SCREAM: A novel multiway methods for regression on tensors with shifts along one mode

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Analytical instrumentation has developed to a point where many techniques provide outcomes that, for each sample, take the form of a landscape or a higher order array. Accordingly, several methods have been proposed during the years to directly process multi-way data, both for exploratory purposes (e.g. PARAFAC [1]) and for regression (multilinear PLS [2]) or classification (NPLS-DA, NSIMCA [3]). However, these same methods become less adequate, when the underlying profiles change shape from sample to sample, for instance in chromatography when there are retention time shifts in the elution profiles or in process analysis, when the batches have different lengths and/or are not synchronized. In such cases, if only a decomposition of the array is sought, reliable models can still be calculated using a suitable modification of the PARAFAC algorithm, called PARAFAC2 [4]. On the other hand, in the case of calibration problems, no alternatives to N-PLS have been proposed so far to cope with these limitations. To overcome this problem, in this communication a new regression method called SCREAM (Shifted Covariates REgression Analysis for Multi-way data) is proposed for calculating calibration models on multi-way arrays which present shifts (or shape changes) along one of the modes. The algorithm combines a PARAFAC-2 decomposition of the X array and a Principal Covariate Regression-like least squares criterion for the computation of the regression coefficients in a way which is analogous to what already described by Smilde and Kiers in the case of other multi-way PCovR algorithms [5]. The method is tested on real and simulated datasets providing good results and performing as well or better than other available regression approaches for multi-way data.

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