




WSC-2021 Program




3rd Winter School of Chemometrics

31 January - 3 February 2021

Department of Chemistry, Sharif University of
Technology, Tehran, Iran

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Sunday 31 January (Theory)

Time	Title	Presenter
8:30-9:00	Opening	---
9:00-9:50	Introduction to multivariate analysis	H. Abdollahi
9:50-10:35	Univariate linear regression	A. Naseri
10:35-10:45	Break ☕	---
10:45-11:45	Principal component analysis (PCA)	D. Kirsanov
11:45-12:30	Multiple linear regression (MLR)	A. Naseri
12:30-14:00	Lunch 🍱	---
14:00-15:00	Preprocessing methods	H. Parastar
15:00-16:00	Multivariate calibration, inverse least squares (ILS), principal component regression (PCR) (1)	A. Olivieri
16:00-16:15	Break 🍰	---
16:15-17:15	Classical least squares (CLS)	H. Abdollahi
17:15-18:15	Principal component regression (PCR) (2) and partial least squares (PLS)	A. Olivieri

Monday 1 February (Theory)

Time	Title	Presenter
8:30-9:30	Quantitative structure-property relationship (QSPR) (1)	M. Jalali-Heravi
9:30-10:30	Exploratory data analysis (EDA)	B. Hemmateenejad
10:30-10:45	Break ☕	---
10:45-11:45	Linear/quadratic discriminant analysis (L/QDA)	B. Hemmateenejad
11:45-12:45	Partial least squares-discriminant analysis (PLS-DA)	D. Kirsanov
12:45-14:00	Lunch 🍱	---
14:00-15:00	Soft independent modeling of class analogy (SIMCA)	R. Vitale
15:00-16:00	Model validation	H. Parastar
16:00-16:30	Break 🍱	---
16:30-17:30	Machine learning (1)	P. Harrington
17:30-18:30	Machine learning (2)	P. Harrington

Tuesday 2 February (Theory)

Time	Title	Presenter
8:30-9:30	Quantitative structure-property relationship (QSPR) (2)	M. Jalali-Heravi
9:30-10:30	Multivariate curve resolution (MCR)	H. Abdollahi
10:30-10:45	Break 🍰	---
10:45-11:45	Multivariate curve resolution-alternating least squares (MCR-ALS)	C. Ruckebusch
11:45-12:45	MCR-based second-order calibration (1)	M. Vosough
12:45-14:00	Lunch 🍱	---
14:00-15:00	MCR-based second-order calibration (2)	M. Vosough
15:00-16:00	Analytical figures of merit (AFOMs)	A. Olivieri
16:00-16:30	Break 🍌	---
16:30-17:30	Machine learning (3)	P. Harrington

Wednesday 3 February (Practice)

Time	Title	Presenter
8:30-10:30	Multivariate classification (1)	H. Parastar
10:30-10:45	Break 🍰	---
10:45-13:00	Multivariate classification (2)	M. Vosough
13:00-14:30	Lunch 🍱	---
14:30-16:00	Multivariate calibration (1)	A. Olivieri
16:00-16:15	Break 🍰	---
16:15-18:00	Multivariate calibration (2)	A. Olivieri