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Vrije Universiteit Brussel

Faculteit Geneeskunde en Farmacie

Doctoraat
Farmaceutische Wetenschappen
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UITNODIGING

voor de openbare verdediging van het
doctoraatsproefschrift van

Xavier Capron

26 februari 2007

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

Xavier Capron

Updating and maintenance of multivariate regression and classification models

Op 26 februari 2007 om 14h
in auditorium P. Brouwer van de Faculteit
Geneeskunde & Farmacie, Laarbeeklaan 103,
1090 Brussel

Situering van het proefschrift

One of the main goals of chemometrics is to take advantage of the progresses made in analytical chemistry and mathematics to solve in an efficient and economical way practical problems. In particular, the combination of multivariate modelling techniques with analytical devices such as NIR (Near InfraRed) spectrometer has proven to be very useful. The association of those tools indeed led to the development of analytical methods which have many advantages compared to reference methods. Those new methods are fast, accurate, economical, simple to use and can estimate several properties at once. However, the calibration of the mathematical model requires the careful preparation of a representative training set. This set must carry all the possible sources of variation which are likely to occur in the future. The preparation and analysis of those calibration samples is therefore an important investment. Nonetheless, it is seldom impossible to foresee all possible sources of variation and a regression model might need to be updated from time to time. The aim of this PhD was therefore to study and design effective maintenance procedure.

Although the choice of the updating approach certainly depends on the data, the work performed during this thesis shows that the recalibration method, though the simplest one, also is the most versatile one. Hence, a particular effort was done to solve the problems related to this approach and especially the validation issue.

Curriculum Vitae

Xavier Capron was born in Lille, France on the 4th of January 1978. He studied chemistry in Lille and Brest and he has a master degree in chemometrics since June 2001.

He started his PhD on the 1st of October 2002 in the department of analytical chemistry and pharmaceutical technology (FABI) under the supervision of prof. D.L. Massart, prof. J. Smeyers-Verbeke, and Prof. B. Walczak. During his PhD he studied many chemometrics techniques for regression and classification problems and his work mainly focused on updating and maintaining the mathematical models derived from these methods. He worked in collaboration with partners from the petrochemical industry such as Shell and a significant part of the work performed during his thesis was accomplished in the framework of the WineDB European project. During this project, he had the opportunity to show that advanced modelling techniques such as non-linear classification methods can lead to improved results and solve efficiently practical food authentication problems.

He is the first author of five scientific publications and he is the co-author of five more articles which were published in international scientific reviews.