Strategy for introducing NIR spectroscopy and multivariate calibration techniques in industry

M.S. Larrechi, M.P. Callao

Analytical methods based on near infrared spectroscopy (NIR) and multivariate calibration techniques have important characteristics for industrial applications because they are quick and can be used to make direct determinations and extract information from several parameters from one single measurement. They can also be used in on-line applications. However, they have not been used in industry as much as one might expect because the validity of the calibration model must be assured when the signal is transformed. There are chemometric techniques for tackling every problem, but there are no specific guidelines about which procedure to use. In this article, we describe a practical strategy for introducing these methods. We discuss the relative merits of the various univariate and multivariate control techniques and describe how they might be used. We also discuss the standardisation of the calibration models and describe how to obtain robust models at low experimental cost. Finally, we illustrate our strategy with a practical case study from the petrochemical industry.

Keywords: Multivariate statistical process control (MSPC); Near infrared spectroscopy (NIR); Petrochemical industry; Robust model; Standardisation

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1. Introduction

NIR combined with multivariate processing techniques has been widely studied in recent years. There have been important applications, for example in the agri-food industry [1], the pharmaceutical industry [2] and the petrochemical industry [3].

In the petrochemical industry, the method made a strong impact when it was used to determine the number of octanes in different types of petrol [4]. The method is interesting because a wide variety of samples can be measured without the need for pre-treatment and because the determinations can be made quickly. Both of these are highly desirable features for on-line applications.

However, NIR has not been fully introduced in the above areas as an alternative to conventional analytical methods. We believe this may partly be because it is sensitive to factors such as temperature, the ageing of the source, and small instrumental disturbances that can affect the validity of the models over time. This suggests that the system needs to be controlled. It may also be because the goodness of the results depends on whether the samples analysed are of the same type as those used as calibration samples. Outliers in prediction should therefore be easily detected.

These problems (control, suitability of the system if a change is detected, and outlier detection) have been widely studied [5–7]. Such studies have illustrated the chemometric approaches to solving the problems, but, in our opinion, they have always dealt with just one of the problems and have been too theoretical. We think that these techniques need general practical guidelines that can be applied to each particular field.

Another problem is that these methods are normally implemented by specialised personnel but are used on a day-to-day basis by operators who are unfamiliar with the science on which they are based. It would be useful, therefore, if they contained means by which the operators could feel that they were involved in analysing the results they helped to produce.

We are developing NIR methods for use in the petrochemical industry [8–10]. In this article, we use this experience to discuss a practical strategy for using these methods effectively. As an example, we will discuss the determination of the ethylene

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Application Of Multivariate Calibration And Nir

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Application Of Multivariate Calibration And Nir:

Multi- and Megavariate Data Analysis Basic Principles and Applications L. Eriksson,T. Byrne,E. Johansson,J. Trygg,C. Vikström,2013-07-01 To understand the world around us as well as ourselves we need to measure many things many variables many properties of the systems and processes we investigate Hence data collected in science technology and almost everywhere else are multivariate a data table with multiple variables measured on multiple observations cases samples items process time points experiments This book describes a remarkably simple minimalistic and practical approach to the analysis of data tables multivariate data The approach is based on projection methods which are PCA principal components analysis and PLS projection to latent structures and the book shows how this works in science and technology for a wide variety of applications In particular it is shown how the great information content in well collected multivariate data can be expressed in terms of simple but illuminating plots facilitating the understanding and interpretation of the data The projection approach applies to a variety of data analytical objectives i e i summarizing and visualizing a data set ii multivariate classification and discriminant analysis and iii finding quantitative relationships among the variables This works with any shape of data table with many or few variables columns many or few observations rows and complete or incomplete data tables missing data In particular projections handle data matrices with more variables than observations very well and the data can be noisy and highly collinear Authors The five authors are all connected to the Umetrics company www umetrics com which has developed and sold software for multivariate analysis since 1987 as well as supports customers with training and consultations Umetrics customers include most large and medium sized companies in the pharmaceutical biopharm chemical and semiconductor sectors *Handbook of Near-Infrared Analysis* Donald A. Burns,Emil W. Ciurczak,2007-09-07 Fast inexpensive and easy to use near infrared NIR spectroscopy can be used to analyze small samples of virtually any composition The Handbook of Near Infrared Analysis Third Edition explains how to perform accurate as well as time and cost effective analyses across a growing spectrum of disciplines Presenting nearly 50% new and re Portable Spectroscopy and Spectrometry, Applications Richard A. Crocombe,Pauline E. Leary,Brooke W. Kammrath,2021-04-26 The most comprehensive resource available on the many applications of portable spectrometers including material not found in any other published work Portable Spectroscopy and Spectrometry Volume Two is an authoritative and up to date compendium of the diverse applications for portable spectrometers across numerous disciplines Whereas Volume One focuses on the specific technologies of the portable spectrometers themselves Volume Two explores the use of portable instruments in wide range of fields including pharmaceutical development clinical research food analysis forensic science geology astrobiology cultural heritage and archaeology Volume Two features contributions by a multidisciplinary team of experts with hands on experience using portable instruments in their respective areas of expertise Organized both by instrumentation type and by scientific or technical discipline 21 detailed chapters cover various applications of portable ion mobility spectrometry IMS infrared and

