

On MCR-BANDS and FACPAC under unimodality constraints

*Somaye Vali Zade¹, Klaus Neymeyr², Hamid Abdollahi^{*1}, Mathias Sawall³*

¹ *Institute for Advanced Studies in Basic Sciences (IASBS)*

² *Universität Rostock, Institut für Mathematik, Ulmenstrasse 69, 18057 Rostock, Germany*

³ *Leibniz-Institut für Katalyse, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany*

E-mail address: abd@iasbs.ac.ir

ABSTRACT

Multivariate curve resolution methods suffer from non-unique solutions. Due to the rotational ambiguity there is often a range of feasible solutions for the decomposition of the data set. This ambiguity is covered in a low-dimensional way by the so-called area feasible solutions (AFS-sets). Several methods have been proposed for the estimation of the AFS-sets. One of them is the polygon inflation algorithms, implemented in FACPAC [1]. Another method in order to analyze the rotational ambiguity of spectral data is the MCR-BANDS method [2] that provides an easy and flexible estimation of the extension of the ambiguity for any number of components and different types of constraints. In this work, results obtained by MCR-BANDS are compared with the AFS-sets obtained by FACPAC. In particular we apply both approaches only with nonnegativity constraints as well as with nonnegativity and unimodality constraints. For a three-component model problem we demonstrate how the MCR-BANDS solutions shift from the boundary of the AFS-sets by nonnegativity constraints to the boundary of the AFS-sets by nonnegativity and unimodality constraints.

Keywords: “Multivariate curve resolution”, “self-modeling curve resolution”, “area of feasible solutions”, “FACPAC”, “MCR-BANDS”, “unimodality constraint”

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