

MULTIVARIATE AND MULTIWAY CALIBRATION

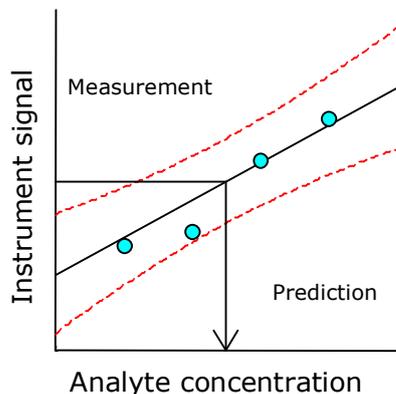
with special focus on uncertainty estimation and analytical figures of merit

27–29 September 2006, Utrecht, The Netherlands

Course leader: Klaas Faber

Univariate calibration

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



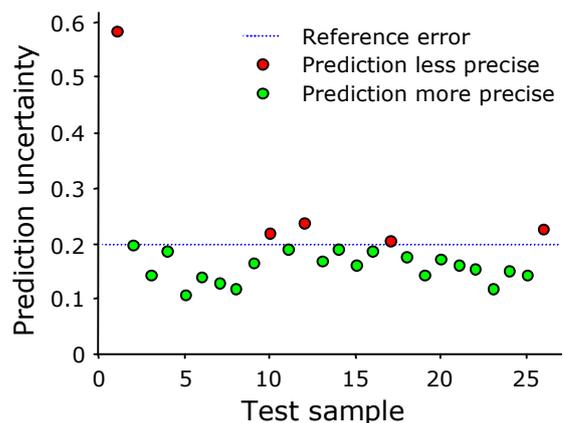
Least-squares straight-line fit with the familiar prediction bands. The prediction intervals are relatively narrow close to the mean, where the model is most precise.

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 prediction 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 newly developed theory 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.

Organizational

The course will be held from September 27-29 at the Jaarbeurs in Utrecht, The Netherlands, see www.jaarbeursutrecht.nl. A route description to the Jaarbeurs will be sent along with the confirmation of the application. Day 1 (September 27) 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 800 for participants from non-commercial and Euro 1000 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. 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, uncertainty estimation and analytical figures of merit are reviewed under www.chemometry.com/Expertise.

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Day 1 – Introduction (27 September)

- Setting the stage
- Linear algebra
- Statistics
- Principal component analysis (PCA)

Day 2 – Calibration (28 September)

- Regression-based calibration
- Curve resolution-based calibration
- Outlier detection
- Validation
- Model selection

Day 3 – Uncertainty estimation (29 September)

- Uncertainty estimation: standard error and bias
- Expression-based approach to uncertainty estimation
- Resampling-based approach to uncertainty estimation
- Uncertainty estimation for PCA
- Uncertainty estimation and analytical figures of merit for regression-based calibration
- Uncertainty estimation and analytical figures of merit for curve resolution-based calibration

APPLICATION FORM

Family name First name

Affiliation

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Tel..... Fax

E-mail.....

Invoice address (if different from above)

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The course fee is due before September 1. I have taken notice of the general conditions on payment and cancellation^{*}

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Signature of applicant

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Date and place

How would you like to be contacted (choose one)?

Surface/air mail

Fax

E-mail

Please return this form to

Chemometry Consultancy, Rubensstraat 7, 6717 VD Ede, The Netherlands

T: +31 (0) 318 641985, F: +31 (0) 318 642150, E: nmf@chemometry.com

*** 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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