

KEMOMETRIJA

UČNI NAČRT PREDMETA/COURSE SYLLABUS

Predmet:	Kemometrija
Course title:	Chemometrics
Članica nosilka/UL Member:	UL FKKT

Študijski programi in stopnja	Študijska smer	Letnik	Semestri	Izbirnost
Kemija, druga stopnja, magistrski	Ni členitve (študijski program)	1. letnik, 2. letnik		izbirni

Univerzitetna koda predmeta/University course code:	0072217
Koda učne enote na članici/UL Member course code:	K2I11S

Predavanja /Lectures	Seminar /Seminar	Vaje /Tutorials	Klinične vaje /Clinical tutorials	Druge oblike študija /Other forms of study	Samostojno delo /Individual student work	ECTS
45	15	15 SV			75	5

Nosilec predmeta/Lecturer:	prof. dr. Matevž Pompe
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Vrsta predmeta/Course type:	izbirni strokovni/Elective Professional
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Jeziki/Languages:	Predavanja/Lectures:	Angleščina, Slovenščina
	Vaje/Tutorial:	Angleščina, Slovenščina

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	Prerequisites:
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	The course has to be assigned to the student.

Vsebina:	Content (Syllabus outline):
Definicija merskega prostora (skalarji, vektorji, razdalje) Predstavili bomo definicije merskega prostora ter opisov populacije ter vzorca. Osnove napovedne statistike Študenti se bodo spoznali z osnovnimi porazdelitvami, ki jih srečamo pri statističnih testih. Prav tako bodo dobili vpogled v predpostavke na katerih temeljijo obravnavani test. Detekcija izvenležečih točk. Kalibracijska premica, meja zaznavnosti Obravnavali bomo kalibracijsko premico na primeru enakih ali neenakih varianc v merskem prostoru. Poudarek bo na kasnejšem testiranju modela ter izračunu merske negotovosti ob upoštevanju enačbe premice.	Definition of the measurement space (scalar , vector , distance) We will present the definition of the measurement area and descriptions of the population and the sample. Basics of predictive statistics Students will learn the basic distributions encountered in statistical tests. They will also get an insight into the assumptions underlying the present test. Detection of outliers. The calibration line , the limit of detection The procedure to obtain calibration line will be explained in the case of equal or unequal variances in metric space. The focus will be on model validation and measurement uncertainty calculation taking into account the calibration line equation.

Izdelava modelov (linearni, nelinearni) V okviru tega poglavja bodo študenti spoznali osnove večkratne linearne regresije, PLS, PCR kot primeri linearne regresije, med nelinearnimi tehnikami pa bomo predstavili različne umetne nevronske mreže. Transformacije merskega prostora Predstavili bomo nekatere pogoste transformacije merskega prostora (npr. PCA,...), ki jih uporabljamo za boljšo predstavitev več dimenzionalnih merskih prostorov. Optimizacija (genetski algoritem) ter eksperimentalni načrt Študenti bodo spoznali oba navedena postopka optimizacije v večdimenzionalnem merskem sistemu, kot tudi postopke večnivojskega načrtovanja eksperimentov z namenov zmanjšanja potrebnega števila meritev. Grupiranje Predstavili bomo enostavne postopke grupiranja podatkov v večdimenzionalnem merskem prostoru, kot tudi uporabo umetnih nevronske mreže v te namene. Vrednotenje modelov Spoznali bomo osnovne postopke za delitev podatkov v več setov potrebnih za učenje in testiranje modela. Prav tako bomo obravnavali metode, ki jih uporabljamo pri testiranju različnih modelov. Matematične reprezentacije kemijskih struktur Spoznali bomo nekatere enostavne reprezentacije kemijskih struktur, ki jih lahko uporabljamo pri modeliranju povezav med kemijsko strukturo in lastnostmi molekul (QSAR, QSPR). Osnove topoloških indeksov- Razlike med različnimi tipi QSAR modelov Modeli za odkrivanje novih zdravil, modeli za regulativo novih zdravil, modeli za regulativo	Modeling (linear and nonlinear) In this chapter, students will learn the basics of multiple linear regression , PLS, PCR as examples of the linear regression. As example of the non-linear techniques various artificial neural networks will be presented. Transformation of the measurement space Some common measurement space transformation will be presented (eg PCA , ...), which are used to enable the graphical presentation of the multi-dimensional metric spaces . 6 Filtering of noise Students will learn simple procedures for noise filtrations in the experimental measurements. Optimization (genetic algorithm) and experimental design Students will learn about both procedures for optimization in multi-dimensional measurement system. They will gain knowledge on multi-level experimental design in order to reduce the number of required experiments. Clustering We will present a simple procedure for clustering of data in a multidimensional space of measurements, as well as the use of artificial neural networks for the same purpose. Model validation We will learn the basic procedures for dividing data in different sets needed for model validation (learning and testing set). We will also discuss the methods used in various model validation. Mathematical representation of chemical structures Some simple representations of chemical structures that can be used in modeling the relationship between chemical structure and properties of molecules (QSAR , QSPR) will be discussed. Basic concepts of topological indices. Differences between various types of QSAR models. Models used for drug discovery, models for regulatory purposes
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Temeljna literatura in viri/Readings:

- D.L. Massart, B.G.M. Vandeginste, L.C.C. Buydens, S. De Yong, P.J.Lewi, J. Smeyers-Verbeke: handbook of Chemometrics and Qualimetrics, Elsevier, 2003 (700 strani, 30%).

