2018 Copenhagen School of Chemometrics

World-class teaching...
...in a World-class environment

COPENHAGEN
7th May – 8th June, 2018

CSC – 2018

COPENHAGEN SCHOOL OF CHEMOMETRICS

May 7th – June 8th, 2018

Main responsible: José Manuel Amigo

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Description of the course:

Chemometrics Analytical Technologies (CAT – www.models.life.ku.dk) is more than happy to announce the new edition of the PhD course:

Copenhagen School of Chemometrics - CSC

CSC-2018 is a five-week school designed to be an introduction to different key aspects of advanced data analysis in different brands of Science (Chemistry, physics, environmental, political economics, etc). **CSC-2018** addresses to MsC, PhD students/post-docs, associate professors, etc. who want to acquire or refresh basic knowledge on multivariate data analysis from different disciplines. **CSC-2018** also addresses to researchers working in industry or research laboratories who want to implement multivariate data analysis in their daily research environment.

CSC-2018 is thought to be an intensive school. Therefore, **CSC-2018** will be held in five weeks structured in different seminars/workshops where the students will be more than welcome to work with their own data together with high-qualified teachers. Moreover, anyone can choose the seminars to participate, not having a minimum of seminars request.

Targets of CSC-2018:

CSC-2018 aims at being a platform for:
- Learning basic and advanced data analysis methods: CSC-2018 is specifically designed for researchers who want to start using data analysis in their routine work.

- Sharing knowledge and interchange ideas between students covering different scientific backgrounds: One of the key points of **CSC-2018** is the interaction between the students to discuss issues and troubleshooting always within the framework of scientific data analysis and performance. The reports days and the workshop will offer the opportunity to the students to discuss, share and improve their main issues and initiatives in a professional environment.

- Meeting world-wide recognized experts of Multivariate Data Analysis in an open discussion forum environment: **CSC-2018** will count on teachers that are well-recognized experts on chemometrics and multivariate data analysis in their respective fields. This, at the same time, will offer the possibility of opening new collaborative frameworks between students and teachers.

- Flexibility in the seminars and ECTS credits: The students can choose to attend the seminars which they consider more relevant for their research. There is no a minimum of seminars that the student must attend. Also, they will have the opportunity to deepen into any multivariate method. In total, attending the whole school, one student can obtain **12 ECTS credits**.

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Timetable, topics and lecturers:

The timetable and topics for CSC-2018 are:

May						
Monday	Tuesday	Wednesday	Thursday	Friday	SAT	SUN
	1*	2	3	4	5	6
7 Chemom/LinMod	8 LinMod	9 LinMod/Free	10 LinAl	11 LinAl	12	13
14 Explore	15 Explore	16 Regress	17 Regress	18 DoE	19	20
21* DoE	22 DoE	23 Class	24 Class	25 Class	26	27
28 VarSel	29 VarSel	30 MCR	31 MCR			

June						
Monday	Tuesday	Wednesday	Thursday	Friday	SAT	SUN
				1 OwnData	2	3
4 HYPER	5 HYPER	6 HYPER	7 HYPER	8 Glue	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	

All seminars run from 9 a.m. to 5 p.m. with a lunch break. Organization of the breaks and the final timetable for each seminar will be under the responsibility of the corresponding teacher/lecturer.

Seminars, lecturers and ECTS points:

	Acronym	Name	Teacher	ECTS
1	**Chemom**	What's Chemometrics	Tormod Næs	0.5
2	**LinMod**	Linear Models	A. Smilde/F. Marini	1
3	**LinAl**	Lineal Algebra	Morten A. Rasmussen	1
4	**Explore**	Multivariate exploration	rasmus Bro	1
5	**Regress**	Multivariate regression	José Manuel Amigo	1
6	**DoE**	Design of Experiments	Riccardo Leardi	1.5
7	**Class**	Linear Classification	Davide Ballabio	1.5
8	**VarSel**	Variable selection methods	Åsmund Rinnan	1
9	**MCR**	Multivariate Curve resolution	Anna de Juan	1
10	**OwnData**	Analysis of your Own Data	J.M. Amigo/A. De Juan	0
11	**HYPER**	Hyperspectral Image Analysis	José Manuel Amigo	2
12	**GLUE**	How not to make chemometrics	R. Bro/J.M. Amigo	0.5

For PhD students:

Each seminar accounts for **0.5, 1, 1.5 or 2 ECTS** (see previous list). All PhD students who want to obtain the corresponding ECTS credits from the seminars will be obliged:

1) To attend the corresponding seminars.

