



World-class Teaching...

... in a World-class Environment

BILBAO, 8 October – 30 October, 2020

COPENHAGEN, 2 November – 20 November, 2020

International School of Chemometrics - ISC



ISC – 2020

INTERNATIONAL SCHOOL OF CHEMOMETRICS

October 8th – November 20th, 2020

Main responsible: José Manuel Amigo

Co-organizers: Rasmus Bro and Nestor Etxebarria



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Description of the course:

The **Research and Analytical Innovation (IBeA)** - <https://www.ehu.eus/es/web/ibea/home>) and the **Chemometrics Analytical Technologies (CAT)** – www.models.life.ku.dk) groups are more than happy to announce the brand new edition of the School of Chemometrics, now named:

International School of Chemometrics - ISC

ISC-2020 is a six-week school designed to be an introduction to different key aspects of advanced data analysis in different brands of science (chemistry, food & feed, physics, environmental, political economics, etc). **ISC-2020** addresses to BSc, MSc, PhD students/post-docs, associate professors, etc. who want to acquire or refresh basic knowledge on multivariate data analysis from different disciplines. **ISC-2020** is also addressed to researchers working in industry or research laboratories wanting to implement multivariate data analysis in their daily research environment.

ISC-2020 is an intensive school. **ISC-2020** is held in six consecutive weeks structured in different seminars/modules where the students will be more than welcome to work with their own data together with high-qualified teachers. Moreover, anyone can choose which seminars to participate in. There is no minimum of seminars requested for participating.

Targets of ISC-2020:

ISC-2020 aims at being a platform for:

- **Learning basic and advanced data analysis methods:** **ISC-2020** 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 **ISC-2020** is the interaction between the students discussing 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:** **ISC-2020** 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 dive into any multivariate method. In total, attending the whole school, one student can obtain up to **14 ECTS credits**.



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Timetable, topics and lecturers:

The timetable and topics for ISC-2020 are:

October						
			1	2	3	4
5	6	7	8	9	10	11
			Matlab	Matlab		
12	13	14	15	16	17	18
Matlab	Matlab	Matlab	Matlab	Matlab		
19	20	21	22	23	24	25
Basic	Basic	Basic	Basic	Basic		
26	27	28	29	30	31	
Intermediate	Intermediate	Intermediate	Intermediate	Intermediate		

November						
						1
2	3	4	5	6	7	8
Error	Error	Error	Multiblock	Multiblock		
9	10	11	12	13	14	15
Sparse	Sparse	Nonlin	Nonlin	GLUE		
16	17	18	19	20	21	22
Special	Special	Special	Special	Special		
23	24	25	26	27	28	29

All seminars run from 9 a.m. to 5 p.m. with one hour for lunch. 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:

Dates	Topic	Title	ECTS	Teacher	Place
8 - 16 Oct	Matlab:	Introduction to Matlab for Multivariate Data Analysis	3	José Manuel Amigo	BIO
19 - 21 Oct	Basics.Chem:	Exploratory (PCA), preprocessing, Multivariate Regression	1.5	José Manuel Amigo	BIO
22 - 23 Oct	Basics.DoE:	Design of Experiments	1	Nestor Etxebarria	BIO
26 - Oct	Int.VarSel:	Variable selection	0.5	José Manuel Amigo	BIO
27 - 28 Oct	Int.Class:	Multivariate Classification	1	Davide Ballabio	BIO
29 - 30 Oct	Int.MCR:	Multivariate Curve Resolution	1	Anna de Juan	BIO
2 - 4 Nov	Chall.Error:	Multivariate Error	1	Ricard Boqué	CPH
5 - 6 Nov	Chall.Multiblock:	Multiblock analysis	1	Federico Marini	CPH
9 - 10 Nov	Chall.Sparse:	Sparse Modelling	1	Morten A. Rasmusen	CPH
11 - 12 Nov	Chall.Nonlin:	Non-linear modelling	1	Rasmus Bro	CPH
13 - Nov	Chall.GLUE:	How not to make chemometrics	0	José Manuel Amigo	CPH
16 - 20 Nov	Spe.Multiway:	Multiway data analysis	2	Rasmus Bro	CPH
16 - 20 Nov	Spe.Hyperspectral:	Hyperspectral Image Analysis	2	José Manuel Amigo	CPH

