

ODIN Autumn Courses 2015

Infrared and Raman Spectroscopy:

Week 39: Wednesday, September 23rd, 2015

Background: The vibrational spectroscopic techniques Infrared (IR) absorbance and Raman scattering are widely used in quantitative and qualitative analysis. Both have much stronger spectral interpretation abilities compared to e.g. Near-Infrared or UV/Vis measurements (albeit frequently with poorer quantification performance). Although typically applied for similar research tasks, they can be considered complementary from an information point of view. In this one-day course we will go over the theoretical mechanisms of IR and Raman, the practical principles of measurements and spectral interpretation. Part of the course is hands-on experience in our laboratory.

Audience: This one-day course is intended for people with an interest in or modest knowledge of vibrational spectroscopy and analytical chemistry.

Due to restrictions in the hands-on facilities, we limit this course to a maximum of 12 participants.

Teachers: Søren Balling Engelsen and Frans van den Berg.

Location: University of Copenhagen, Frederiksberg Campus.

Lunch and coffee will be included. If you have special dietary needs, please let us know by enrollment.

This ODIN course is limited to three persons per membership. Enroll to Carl Emil Eskildsen (carle@food.ku.dk) September 9th at the latest. Enrollment will be accepted only through your ODIN representative. Please provide e-mail address of course participants so last minute details can be provided. Cancellations must be made no later than four days in advance or a fee of 500 DKK will be charged.



data • information • control

All the Pitfalls in Chemometrics

Week 43: Tuesday, October 20th, 2015

Background: This course is for people who are working with chemometric models and have doubts on how to really be sure the models are fine. Through numerous examples, we will explain and highlight all the most common problems, mistakes and pitfalls you run into when developing chemometric models. The course is designed to make the participants more critical and confident in their day to day work. Attendees can also bring their own data together with specific questions (these must be provided well in advance of the course).

The course will, amongst others, provide the participants with insight on:

- Practical outlier detection
- How to perform cross-validation
- How to handle reference method errors
- How to avoid spurious results and over-fitting
- How to make good use of replicates
- How to properly assess the quality of a model

Software: Demonstrations are given in matlab using PLS_Toolbox. No prior knowledge of the software is needed.

Audience: The course is of importance to engineers and technologists working e.g. in the food and medicinal industry engaged in developing chemometric models and also to people involved in assessing such models.

Teacher: Rasmus Bro.

Location: University of Copenhagen, Frederiksberg Campus.

Lunch and coffee will be included. If you have special dietary needs, please let us know by enrollment. Lectures and notes are in English.

This ODIN course is limited to three persons per membership. Enroll to Carl Emil Eskildsen (carle@food.ku.dk) October 6th at the latest. Enrollment will be accepted only through your ODIN representative. Please provide e-mail address of course participants so last minute details can be provided. Cancellations must be made no later than four days in advance or a fee of 500 DKK will be charged.



Network Meeting: Experiences and Problems getting Chemometrics and Spectroscopy into the Process

Week 46: Wednesday, November 11th, 2015

Background: In this meeting, the participants will share their experiences in getting the PAT and QbD tools into the production and related areas. Each participant will give a 20-30 min. presentation followed by open discussion. The presentation can be focused on problems, challenges, solutions or any kind of aspect that the presenter would like to share or have feedback on.

Note: All attendees at this meeting must give a presentation.

Audience: This network meeting is intended for engineers and technologists working e.g. in the food and medicinal industry engaged in process monitoring/control using spectroscopy and chemometrics.

Responsible: Rasmus Bro and Thomas Skov.

Location: University of Copenhagen, Frederiksberg Campus.

Lunch and coffee will be included. If you have special dietary needs, please let us know by enrollment. Lectures and notes are in English.

This ODIN course is limited to three persons per membership. Enroll to Carl Emil Eskildsen (carle@food.ku.dk) October 28th at the latest. Enrollment will be accepted only through your ODIN representative. Please provide e-mail address of course participants so last minute details can be provided. Cancellations must be made no later than four days in advance or a fee of 500 DKK will be charged.

Data Fusion

Week 48: Wednesday, November 25th, 2015

Background: This course aims to provide a general overview of data fusion methods (also known as multi-block or multi-set analysis techniques) based on joint factorization of data sets. The course is designed to give the participants an introduction to basic mathematical background for coupled matrix factorizations and coupled tensor factorizations, an advanced understanding of the state-of-the-art data fusion methods and hands-on experience with the MATLAB CMTF Toolbox to practice exploratory analysis using coupled factorizations. The course will primarily focus on unsupervised data fusion methods. We will also briefly discuss supervised data fusion methods (a.k.a. multi-view learning, collective learning).

Software: Course participants are expected to be experienced in MATLAB and able to write simple scripts.

Audience: The course is intended for people working on problems which can potentially benefit from joint analysis of multiple data sets, e.g., measurements from different analytical platforms, or people having a general interest in learning more about data fusion methods and their applications.

Teacher: Evrim Acar.

Location: University of Copenhagen, Frederiksberg Campus.

Lunch and coffee will be included. If you have special dietary needs, please let us know by enrollment. Lectures and notes are in English.

This ODIN course is limited to three persons per membership. Enroll to Carl Emil Eskildsen (carle@food.ku.dk) November 11th at the latest. Enrollment will be accepted only through your ODIN representative. Please provide e-mail address of course participants so last minute details can be provided. Cancellations must be made no later than four days in advance or a fee of 500 DKK will be charged.



data • information • control

Design of Experiments

Week 50: Wednesday and Thursday, December 9th and 10th, 2015

Background: Proper analysis of data and efficient planning of experiment is (or should be!) a part of every scientist's toolbox. In this short course, an outline of different terms within Design of experiments and the theory behind when to use what are given. After a reminder on the basics of statistics and populations required for experimental planning (sampling, univariate linear regression, etc.) we will look at the setup and analysis of designed experiments and statistical inference from designed data (Designs, ANOVA, etc.). Furthermore we will discuss efficient planning and performance of fixed pattern and sequential optimizations techniques useful in e.g. yield optimization in production processes or instrumental optimization in analytical chemistry procedures.

Software: JMP (SAS) or MODDE (Umetrics) can be used during exercises.

Audience: The course is intended for people handling problems where using Design of experiments can be an advantage when setting up the experiments or people who have general interest in knowing how to setup and use experimental designs. Simple mathematical and statistical terms will be used in the course and the theory will be accompanied by computer exercises.

Teacher: Frans van den Berg.

Location: University of Copenhagen, Frederiksberg Campus.

Lunch and coffee will be included. If you have special dietary needs, please let us know by enrollment. Lectures and notes are in English.

Please note that a minimum of 8 participants must sign up for this course to take place.

This course is limited to three persons per membership. Enroll to Carl Emil Eskildsen (carle@food.ku.dk) November 25th at the latest. Enrollment will be accepted only through your ODIN representative. Please provide e-mail address of course participants so last minute details can be provided. Cancellations must be made no later than four days in advance or a fee of 500 DKK will be charged.