

CHIMIOMÉTRIE 2016

Séminaires précongrès - Lundi 18 Janvier

Pre-conference courses - Monday 18 January

Titre du séminaire / Course title

Preprocessing methods for spectral data

Enseignant / Trainer

Tom Fearn, Professor of Applied Statistics, UCL, London. He has 35 years of chemometrics experience with near infrared spectroscopy, and writes the Chemometric Space column in NIR news.

Description / Course details

Before using spectral data to develop regression or classification models it is common to apply a preprocessing step. The aim of this step, in general terms, is to improve the signal to noise ratio in the processed data. The course will review as well as comparing and contrasting some of the common methods of preprocessing, including smoothing, the computation of derivatives, various scatter corrections that aim to remove multiplicative interferences, and an assortment of methods based on orthogonal projections. There will also be some discussion of how to optimize (and how not to over-optimize) choice of preprocessing method. The course will take the form of lectures, delivered in English, with plenty of time for questions. The theory will be described with pictures rather than mathematics wherever possible, and the methods will be illustrated on near infrared spectroscopic data.

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Public / Expected public

This is aimed at those involved in the use of spectral data for qualitative or quantitative purposes.

Prérequis / Specific needs

The course should be accessible without a strong mathematical background. The examples will involve near infrared spectroscopy, so it would help to have a little experience in this area, but this is by no means essential.