Dodatno

ZUPAN, Jure. Kemometrija in obdelava eksperimentalnih podatkov. Ljubljana: Kemijski inštitut: Inštitut Nove revije, Zavod za humanistiko, 2009. 368 str., ilustr. ISBN 978-961-92463-3-7.

Cilji in kompetence:

Cilji: a) Seznaniti študente s teorijo in uporabo kemometričnih metod za:

- Pripravo eksperimentov
- Predobdelavo merskih podatkov
- Vrednotenje podatkov in rezultatov dobljenih pri eksperimentih z večjim številom spremenljivk

Objectives and competences:

Objectives

- a) To acquaint students with the theory and applications of chemometric procedures for:
- Preparation of experiments
 - Pretreatment of experimental data

b) Podati osnove modeliranja, iskanja inverznih modelov ter vrednotenja statistične zanesljivosti dobljenih modelov. c) Omogočiti študentom neposredni dostop do računalnikov ter ustrezne programske opreme za izvedbo naštetih testov. <i>Kompetence:</i> Študent bo usposobljen kritično ovrednotiti eksperimentalne podatke, poiskati vzorce v večdimenzionalnih merskih prostorih ter izdelati nekatere enostavne modele, ki povezujejo merski prostor z določeno lastnostjo opazovanega sistema.	• Evaluation of data and results obtained from experiments with a large number of variables b) Provide the basics of modeling, search for inverse models and the statistical evaluation of the obtained models. c) To allow students direct access to computers and relevant software for carrying out the above tests. Competences Student will be able to critically evaluate experimental data to find patterns in multi-dimensional metric spaces, and create some simple models to use measurement space in order to explain some characteristics of the observed system.
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Predvideni študijski rezultati:

Znanje in razumevanje
Študent se bo naučil kritično uporabljati kemometrične metode. Razumeti bo moral njihovo delovanje. Pri predmetu bo spoznal njihove bistvene prednosti ter omejitve.

Uporaba
Znanja bodo uporabljena v analiznih laboratorijih za zagotavljanje kakovosti rezultatov. Prav tako se bodo znanja uporabljala pri raziskavah v okolju ter analizi živil za razpoznavanje vzorcev ter izdelavi napovednih modelov.

Refleksija
Študent bo sposoben samostojno obdelovati eksperimentalne podatke v večdimenzionalnem vektorskem prostoru, v njih poiskati skrite vzorce ter izdelati in validirati enostavne linearne modele.

Prenosljive spretnosti
Študenti se naučijo kritično podajati in interpretirati eksperimentalne rezultate in izdelati ter validirati enostavne modele.

Intended learning outcomes:

Knowledge and Comprehension
The students will learn to critically apply chemometric methods. They will understand their operation as well as their main advantages and limitations.

Application
Knowledge will be used in analytical laboratories to ensure the quality of the results. The obtained knowledge will be used in the environmental and food research for pattern recognition and the creation of predictive models.

Analysis
Students will be able to independently process the experimental data in multi-dimensional vector space and find the hidden patterns and to establish and validate a simple linear models.

Skill-transference Ability
Students learn to critically present and interpret experimental results and to create and validate simple models.

Metode poučevanja in učenja:

Predavanja s seminarji.

Learning and teaching methods:

Lectures and seminar work.

Načini ocenjevanja:

Pisni in ustni izpit. ocene od 6-10 (pozitivno) oz. 1-5 (negativno).

Delež/Weight

Assessment:

Written and oral exam Grades: positive 6-10; negative 1-5.

Reference nosilca/Lecturer's references:

1. **POMPE, Matevž**, DAVIS, Joe M., SAMUEL, Clint D. Prediction of thermodynamic parameters in gas chromatography from molecular structure : hydrocarbons. *J. chem. inf. comput. sci.*, 2004, vol. 44, no. 2, str. 399-409.
2. **POMPE, Matevž**. Variable connectivity index as a tool for solving the 'anti-connectivity' problem. *Chem. Phys. Lett.* [Print ed.], 2005, vol. 404, no. 4/6, str. 296-299.
3. KOLAR, Jana, ŠTOLFA, Andrej, STRLIČ, Matija, **POMPE, Matevž**, PIHLAR, Boris, BUDNAR, Miloš, SIMČIČ, Jurij, REISSLAND, Birgit. Historical iron gall ink containing documents - properties affecting their condition. *Anal. chim. acta*. [Print ed.], 2006, vol. 555, str. 167-174.