CHEMOMETRICAL APPROACHES IN ENVIRONMENTAL AND HUMAN HEALTH RISK ASSESSMENT STUDIES

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Horarium: 30 academic hours (15 hours lectures + 15 hours seminars)

Visiting period: January 13 – January 31, 2020

Abstract:

The goal of the course is to deepen participants' knowledge in statistical concepts used in risk assessment studies. The course will start with introduction of risk assessment concept and its relevance to the decision making and regulation management. In the second part of the course, risk assessment data analysis will be presented by the basic (univariate) statistics and multivariate statistics approaches. In the third part the most widely used chemometrical methods like Cluster analysis, Principal component analysis, Partial least squares and some more advanced methods will be introduced. The use of a variety of risk assessment data sets and software packages during seminars will provide the students basic practical skills in uni- and multivariate risk data analysis.

At the end of the course, each participant will be able to:

- apply basic concept in chemical risk assessment;
- apply Cluster analysis, Principal component analysis, Partial least squares on new data and analyse the results;
- compare and contrast the methods for a given risk assessment study considering methods' benefits and pitfalls;
- interpret risk assessment studies described in scientific literature and perform his/her own studies.

Lecture modules:

1. Risk analysis and Risk assessment: approaches, experiences and metrics.
2. Multivariate data analysis: Cluster analysis, Principal component analysis, Partial least squares (modelling and discrimination). Introduction to Self organizing maps and Hasse diagram techniques.
3. Selection and application of appropriate chemometrical approaches for particular risk assessment study.

Seminar key topics:

1. Data quality and evaluation of experimental factors: risk quotient, parametric and non-parametric (robust) statistical tests, ANOVA.
2. Multivariate data analysis: data arrangement, pretreatment, transformation, handling of missing data.
3. Clusters analysis. Similarity measures. Agglomerative hierarchical algorithms.

4. Principal component analysis (PCA). Loading plots. Score plots. Choice of principal components (rank analysis), both numerically and graphically (scree plot). Data exploration.
5. Partial least squares (PLS). Loadings, weights and score plots. Importance of "original" variables. Evaluation parameters for a regression model.
6. Classification applications based on PLS: PLS- discriminant analysis (PLS-DA).
7. Advanced chemometrical methods: Self organizing maps, Hasse diagram techniques - principles and available software packages.

Consultations (30 hours):

Prof. Tsakovski will be available for consultation and discussion about the material presented during the lectures and key topics covered in the seminars. Consultation concerning proper selection of chemometrical treatment of participants' data sets will be available.

Termin	Dzień tygodnia	Godzina	Miejsce
~~13.01.2020~~	~~Poniedziałek~~	~~12.15 – 15.00~~	~~Minicentrum Konferencyjne WCH~~
14.01.2020	Wtorek	12.15 – 15.00	Minicentrum Konferencyjne WCH
15.01.2020	Środa	12.15 – 15.00	Minicentrum Konferencyjne WCH
16.01.2020	Czwartek	12.15 – 15.00	Minicentrum Konferencyjne WCH
17.01.2020	Piątek	13.15 – 16.00	Minicentrum Konferencyjne WCH
20.01.2020	Poniedziałek	12.15 – 15.00	Minicentrum Konferencyjne WCH
21.01.2020	Wtorek	12.15 – 15.00	Minicentrum Konferencyjne WCH
22.01.2020	Środa	12.15 – 15.00	Minicentrum Konferencyjne WCH
23.01.2020	Czwartek	12.15 – 15.00	Minicentrum Konferencyjne WCH
24.01.2020	Piątek	13.15 – 16.00	Minicentrum Konferencyjne WCH
27.01.2020	Poniedziałek	9.15 – 12.00	Minicentrum Konferencyjne WCH