2) To deliver the corresponding reports (see below). The length, content and the final delivering date of the reports will be **specified by the corresponding lecturer**.

Optional "Introduction to Matlab for Multivariate Data Analysis" course offered:

Matlab is one of the main software packages that will be used in the **CSC-2018**. Therefore, attending some suggestions from the students of previous editions, we have decided to merge our PhD course "Introduction to Matlab for Multivariate Data Analysis" with **CSC-2018**.

"Introduction to Matlab for Multivariate Data Analysis" will be held from **April 23rd to May 3rd 2018**, and the students will be able to obtain 3 ECTS credits. This PhD course is totally independent from the **CSC–2018** course.

If any student of the **CSC–2018** is interested in attending the "Introduction to Matlab for Multivariate Data Analysis" course, please, join at:

https://phdcourses.ku.dk/DetailKursus.aspx?id=103960&sitepath=NAT

For further information, write to José Manuel Amigo (jmar@life.ku.dk – jmar@food.ku.dk).

Detailed description for each seminar of CSC-2018:

1.- Chemom. What's Chemometrics?

This seminar will serve as opening seminar to shed light into several general questions about Chemometrics: What is Chemometrics? And what is the difference between chemometrics and statistics? The seminar will last for 3 hours and it will officially open the CSC-2018.

Previous knowledge needed: None.
Software: None.
Dates: 7th May. Morning.
Teacher: Prof. Tormod Næs
ECTS: 0.5

2. LinMod. Linear Models

Linear models are at the basis of many methods in statistics and chemometrics. We will give an introduction to the theory and application of these models along the following lines:
i) Introduction to the theory of linear models, ii) factorial designs: fixed vs random effects; crossed, nested, replicated measurements and mixed designs, iii) fixed effect models, iv) mixed-effect models, v) extensions to multivariate data, specifically, MANOVA. The models will be illustrated with real-life examples and exercises.

Previous knowledge needed: None.
Software: Matlab.
Dates: 7th May. Afternoon, 8th May, 9th May morning.
Teacher: Prof. Age Smilde and Dr. Federico Marini
ECTS: 1

3.- LinAl. Linear Algebra for Multivariate Data Analysis

Linear Algebra is the basis of the Multivariate Data Analysis. Therefore, it is important to give it a central position in any school about multivariate data analysis. This seminar will be a clear introduction to the linear algebra behind the multivariate models that will be presented in the school.

Previous knowledge needed: None.
Software: Matlab.
Dates: 10th and 11th May
Teacher: Dr. Morten A. Rasmussen
ECTS: 1

4.- Explore. Multivariate data exploration.

Principal Component Analysis has become the most powerful and versatile tool for exploring data tables in Analytical Sciences. Here we present a course to show the main benefits and drawbacks of PCA when it is used for different kind of analytical data: Spectroscopy, environmental assessment, sensory, experiments performance, chromatography, etc. Moreover, preprocessing of different type of data will be also addressed in the seminar as a prerequisite for having the optimal possibility for exploring the data.

Previous knowledge needed: None.
Software: Matlab and/or PLS-Toolbox. A full demo available at: http://www.eigenvector.com/
Dates: 14th and 15th May
Teacher: Prof. Rasmus Bro
ECTS: 1

5.- Regress. Multivariate Regression

If PCA is the keystone of pattern recognition methods, PLS is the keystone of multivariate calibration methods. This seminar will give a general overview of different multivariate calibration strategies and will focus in Partial Least Squares regression.

