Abstract

A new NMF algorithm has been proposed for the deconvolution of overlapping chromatograms of chemical mixture. Most of the NMF algorithms used so far for chromatogram separation do not converge to a stable limit point. To get same results for all the runs, instead of random initialization, three different initialization methods have been used namely, ALS-NMF (robust initialization), NNDSVD based initialization and EFA based initializations. To improve the convergence, a new sNMF algorithm with modified multiplicative update (ML-sNMF) has been proposed in this work for overlapped chromatogram separation. The algorithm has been validated with the help of simulated partially, severely overlapped and embedded chromatograms. The proposed ML-sNMF algorithm has also been validated with the help of experimental overlapping chromatograms obtained using Gas Chromatography –Flame Ionization Detector (GC-FID) for the chemical mixture of acetone and acrolein.
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539-548.
- Hong-Tao Gao, Tong-Hua Li, Kai Chen, Wei-Guang Li, Xian Bi, Overlapping spectra resolution using non-negative matrix factorization, Talanta, 66 (2005) 65-73.

Index Terms

Computer Science  Applied Sciences
Keywords
ML-sNMF  modified update for convergence  ALS-NMF (Robust)  EFA and NNDSVD based initializations

Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS)

Resolution

overlapped and embedded chromatograms

acetone and acrolein mixture