

MULTIVARIATE AND MULTIWAY CALIBRATION

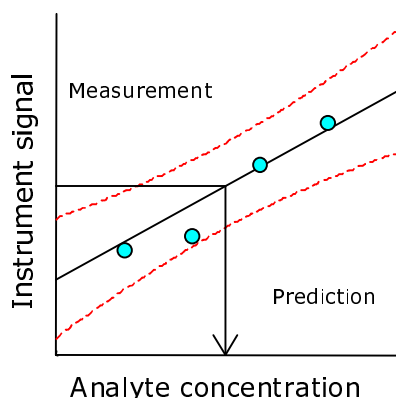
with special focus on uncertainty estimation and analytical figures of merit

28–30 September 2005, 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:



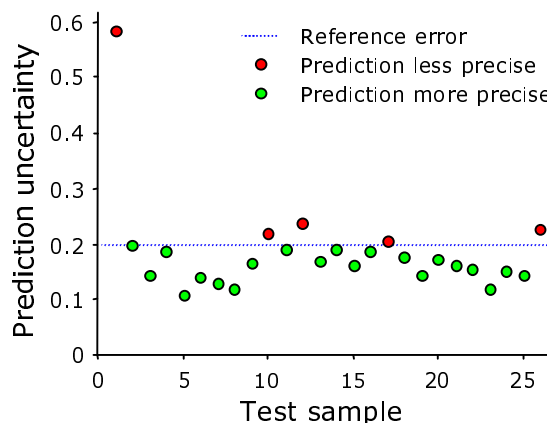
Least-squares straight-line fit with the familiar prediction bands. The prediction intervals are relatively narrow close to the mean, where the model is most precise.

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 the 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 28-30, from 9 am to 5 pm at the Jaarbeurs in Utrecht, The Netherlands (www.jaarbeursutrecht.nl). A route description to the Jaarbeurs will be sent along with the confirmation of the application. Day 1 provides an optional introduction to the actual course held during days 2 and 3.

To apply, please return the attached application form no later than **September 1**. The fee for the 2-days course is Euro 450 for participants from academia, Euro 600 for participants from non-commercial and Euro 750 for participants from commercial organizations. The fee for the 1-day introduction is Euro 150, Euro 200 and Euro 250, respectively.

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. Since these programs are made available, Matlab-users are encouraged to bring their own laptop. 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 (28 September)

- Linear algebra and statistics
- Principal component analysis (PCA)
- Regression
 - Classical vs. inverse model
 - Full-rank predictors (\mathbf{X}): multiple linear regression (MLR)
 - Reduced-rank predictors (\mathbf{X}): principal component regression (PCR) and partial least squares (PLS)
- Outlier detection and validation

Day 2 – Multivariate and multiway calibration (29 September)

- Uncertainty estimation: standard error and bias
- Expression-based approach to uncertainty estimation
 - Taylor series expansion
- Resampling- based approach to uncertainty estimation
 - Cross-validation, jackknife, bootstrap and noise addition
- Uncertainty estimation for PCA

Day 3 – Multivariate and multiway calibration (30 September)

- Uncertainty estimation and analytical figures of merit for univariate calibration
 - Least-squares straight-line fit
- Uncertainty estimation and analytical figures of merit for multivariate calibration
 - MLR, PCR and PLS
- Uncertainty estimation and analytical figures of merit for multiway calibration
 - Unfold-PCR, unfold-PLS, multilinear PLS, bilinear least squares (BLLS) with pure samples and mixtures
 - Generalized rank annihilation method (GRAM) and parallel factor analysis (PARAFAC)
- Calibration model selection

APPLICATION FORM

Family name..... First name

Affiliation.....
.....

Tel Fax

E-mail

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

VAT number

Indicate which module(s) you wish to attend

Introduction (28 September)

Multivariate and multiway calibration (29–30 September)

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

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 course start, half of the course fee is due. After that the full amount needs to be paid. In case you cannot attend the course you applied for, 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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