Previous knowledge needed: Basic knowledge of PCA and linear algebra.
Software: Matlab and PLS-Toolbox. A full demo available at: http://www.eigenvector.com/
Dates: 16th and 17th May
Teacher: Dr. José Manuel Amigo
ECTS: 1

6.- DoE. Introduction to Design of Experiments

DoE. Design of Experiments (Riccardo) The basic theory and practice of Design of Experiments is revisited. The aim is to give a practitioner idea or reminder about the main features and uses of DoE. Several real examples in very different fields will be shown. The seminar will be based on teaching hours and some guided exercises.

Previous knowledge needed: Very basic statistics.
Software: Free R-based software: http://gruppochemiometria.it/gruppo-lavoro-r-in-chemiometria.html
Dates: 18th, 21st and 22nd May
Teacher: Prof. Riccardo Leardi
ECTS: 1.5
NOTE: 21st is Holyday

7. CLASS. Linear Classification

The seminar is focused on the theory and practice of two linear classification tools (SIMCA and PLS-DA). The seminar will be based on teaching hours with guided exercises and practical sessions with real cases.

Previous knowledge needed: Basic knowledge of PCA.
Software: Matlab and free Classification Toolbox: http://michem.disat.unimib.it/chm/download/classificationinfo.htm
Dates: 23rd, 24th and 25th May
Teacher: Dr. Davide Ballabio
ECTS: 1.5

8.- VarSel. Variables selection methods

This seminar aims at revisiting the most important variable selection methods for regression and classification purposes with the aim at improving the performance of the models. The emphasis will be on practical applications, and what methods could be applied to which problem. There will also be hints as to what methods are good, and which ones to stay away from.

Previous knowledge needed: Basic knowledge of multivariate regression methods.
Software: Matlab (plus in-house routines, will be provided).
Dates: 28th and 29th May
Teacher: Dr. Åsmund Rinnan
ECTS: 1

9. MCR. Multivariate Curve Resolution

Curve resolution techniques are gaining importance in modeling of different analytical data types. Especially, Multivariate Curve Resolution has widely demonstrated its usefulness in kinetic modeling, solving problems in chromatographic data (peak resolution/deconvolution) and hyperspectral images. This seminar will offer a general overview of curve resolution methodologies and will focus in multivariate curve resolution applied to different analytical problems.

Previous knowledge needed: Basic knowledge of PCA.
Software: Matlab and free MCR-ALS Toolbox: http://www.mcrals.info/
Dates: 30th and 31st May
Teacher: Prof. Anna de Juan
ECTS: 1

10.- OwnData. Analysis of your own data

For those who bring own data and want to consult different perspectives of analysis of the data, CSC-2018 offers the opportunity of showing the data and have a "consultancy" about what is best to achieve good results. Bring your own data and we can have a look together!

Previous knowledge needed: None
Software: Is up to you! We know some of them!
Dates: 1st June
Teacher: Dr. José Manuel Amigo and Prof. Anna de Juan
ECTS: 0

11.- HYPER. Hyperspectral Image Analysis

Multivariate or Hyperspecral imaging techniques are gaining in popularity due to their high information content. Images are now acquired using a wide variety of spectroscopic techniques (e.g., infra-red, mass spectroscopy, Raman, etc.) and the course will cover a variety of multivariate methodologies that can be applied to analysis and interpretation of hyperspectral data. This will start by examining how images are represented in the MATLAB environment to target detection techniques used to find analytes of interest within an image. The course content will be useful for those involved in chemical, food, pharmaceutical and medical imaging, remote and standoff imaging.

Previous knowledge needed: Basic knowledge of Chemometrics
Software: Matlab will be used for demonstrations. Software and data will be provided.
Dates: 4th, 5th, 6th, 7th June
Teacher: Dr. José Manuel Amigo
ECTS: 2

12.- GLUE. Or how NOT to make chemometrics

In this course, we will take a very close look at all the most common mistakes that even experienced people will do when doing multivariate analysis. We will cover exploration, calibration, interpretation, visualization and many other subjects. And always with a focus on what is the most common problem as well as a sounder alternative.

Previous knowledge needed: Basic knowledge of Chemometrics
Software: Matlab will be used for demonstrations. Software and data will be provided.
Dates: 8th June
Teacher: Prof. Rasmus Bro
ECTS: 0.5

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Location and subscription:

Location: CSC-2018 will be held by the department of food sciences of the University of Copenhagen, Denmark. The classrooms will be announced soon.

