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(54) Title: MUTIVARIATE SAMPLE ANALYSIS

(57) Abstract

In a process for analyzing a sample of unknown constitution by an analytical apparatus, a set of analytical measurements and a set of reference measurements, each comprising a set of multivariate signal responses obtained from a set of samples by a first and a second analytical apparatus, are adjusted to remove operational variabilities associated with the apparatus, thereby providing a first and a second matrix of adjusted signal responses. One of the two matrices of adjusted signal responses is decomposed into a matrix product of a matrix comprising a set of principal factors and a matrix comprising the amounts associated with each of the principal factors. A compressed signal response matrix product is constructed that comprises a matrix comprising a subset of the set of principal factors and a matrix comprising the amounts associated with each of the principal factors included in the subset. From the latter matrix a projection matrix is computed. Using this projection matrix and a first normalized matrix product that comprises a normalization matrix and the other of the two matrices of adjusted signal responses, a compressed normalized matrix product is constructed. Values of the normalization matrix that minimize the difference between the first normalized matrix product and the compressed normalized matrix product are computed, thereby producing an optimal normalization matrix. A second normalized matrix product comprising the optimal normalization matrix and the one matrix of adjusted signal responses that had been decomposed into a matrix product is constructed. Using the other matrix of adjusted signal responses and the second normalized matrix product, a calibration useful for analyzing the signal responses obtained from the sample of unknown constitution by the first analytical apparatus is constructed and applied to the signal responses from the sample to determine its constitution.