MULTIVARIATE LATENT VARIABLE MODELING FOR PROCESS DESIGN AND OPERATION IMPROVEMENT

16-17 July 2018

The participants will be introduced to the concept of “Latent Variable Modeling” (LVM) through lectures and hands on applications (Workshops). The syllabus is geared towards general concepts, and depending on time multiple advanced topics can be added. LVM is a data-driven modeling technique particularly useful to understand processes where acquired data is: abundant, complex, correlated and noisy. Basic knowledge of statistics, engineering principles, linear algebra and geometry are helpful to fully understand the concepts of this course.

Course Instructor: Dr Salvador Garcia-Munoz.

The course will take place in Skempton Room 165-163, Skempton Building, Imperial College London, South Kensington Campus, London SW7 2AZ.

Dr Salvador Garcia-Munoz is a Visiting Professor at Imperial College London, with +20 years of experience in the implementation of systems engineering tools to industrial problems. He works for the pharmaceutical R&D sector leading the application of digital design tools for the development of new products and accelerated process design. He is an active member of AIChE, a founder of the Systems Based Pharmaceutics Alliance and associate editor for Chemical Engineering Research and Design. His research in multivariate modeling spans from industrial applications to the development of new methods and algorithms to analyze complex datasets common in contemporary industrial scenarios.

CPSE is a Multi-institutional research centre of world-class departments at Imperial College London and University College London. CPSE was inaugurated in 1989 by Professor Roger W.H. Sargent, the founding Director of the Centre from 1989 to his retirement in 1992. Since then, CPSE has continued the legacy of Professor Sargent and remains a Centre of Excellence. CPSE academics come from multi-disciplinary backgrounds, including: chemical engineering, mathematics, physics and chemistry and are international leaders in their fields.

Course Summary

DAY 1—16 July 2018, 9am - 5pm
Principal Components Analysis (PCA)
Overview of LVM methods and reported applications
Ordinary Least Squares
The objective function
The model
The solution to the parameter estimation problem
1 PCA
WORKSHOPS 1-2-3-4

DAY 2—17 July 2018, 9am - 5pm
Projection to Latent Structures (PLS)
2. PLS
WORKSHOPS 5-6
3. Practical Issues in Data Based Modeling
WORKSHOP 7
4.0. The PLS Model Inversion via non-linear programming for Process and Product Design, Process Control and operations advisory systems
WORKSHOP 8: Process design using Inverse PLS models.

Registration Fee:

£480 for industry participants
(20% discount for CPSE Consortium companies)
£240 for non-CPSE researchers
£80 for non-CPSE students
Free for CPSE students and researchers
To register please email Dr Cristina Bertulli at c.bertulli@imperial.ac.uk

Cancellations: cancellations must be received in writing before or on 9 July. After this date cancellations will be subject to an administration charge of £50.00. Substitutions may be made at any time, whilst a valid place is held. The organizer cannot accept liability for costs incurred in the event of a course having to be cancelled as a result of circumstances beyond its reasonable control. If you would like to discuss the course, please contact Dr Cristina Bertulli c.bertulli@imperial.ac.uk
Detailed Course Summary

DAY 1—16 July 2018, 9am - 5pm
Principal Components Analysis (PCA)
Overview of LVM methods and reported applications
Ordinary Least Squares
The objective function
The model
The solution to the parameter estimation problem
1 PCA
1.1. Projection Mechanisms
1.2. The dot Product and coordinate transformation of data
1.3. The objective function behind PCA
1.4. Solving the parameter estimation problem
1.5. The PCA Model and its basic parameters
1.5.1. Scores, Loadings, R2
1.5.2. Contribution plots
WORKSHOPS 1 and 2
1.6. The PCA Model and its diagnostics
1.6.1. SPE,Hotelling’s T2
1.6.2. Cross-validation
1.7. Outlier detection
1.8. Handling of missing data
WORKSHOP 3
1.9 Multivariate Statistical Process Control
WORKSHOP 4
1.10 Establishment of multivariate specifications for raw materials

DAY 2—17 July 2018, 9am - 5pm
Projection to Latent Structures (PLS)
2. PLS
2.1. Fundamentals
2.1.1. From PCA to PCR to PLS
2.1.2. The PLS model, objective function and parameter estimation solutions
2.1.3. PLS Parameters and Diagnostics
2.1.4. The unique features of the PLS model
WORKSHOPS 5 and 6
3. Practical Issues in Data Based Modeling
3.1. Handling of Missing Samples
3.2. Modeling Systems under Feedback
3.3. Non-linear Data
WORKSHOP 7
4.0. The PLS Model Inversion via non-linear programming for Process and Product Design, Process Control and operations advisory systems
4.1 The analytical solution to the inversion problem
4.2 Rank deficiencies and null spaces
4.3 Handling the inversion of underspecified scenarios with unconstrained variables.
WORKSHOP 8: Process design using Inverse PLS models.