

TOPICS IN CHEMOMETRICS FOR NEAR INFRARED SPECTROSCOPY

Practical guidelines for reporting calibration results using NIR, including figures of merit

Comparison of average errors for test sample sets. Linear versus non-linear calibration models: when and why. PLS-1 vs. PLS-2, PLS vs. PCR, PLS vs. MLR. Regression coefficients: use and abuse. Figures of merit: sensitivity, selectivity, limits of detection and quantitation.

The Successive Projections Algorithm for Variable Selection in NIR

Variable selection in multivariate calibration and classification tasks: Motivation and challenges. Collinearity problems in multiple linear regression (MLR). The Successive Projections Algorithm for MLR modelling (SPA-MLR): Phase 1 (construction of chains of variables), Phase 2 (evaluation of subsets of variables) and Phase 3 (final elimination of variables). Choice of validation samples for use in Phase 2. Applications reported in the literature. Overview of the graphic user interface for SPA-MLR. Example using NIR data. Use of SPA-MLR for selection of robust variables in calibration transfer. Collinearity problems in linear discriminant analysis (LDA). The Successive Projections Algorithm for LDA modelling (SPA-LDA): Phases 1 and 2. Choice of validation samples for use in Phase 2. Applications reported in the literature and example using NIR data. Comparison with other variable selection methods. Limitations and possible drawbacks of SPA.

Requirements: Basic notions of linear algebra, regression analysis, multivariate calibration and multivariate classification and MATLAB.

**Schedule: 8 am – 12 am
13:30 pm – 17:30 pm
(October 18, 2015)**

TRAINER PROFILE



Alejandro Olivieri was born in Rosario, Argentina, on July 28, 1958. B.Sc. in Industrial Chemistry, Catholic Faculty of Chemistry and Engineering (1982), Ph.D., Faculty of Biochemical and Pharmaceutical Sciences, University of Rosario (1986). Professor at the Department of Analytical Chemistry of the latter Faculty and fellow of the National Research Council of Argentina (CONICET). About 200 scientific papers in international journals, several books and book chapters and nine supervised Ph.D. Theses. John Simon Guggenheim Memorial Foundation fellow (2001-2002).

Roberto Kawakami Harrop Galvão graduated in Electronic Engineering with Summa cum Laude honours at Instituto Tecnológico de Aeronáutica (1995), where he also obtained the Doctorate degree in Systems and Control (1999). He is currently an Associate Professor at the Electronic Engineering Department of ITA.



Mário César Ugulino de Araújo received the B.S. degree in Industrial Chemistry from Universidade Federal da Paraíba (1979) and the Doctorate degree in Analytical Chemistry from Universidade Estadual de Campinas (1987). He is currently head of the Laboratório de Instrumentação e Automação em Química Analítica/Quimiometria at UFPB.

