



Course Chemometrics in Excel

Monday, October 18, 2010, Antwerp, Belgium, Conference CAC-2010



The aim of the course is to provide the participants with simple and powerful tool for basic multivariate analysis. The core functions for projection methods are presented as worksheet functions in Excel, a most widely spread data handling environment. All calculations are carried out in Excel books, and all regular Excel capacities can be applied for additional calculations: charts, data export and import, templates, etc. During the course, attendees will have a wide opportunity for the hands-on data analysis. The course consists of two blocks: part 1 – Introduction, and part 2 - Advanced

Audience: (postgraduate) students, specialists, scientists with a basic knowledge in chemometrics and Excel

Language: English

Instructors: DSc. [Alexey Pomerantsev](#) (ICP RAS, Moscow)
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Course materials:

- Matrix calculations in Excel ([web tutorial](#))
- Projection methods in Excel ([web tutorial](#))
- Useful Formulae for Chemometrics Add-In ([web tutorial](#))
- Supplementary xls-files ([ZIP archive](#))
- Chemometrics Add-In software ([ZIP archive](#))

will be available for the participants since Sep. 15, 2010. To refresh the Excel skills it is highly recommended to read the tutorials and to look through the exercises.

Course Outline:

Part 1, Introduction 9h00 - 13h00 deals with:

- Matrix calculations in Excel
- Computer exercises: basic calculation, regression, plots, etc

Part 2 Advanced 14h00 - 18h00 deals with:

- Projection methods: PCA, PLS
- Main features of *Chemometrics.Add-In*
- Computer exercises: data analysis, multivariate calibration

Chemometrics Add-In is specially designed software for Microsoft Excel. The package consists of two files Chemometrics.dll and Chemometrics.xla. The main projection functions can be applied as ordinary user-defined functions in Excel

The core functions for the PCA/PLS decompositions are designed to ensure very fast calculations even for the rather large data sets (200 samples by 4500 variables). They are programmed in C++ language and linked to Excel via DLL.

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1							
2							
3							
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7							
8							
9							
10							

Window Factor Analysis			
Component A			
Rows omitted from top		15	
	P _a	t _z	
220	=LoadingsPCA(OFFSET(Xdata,\$F\$3,0,-\$F\$3))		
225	0.223	2	0.091
230	0.170	3	0.522
235	0.149	4	1.000
240	0.182	5	1.131
245	0.213	6	1.018

***Full individual license for Chemometrics Add-In software
will be provided for all registered attendees.***

Participants are encouraged to use their **own laptops** with Excel 2007 and Chemometrics Add-In installed.

Registration via [conference site](#)

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