Statistical Engineering Division Seminar

Wednesday September 4, 1996, 11:00 am
Lecture Room D, Administration Bldg.
NIST
Gaithersburg, MD

Uncertainty in Predicted Concentrations Using Multivariate Calibration Technologies

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Multivariate calibration aims to obtain a predictive relation between analyte concentrations and measured spectral values of complex mixtures. Model parameters are estimated in the form of a regression vector using methods like ordinary least squares (OLS), principal component regression (PCR) and partial least squares (PLS). The covariance matrix of the estimated regression vector is indispensable for the construction of confidence intervals for the predicted analyte concentrations. Previously proposed confidence intervals for predictions obtained by PCR and PLS only take the uncertainty in the concentrations of the calibration samples into account. This limits their capability for establishing realistic intervals. This seminar gives an overview of recently derived expressions that include uncertainties in the spectral data.

Klaas Faber holds a Ph.D. from the Katholieke Universiteit Nijmegen, The Netherlands. He has worked with Dutch, Swedish and U.S. chemometric research groups. He is now a Research Associate at the Center for Process Analytical Chemistry. His research focus has and continues to be improving the reliability of analytical chemistry's emerging multivariate technologies.

(A NIST Shuttle is scheduled 30 minutes before the talk for pickup from NIST North.)

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