MULTIVARIATE AND MULTIWAY CALIBRATION

with special focus on uncertainty estimation and analytical figures of merit

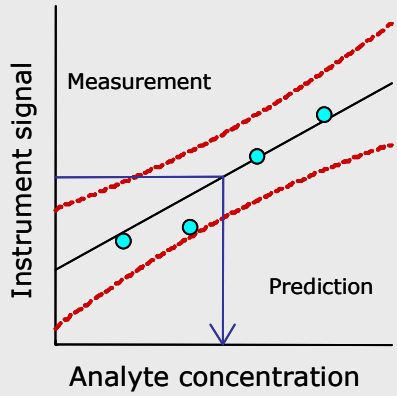
13–15 October 2008, Nijmegen, The Netherlands

Course leader: Klaas Faber

Introduction

Univariate calibration

Univariate calibration leads to relatively simple models with a sound statistical underpinning; the uncertainty estimation is a topic taught in courses on basic statistics. Consider the straight-line fit:



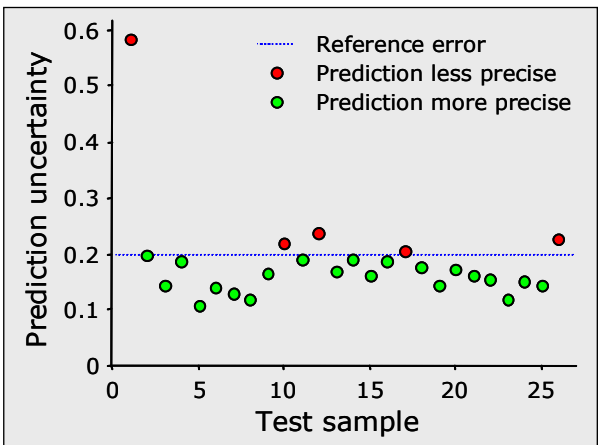
Least-squares straight-line fit with the familiar prediction bands. The prediction intervals are relatively narrow close to the mean, where the model is most precise.

Analytical figures of merit are performance characteristics of the data that are closely related to prediction uncertainty. The sensitivity, for example, is the slope of the calibration graph. Analytical figures of merit can be used to select between potentially useful methods or to evaluate or optimize a determination that is already in use.

Multivariate and multiway calibration

Multivariate and multiway calibration models are inherently much more complex than a straight-line fit. However, considerable progress has been made over the last two decades to extend the generally accepted univariate methodology to the multivariate and multiway domain. A consistent generalization implies many benefits:

- evidence that target limits are (not) too stringent for that analyte and measurement method, without the need for extensive calibration;
- tighter confidence and prediction intervals;
- lower detection limits;
- improved outlier detection;
- improved validation.



Sample-specific uncertainties for a near-infrared calibration using partial least-squares. Sample 1 is an extreme outlier.

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Goal of the course and target audience

The course provides a critical discussion of uncertainty estimation and analytical figures of merit for a large variety of modeling procedures. Upon completing the course, the applicant should be able to assess the relevance or irrelevance of a certain approach for his/her applications. This is believed to be of interest to a broad audience of varying level and background, e.g.:

- end-users who have to choose among commercial analytical software packages;
- experimental chemometricians who consider applying novel methodology in their research;
- traditional analytical chemists who want to extract quantitative information, e.g. limit of detection, from non-selective multivariate data such as near-infrared spectra or overlapping chromatographic peaks;
- industrial statisticians who want to learn about chemometricians' attempts to bridge the gap between chemical data analysis and statistics.

Background reading

To get familiar with terminology and specific chemometrics jargon, it is recommended to read the seminal paper by Karl Booksh and Bruce Kowalski (*Analytical Chemistry* **1994**, *66*, 782A-791A). An excellent tutorial is Ricard Boqué and Joan Ferré, *LC.GC Europe* **2004**, *22*, 2-6. Finally, introductions to various topics can be found under www.chemometry.com/Research.

Organizational

The course will be held from October 13-15 at the HAN University in Nijmegen, The Netherlands (http://www.han.nl/start/corporate/international/). A route description to the HAN University will be sent along with the confirmation of the application. Day 1 (October 13) starts at 10 am and ends at 5 pm. Days 2 and 3 start at 9 am and end at 5 pm.

Application

To apply, please return the attached application form no later than **September 1**. The course fee is Euro 600 for participants from academia, Euro 900 for participants from non-commercial and Euro 1200 for participants from commercial organizations, respectively. The fee includes course material, as well as lunch and drinks.

Course leader

The course leader is Klaas Faber, who has published extensively on uncertainty estimation (PCA, MLR, PCR, PLS, GRAM, PARAFAC) and analytical figures of merit for multivariate as well as multiway data.

Course set-up

The course language is English. The maximum number of participants is 12. Practical illustrations of theory are based on in-house programs written in Matlab.

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Day 1 – Introduction (13 October)

- Setting the stage
- Linear algebra
- Statistics
- Principal component analysis

Day 2 – Calibration (14 October)

- Regression-based calibration (e.g., partial least-squares)
- Deconvolution-based calibration (e.g., self-modeling curve resolution)
- Outlier detection
- Validation
- Component selection

Day 3 – Uncertainty estimation (15 October)

- Uncertainty components: standard error and bias
- Expression-based approach to uncertainty estimation
- Resampling-based approach to uncertainty estimation
- Illustration for principal component analysis
- Illustration for regression-based calibration
- Illustration for deconvolution-based calibration
- Overall conclusions and outlook

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APPLICATION FORM

Family name ..... First name .....

Affiliation .....

.....

.....

Tel ..... Fax .....

E-mail.....

Invoice address (if different from above) .....

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I have taken notice of the general conditions on payment and cancellation*

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Signature of applicant Date and place

Please return this form to

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***General conditions**

Upon cancellation until twenty days before the start of the course, half of the course fee is due. After that, the full amount needs to be paid. In case you cannot attend, you can let someone else take your place without additional cost. Chemometry Consultancy has the right to cancel a course until twenty days before the start of the course, in which case a complete refund will be provided. Chemometry Consultancy also has the right to reject the application of course candidates without further motivation.

BACKGROUND OF THE APPLICANT

Research experience and current activities

What do you expect to learn from this course?

Please specify the analytical software you are familiar with

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Relevant publications

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