NOTE: The modules BASICS and INTERMEDIATE are indivisible entities. That is, the student joining BASICS will attend the Chem and DoE (total of 2.5 ECTS). At the same time, the student attending the INTERMEDIATE will attend MCR, VarSel and Class (total of 2.5 ECTS).



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For PhD students:

Each module accounts for a specific amount of ECTS credits associated (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. The length, content and the final delivering date of the reports will be **specified by the corresponding lecturer**.

IMPORTANT NOTE FOR LIVE STREAMING STUDENTS: Due to the Covid-19 pandemic situation, we open the possibility of attending the School with a live streaming platform. The students will have access to:

- All the material.
- All the lessons.
- Chat with teachers.

Nevertheless, there will NOT be ECTS granted by any circumstance to live streaming students.



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Brief description for each seminar of ISC-2020:

01.- Matlab:

Matlab is one of the main software packages that will be used in the **ISC-2020**. 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 **ISC-2020**. This course will show the basis of the software Matlab in order to be able to deal with data analysis.

Previous knowledge needed: None

Software: Matlab.

Teacher: Dr. José Manuel Amigo

ECTS: 3

02.- BASICS

This seminar contains 2 topics:

- Basic chemometrics

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. 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.

- Introduction to Design of Experiments

DoE. Design of Experiments 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: None

Software: TBA

Teacher: Dr. José Manuel Amigo (basic chemometrics) and Nestor Etxebarria (Design of Experiments)

ECTS: 2.5

0.3.- Intermediate Chemometrics

This seminar contains three topics:

- 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.

- Variable 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.



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- Linear classification

The seminar is focused on the theory and practice of 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 and multivariate regression methods.

Software: TBA

Teachers: Prof. Anna de Juan (MCR), Prof. José Manuel Amigo (VarSel) and Dr. Davide Ballabio (Class)

ECTS: 2.5

0.4.- Challenges. Multiblock

The multi-block seminar will focus on methods and applications where one is interested in analyzing relations between more than two data sets/blocks. Main emphasis will be given to applications in spectroscopy and sensory science. Some of the most well know methods in the area will be presented and discussed. Both regression situations and situations where all blocks are handled without a predictive direction will be covered. Most methods covered will be extensions of PLS and PCA based methodology. Validation and interpretation will also be covered.

Previous knowledge needed: Knowledge of PCA and multivariate regression methods.

Software: TBA

Teachers: Prof. Federico Marini

ECTS: 1

05.- Challenges. Nonlinear

This module aims at providing a basic introduction to the techniques which may be used in all those situations when a linear relation is not enough to provide accurate results (e.g. due to the presence of multiple sources of variability). In this respect, the most important aspects of data modeling will be considered (exploratory analysis, classification and calibration). Topics such as kernel and dissimilarity-based approaches (including support vector machines), local modeling (kNN and locally weighted regression/classification) and artificial neural networks will be covered.

Previous knowledge needed: Knowledge of PCA and PLS

Software: TBA

Teacher: Prof. Rasmus Bro

ECTS: 1

06.- Challenges. Sparse

Data analytical problems are becoming more and more complex, with more challenging questions and with data of increasing complexity for unraveling of these questions. Ordinary data analysis tools, such as e.g. principal component analysis, will typically lead to a huge number of variables influencing the model significantly. Hence it is difficult to assess which variables are most important for further investigation. One approach to reduce complexity is by forcing less influential variables to have zero influence on the model. This can be achieved by modifying e.g. a regression model such that rather than finding a regression vector that only provides good predictions, a well-predicting regression vector is sought that is also *sparse* (has many zero regression coefficients). This seminar will show how sparse techniques can, when correctly applied, reduce the complexity of datasets.

