods, Parallel Factors Analysis (PARAFAC) and their variants (PARAFAC2, -PARALIND);
- Multivariate curves resolution (MCR);
- Independent component analysis (ICA).
- Residual multilinearization-based methods (U-PLS, N-PLS);
- Data Fusion into calibration and classification. Figures of Merit.

5. Assessment
List of exercises, presentation and discussion of scientific articles, theoretical tests and/or directed works. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:
A: grade equal to or above 9.0
B: grade equal to or above 7.5 and below 9.0
C: grade equal to or above 5.0 and below 7.5
D: grade below 5
FF: lack of frequency

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6. Methodology

Lectures, exercises lists, seminars and examinations.

7. Bibliography

- S. D. Brown, R. Tauler, B. Walczak. Comprehensive Chemometrics, Elsevier Science, 2009.
- A. M. Peña, H. C. Goicoechea, G. M. Escandar, A. C. Olivieri. Fundamentals and Analytical Applications of Multiway Calibration. Data Handling in Science and Technology, Elsevier Science, 2015. - G. M; Escandar, A. C. Olivieri, Practical Three-Way Calibration Elsevier Science, 2014.
- A. Smilde, R. Bro, P. Geladi, Multi-way Analisys: Application in the chemical sciences. John Wiley, LTDA, 2004.
- R. G. Brereton, Chemometrics: Data analysis for the laboratory and chemical plants. John Wiley & Sons Ltd, 2003.
 - Recent papers.