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VUB
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UITNODIGING

voor de openbare verdediging van het doctoraatsproefschrift van

Ling JIN

26 September 2005

U wordt vriendelijk uitgenodigd op de openbare verdediging van het proefschrift van

Ling JIN

'Simplex local methods for multivariate calibration'

Op 26 September 2005 om 15h
in auditorium Vanden Driessche van de Faculteit Geneeskunde & Farmacie,
Laarbeeklaan 103, 1090 Brussel

Situering van het proefschrift

Calibration is one of the most important steps in chemical analysis. A good precision and accuracy can only be obtained when a good calibration procedure is used. Among the multivariate calibration methods, one can distinguish local and global methods. Global calibration methods have some disadvantage, such as in dealing with nonlinear data and in the context of updating. To solve these problems, local calibration methods are proposed. This thesis describes two new simplex local methods, the Law of Mixtures (LM) method and the Delaunay Triangulation (DT) method, for multivariate calibration.

There are two types of local calibration methods. One is based on Principal Component Regression (PCR) or Partial Least Squares Regression (PLS). Another type of local methods, called topological methods, do not use regression. Since the topological methods are based on averaging in some way the concentration of similar samples, they are mathematically much simpler than the one based on PCR/PLS, which should be a bonus to the analytical chemistry. The LM and DT methods belong to the topological methods.

The main question in the local methods is how to select the most similar calibration samples to the unknown sample. To develop better topological methods, it seems to us that methods based on simplexes that enclose the samples to be predicted are to be preferred, which are called simplex local methods. To make the selection of the vertices of the simplex for each unknown sample simpler, in the LM and DT methods, a predefined mesh of simplexes using the calibration data set is constructed.

For further investigation, outlier detection in the calibration set and updating multivariate calibration with the DT method are also evaluated. All examples presented in this thesis are based on near- infrared (NIR) data sets.

Curriculum Vitae

Ling JIN obtained her Bachelor degree in 1994 in Chemistry at Nanchang University (China). She continued studying chemometrics applied in analytical chemistry in the same university and obtained her master degree in 1997.

After that, she worked in the Institue of applied chemisty in Nanchang University for teaching and research in analytical chemistry. The research was in the field of ICP-AES and electroanalysis.

In 2001, she came to Belgium as a visiting scholar to do some research work on chemometrics at the department of Pharmaceutical and Biomedical Analysis (FABI). She started her study at the department to obtain the PhD degree under the guidance of Prof. D.L. Massart. The main part of her thesis concerns the development of new methods for mutlivariate calibration, applied to near-infrared (NIR) data sets.