Previous knowledge needed: Knowledge of PCA and PLS

Software: TBA

Teacher: Dr. Morten A. Rasmussen

ECTS: 1



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07.- Challenges. Multivariate Error

Multivariate measurements are a combination of both the true signal and measurement errors, but the role of the latter is often ignored in the multitude of data analysis methods designed to extract information from chemical data. This course will define the most common sources of multivariate measurement errors and will expose different ways to deal with.

Previous knowledge needed: Knowledge of PCA and PLS

Software: TBA

Teacher: Prof. Ricard Boqué

ECTS: 1

08.- Challenges. GLUE or How *not* to make chemometrics

In this half day seminar 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: TBA

Teacher: Prof. José Manuel Amigo

ECTS: 0

09.- SPECIAL

Here you can choose between either multi-way analysis with Rasmus Bro or hyperspectral imaging with José Manuel Amigo. Both courses run for three days and will give 2 ECTS points.

- Hyperspectral Image Analysis

In this seminar we will study the different types of hyperspectral and multispectral images and their analysis. Concepts like pattern recognition, endmembers, spectral unmixing/curve resolution and classification will be revisited and applied in the framework of hyperspectral and multispectral imaging.

Previous knowledge needed: Basic knowledge of Chemometrics

Software: Matlab and HYPER-Tools (freely downloadable from www.hypertools.org)

Teacher: Prof. José Manuel Amigo

ECTS: 2

- Multi-way analysis

Multi-way data is gaining popularity due to the capability of scientific devices to generate data with, at least, 3 dimensions (elution time – m/z channel – samples, excitation – emission – sample, etc). Therefore, learning the basics of multi-way analysis will help extracting the most of that complex data structure. In this sense, methods like parallel factor analysis (PARAFAC) and PARAFAC2 will be studied and applied to different examples.

Previous knowledge needed: Basic knowledge of Chemometrics

Software: Matlab and PLS_Toolbox

Teacher: Prof. Rasmus Bro

ECTS: 2



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Location and subscription:

- Location:

ISC-2020 will be held by two research groups:

- **Research and Analytical Innovation (IBeA** - <https://www.ehu.es/es/web/ibea/home>)
- **Chemometrics Analytical Technologies (CAT** – www.models.life.ku.dk)

Therefore, the ISC – 2020 will be held in two cities: Bilbao (BIO), Spain and Copenhagen (CPH), Denmark. Check the previous table to see the **place**:

- **Bilbao (BIO):** Research Centre for Experimental Marine Biology & Biotechnology. Areatza Pasealekua. 48620 Plentzia – Bizkaia. Basque Country (Spain) (<http://www.ehu.es/PIE/>)
- **Copenhagen (CPH):** Department of Food Science. University of Copenhagen. Rolighedsvej 26, DK-1958 Frederiksberg (Denmark) (<https://food.ku.dk/english/>)

- Subscription:

The persons interested in joining the ISC-2020 will have to send an e-mail to José Manuel Amigo (josemanuel.amigo@ehu.es)

The information to provide is:

- Full name
- Institution
- Which seminars/modules to attend

Fees:

- Bilbao part (BIO):

- Academia 100 euros per ECTS
- Industry 300 euros per ECTS

- Copenhagen part (CPH):

- Academia 800 DKK per ECTS
- Industry 2000 DKK per ECTS

- Live streaming:

- Unique price of 2000 DKK for all School.



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Important information:

- Read carefully the description for each seminar and the needs regarding software. We will *not* provide laptops or software packages. Therefore, bring your own laptops with the required software already installed. We will provide you with directions on how to obtain the needed software for each course.
- We will provide office material (notebooks, folders, USB, pens, etc.)
- There will be free WI-FI internet connection.
- We can issue letters of participation as a PDF.
- **Lunch is not included.** Nevertheless, there will be free coffee and refreshment for the coffee breaks.