near infrared NIR spectroscopy Raman and x ray fluorescence XRF spectroscopy smartphone spectroscopy and many others Filling a significant gap in literature on the subject the second volume of Portable Spectroscopy and Spectrometry Features a significant amount of content published for the first time or not available in existing literature Brings together work by authors with assorted backgrounds and fields of study Discusses the central role of applications in portable instrument development Covers the algorithms calibrations and libraries that are of critical importance to successful applications of portable instruments Includes chapters on portable spectroscopy applications in areas such as the military agriculture and feed hazardous materials HazMat art conservation and environmental science Portable Spectroscopy and Spectrometry Volume Two is an indispensable resource for developers of portable instruments in universities research institutes instrument companies civilian and government purchasers trainers operators of portable instruments and educators and students in portable spectroscopy courses Process Analytical Technology Katherine A. Bakeev,2010-04-01 Process Analytical Technology explores the concepts of PAT and its application in the chemical and pharmaceutical industry from the point of view of the analytical chemist In this new edition all of the original chapters have been updated and revised and new chapters covering the important topics of sampling NMR fluorescence and acoustic chemometrics have been added Coverage includes Implementation of Process Analytical Technologies UV Visible Spectroscopy for On line Analysis Infrared Spectroscopy for Process Analytical Applications Process Raman Spectroscopy Process NMR Spectrscopy Technology and On line Applications Fluorescent Sensing and Process Analytical Applications Chemometrics in Process Analytical Technology PAT On Line PAT Applications of Spectroscopy in the Pharmaceutical Industry Future Trends for PAT for Increased Process Understanding and Growing Applications in Biomanufacturing NIR Chemical Imaging This volume is an important starting point for anyone wanting to implement PAT and is intended not only to assist a newcomer to the field but also to provide up to date information for those who practice process analytical chemistry and PAT It is relevant for chemists chemical and process engineers and analytical chemists working on process development scale up and production in the pharmaceutical fine and specialty chemicals industries as well as for academic chemistry chemical engineering chemometrics and pharmaceutical science research groups focussing on PAT Review from the First Edition The book provides an excellent first port of call for anyone seeking material and discussions to understand the area better It deserves to be found in every library that serves those who are active in the field of Process Analytical Technology Current Engineering Practice **Computer Applications in Chemical Research and Education** Josef Brandt,Ivar Ugi,1989 **Comprehensive Chemometrics** Steven Brown,Roma Tauler,Beata Walczak,2020-05-26 Comprehensive Chemometrics Second Edition Four Volume Set features expanded and updated coverage along with new content that covers advances in the field since the previous edition published in 2009 Subject of note include updates in the fields of multidimensional and megavariate data analysis omics data analysis big chemical and biochemical data analysis data fusion and sparse methods The book follows a similar structure to

the previous edition using the same section titles to frame articles Many chapters from the previous edition are updated but there are also many new chapters on the latest developments Presents integrated reviews of each chemical and biological method examining their merits and limitations through practical examples and extensive visuals Bridges a gap in knowledge covering developments in the field since the first edition published in 2009 Meticulously organized with articles split into 4 sections and 12 sub sections on key topics to allow students researchers and professionals to find relevant information quickly and easily Written by academics and practitioners from various fields and regions to ensure that the knowledge within is easily understood and applicable to a large audience Presents integrated reviews of each chemical and biological method examining their merits and limitations through practical examples and extensive visuals Bridges a gap in knowledge covering developments in the field since the first edition published in 2009 Meticulously organized with articles split into 4 sections and 12 sub sections on key topics to allow students researchers and professionals to find relevant information quickly and easily Written by academics and practitioners from various fields and regions to ensure that the knowledge within is easily understood and applicable to a large audience Comprehensive Chemometrics ,2009-03-09 Designed to serve as the first point of reference on the subject Comprehensive Chemometrics presents an integrated summary of the present state of chemical and biochemical data analysis and manipulation The work covers all major areas ranging from statistics to data acquisition analysis and applications This major reference work provides broad ranging validated summaries of the major topics in chemometrics with chapter introductions and advanced reviews for each area The level of material is appropriate for graduate students as well as active researchers seeking a ready reference on obtaining and analyzing scientific data Features the contributions of leading experts from 21 countries under the guidance of the Editors in Chief and a team of specialist Section Editors L Buydens D Coomans P Van Espen A De Juan J H Kalivas B K Lavine R Leardi R Phan Tan Luu L A Sarabia and J Trygg Examines the merits and limitations of each technique through practical examples and extensive visuals 368 tables and more than 1 300 illustrations 750 in full color Integrates coverage of chemical and biological methods allowing readers to consider and test a range of techniques Consists of 2 200 pages and more than 90 review articles making it the most comprehensive work of its kind Offers print and online purchase options the latter of which delivers flexibility accessibility and usability through the search tools and other productivity enhancing features of ScienceDirect Near-Infrared Spectroscopy H. W. Siesler,2002-02-15 Over the last few years near infrared NIR spectroscopy has rapidly developed into an important and extremely useful method of analysis In fact for certain research areas and applications ranging from material science via chemistry to life sciences it has become an indispensable tool because this fast and cost effective type of spectroscopy provides qualitative and quantitative information not available from any other technique This book offers a balanced overview of the fundamental theory and instrumentation of NIR spectroscopy introducing the material in a readily comprehensible manner A considerable part of the text is dedicated to

