



Application of non-linear optimization methods to estimation of Tucker3 solutions for investigation of chemical data

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This report is the first application of FMIN in Tucker3 based resolution of a three way data. FMIN is the name for a conventional rotation based procedure used in multivariate curve resolution (MCR) of two way data. Tuck3-FMIN is proposed to rotate a set of Tucker3 loadings to satisfy the desired constraints that are included in the objective function. The proposed Tuck3-FMIN was successfully applied to resolution of three-way excitation-emission fluorescence data. Nonnegative spectral and concentration profiles, in addition to simple Tucker3 core were estimated from application of proper constraints. A main advantage of the Tuck3-FMIN is its application to large data sets for which the least squares based procedures are time consuming. The method is a proper alternative to least square based procedures for the conditions with high overlapped spectral profiles. In presence of spectral overlap alternative least square algorithm becomes divergent and time consuming. Simulated and real fluorescence data were successfully utilized to evaluate the feasibility of this method.

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