Subscription:
The persons interested in joining the CSC-2018 will have to subscribe at:
https://phdcourses.ku.dk

After accessing to the course catalogue, the student will have to sign up for the seminars. There are two ways:
- If the student wants to make the whole school, please, follow the link to **Copenhagen School of Chemometrics - the complete course (12 ECTS)**
- If, on the contrary, the student wants to join specific seminars, follow the links to each individual seminar.
- There is no need to register for the seminar **10.- OwnData. Analysis of your own data**

For further information, just send an e-mail to Dr. José Manuel Amigo (jmar@food.ku.dk / jmar@life.ku.dk).

Note: Please, send us an e-mail after registration (jmar@life.ku.dk / jmar@food.ku.dk)

The complete course:
https://phdcourses.ku.dk/DetailKursus.aspx?id=103964&sitepath=NAT

1.- Chemom. What's Chemometrics?
https://phdcourses.ku.dk/DetailKursus.aspx?id=103965&sitepath=NAT
2. LinMod. Linear Models
https://phdcourses.ku.dk/DetailKursus.aspx?id=103966&sitepath=NAT
3.- LinAl. Linear Algebra for Multivariate Data Analysis
https://phdcourses.ku.dk/DetailKursus.aspx?id=103967&sitepath=NAT
4.- Explore. Multivariate data exploration.
https://phdcourses.ku.dk/DetailKursus.aspx?id=103968&sitepath=NAT
5.- Regress. Multivariate Regression
https://phdcourses.ku.dk/DetailKursus.aspx?id=103969&sitepath=NAT
6.- DoE. Introduction to Design of Experiments
https://phdcourses.ku.dk/DetailKursus.aspx?id=103970&sitepath=NAT
7.- CLASS. Linear Classification
https://phdcourses.ku.dk/DetailKursus.aspx?id=103971&sitepath=NAT
8.- VarSel. Variables selection methods
https://phdcourses.ku.dk/DetailKursus.aspx?id=103972&sitepath=NAT
9.- MCR. Multivariate Curve Resolution
https://phdcourses.ku.dk/DetailKursus.aspx?id=103973&sitepath=NAT
10.- OwnData. Analysis of your own data
No subscription needed
11.- HYPER. Hyperspectral Image Analysis
https://phdcourses.ku.dk/DetailKursus.aspx?id=103974&sitepath=NAT
12.- GLUE. Or how NOT to make chemometrics
https://phdcourses.ku.dk/DetailKursus.aspx?id=103975&sitepath=NAT

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Fees:

Academia:
- 700 DKK (aprox. 100 Eur – 110 US$) per seminar.
- 1200 DKK (aprox. 160 Eur – 190 US$) per week (or two seminars).
- 5000 DKK (aprox. 670 Eur – 800 US$) the whole school (5 weeks).

Industry/Companies:
- 1200 DKK (aprox. 160 Eur – 190 US$) per seminar.
- 5000 DKK (aprox. 670 Eur – 800 US$) per week (or two seminars).

There will be a fee of 3000 Danish Krone for not coming when enrolled.
All payments with no exception will be charged in Danish Krone (DKK).

Best poster award:

In order to encourage communication between students and with the teachers, the students will be able to bring a poster and present his/her work in a flash presentation in the corresponding seminar. Students are invited to bring the poster no matter which seminars they are attending.

The poster can also be a poster presented in another conference.

The poster size should be A1 (594 x 841 mm).

Once the posters are evaluated, the last day of CSC-2018 the winner of the "best poster award" will be announced and the price given. **The price will consist of a diploma and the return of the CSC-2018 fees.**

Important information:

- Read careful the description for each seminar and the needs regarding software. Unless strictly needed, we will **NOT** provide with laptops or software packages. Therefore, bring your own laptops with the required software already installed.

- We will provide with office material (notebooks, folders, USB, pens, etc.)

- There will be **free WI-FI internet** connection.

- We can issue parking permission. But communicate in advance.

- We can issue letters of participation. But communicate in advance.

- **Lunch is not included.** Nevertheless, there will be free coffee and refreshment for the coffee breaks.