practical applications including sample preparation and investigations of polymers textiles drugs food and animal feed However special topics such as two dimensional correlation analysis are also covered in separate chapters Written by eight experts in different fields this book presents an introduction to the current state of developments and is valuable to spectroscopists and to practitioners applying NIR spectroscopy as a daily analytical tool **Multivariate Calibration of Near Infrared Reflectance Data from Food Products** Tomas Isaksson,1990 **Transfer of Multivariate Calibration Models** Hans Bärring,2001 **Textile Technology Digest** ,2002 **3rd European COST E31 Conference, Management of Recovered Wood** Christos Th Gallis,2007 *Real-time Analysis of Light Alkenes at Elevated Temperatures and Pressures by Fiber-optic Near Infrared Spectroscopy* Engin Deniz Yalvac,1996 **Proceedings of the IVth International Symposium on Applications of Modelling as an Innovative Technology in the Agri-Food-Chain** P. Barreiro,2008 Multivariate Calibration Harald Martens,Tormod Næs,1992-08-07 Multivariate Calibration Harald Martens Chemist Norwegian Food Research Institute Aas Norway and Norwegian Computing Center Oslo Norway Tormod N s Statistician Norwegian Food Research Institute Aas Norway The aim of this inter disciplinary book is to present an up to date view of multivariate calibration of analytical instruments for use in research development and routine laboratory and process operation The book is intended to show practitioners in chemistry and technology how to extract the quantitative and understandable information embedded in non selective overwhelming and apparently useless measurements by multivariate data analysis Multivariate calibration is the process of learning how to combine data from several channels in order to overcome selectivity problems gain new insight and allow automatic outlier detection Multivariate calibration is the basis for the present success of high speed Near Infrared NIR diffuse spectroscopy of intact samples But the technique is very general it has shown similar advantages in for instance UV Vis and IR spectrophotometry transmittance reflectance and fluorescence for x ray diffraction NMR MS thermal analysis chromatography GC HPLC and for electrophoresis and image analysis tomography microscopy as well as other techniques The book is written at two levels the main level is structured as a tutorial on the practical use of multivariate calibration techniques It is intended for university courses and self study for chemists and technologists giving one complete and versatile approach based mainly on data compression methodology in self modelling PLS regression with considerations of experimental design data pre processing and model validation A second more methodological level is intended for statisticians and specialists in chemometrics It compares several alternative calibration methods validation approaches and ways to optimize the models The book also outlines some cognitive changes needed in analytical chemistry and suggests ways to overcome some communication problems between statistics and chemistry and technology **Book of Abstracts** ,1992 *Near Infrared Spectroscopy* Anthony M. C. Davies,Phil Williams,1996 **Applied Spectroscopy** ,2007 Making Light Work: Advances in Near Infrared Spectroscopy Ian Murray,Ian A. Cowe,1992-06 Making Light Work Advances in Near Infrared Spectroscopy Edited by Ian Murray and Ian A Cowe This book

presents a cross section of the most recent developments in near infrared spectroscopy Applications spectroscopic theory chemometrics and instrumentation are all covered The variety of contributors is a striking reflection of the broad range of applications of this technique Workers in agriculture food science medicine life sciences pharmaceuticals textiles general chemicals and polymers have all contributed the latest developments from their fields This book is essential reading for workers in NIR spectroscopy and will greatly benefit those considering implementing NIR in their work Near-infrared Spectroscopy in Agriculture Craig Arthur Roberts,Jerry Workman,James B. Reeves,2004 This monograph highlights the practical use of NIR technology providing the latest information on NIR use in agricultural applications as well as the fundamentals of spectroscopy and chemometrics Unique among NIR publications the majority of the book details the widespread application of NIR analysis in crop production food processing and non food agriculture Forage fruits baking products timber meats and more If it has been analyzed with near infrared technology you will find it here

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