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Implementing partial knowledge based on Duality

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Abstract

Self-modeling curve resolution (SMCR) methods resolve data set to a range of feasible solutions assuming minimal constraints (non-negativity) analytically. Such a direct method for a two and three component system have been introduced by Lawton-Sylvestre in 1971 [1] and Borgen in 1985 [2], respectively. How to incorporate additional knowledge during SMCR and How to reduce the extent of feasible regions are among important questions in the SMCR field of study. Recently it has been highlighted that in order to elucidate the principles of existing theory in SMCR methods, geometrical view is required too [3-4]. In this study the well-known duality concept that first has been used by Henry [5] in chemometrics and generalized by Rajko for SMCR [6] is considered. The aim of research is to clarify the similarity between duality and algebraic Complementarity theorem introduced by Sawall et al [7].

Keywords: Self-Modeling Curve Resolution (SMCR); Duality; Complementarity theorem.

1. Introduction

The duality concept provides a very rigorous mathematical relationship between two spaces of a given data matrix. For the First time in the literature of chemometrics Henry [5] has introduced duality relationship with the analytical formulae for a three component data set containing multivariate receptor modeling of compositional data of airborne pollution. Considering that singular value decomposition (SVD) of the data leads to two sets of eigenvectors it has been shown that one set of eigenvectors spans a space in which source compositions are points and source contributions are hyperplanes and this space is dual to the space spanned by the second set of eigenvectors of the data in which source compositions are hyperplanes and source contributions are points. Later the concept of duality has been generalized by Rajko for SMCR which is based on singular value decomposition or principal component analysis (PCA) [6].In the presence of the partial knowledge, duality helps to extract more information of the data set. Another approach which uses partial knowledge of the pure components in order to reduce the feasible solutions is the complementarity theorem which has been introduced by Sawall et al [7]. They investigated that the knowledge of spectrum leads to linear restrictions on the concentration profiles of the other components. The aim of this study is to clarify the similarity between duality and algebraic Complementarity theorem.

2. Results and discussion

For any spectroscopic process that is measured as a bilinear two-way data (**M**) ,decomposition of the response matrix to concentration profile matrix (**C**) and spectral profile matrix (**A**) ,based on Bouguer–Lambert– Beer law is:

$$\mathbf{M}_{I\times J} = \mathbf{C}_{I\times N}\mathbf{A}^{T}_{N\times J} \qquad (1)$$

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Where **M** has dimension (I×J), **C** has dimension (I×N) and $\mathbf{A}^T$ has dimension (N×J). I is the number of measured spectra, J is the number of wavelengths and N is the number of components.

According to SVD:

$$\mathbf{M}_{I\times J} = \mathbf{U}_{I\times N}\mathbf{D}_{N\times N}\mathbf{V}^T_{N\times J} = \mathbf{X}_{I\times N}\mathbf{V}^T_{N\times J} = \mathbf{U}_{I\times N}\mathbf{Y}^T_{N\times J} = (\mathbf{X}_{I\times N}\mathbf{Z}_{N\times N})(\mathbf{T}_{N\times N}\mathbf{V}^T_{N\times J}) = \mathbf{C}_{I\times N}\mathbf{A}^T_{N\times J} \quad (2)$$

where $\mathbf{C}_{I\times N} = \mathbf{X}_{I\times N}\mathbf{Z}_{N\times N}$ and $\mathbf{A}^T_{N\times J} = \mathbf{T}_{N\times N}\mathbf{V}^T_{N\times J}$ (3)

So transformation of the **X** and **V** by any invertible transformation matrix like **T** and **Z** to **C** and **A** can be based on Eq. (2), note that $\mathbf{TZ} = \mathbf{I}$ and $\mathbf{Z} = \mathbf{T}^{-1}$.

Generating duality concept for a two component system with a known spectrum of the analyte ($\mathbf{A}_i$) leads to the following equations:

$\mathbf{t} = \mathbf{A}_i\mathbf{V}$ (4) $\qquad$ $\mathbf{tz} = \mathbf{0}$ (5)

where **t** is a vector of the coordination of the known spectrum in the **V**-space and **z** is the general variable in the **U**-space. Both vectors, **t** and **z** have dimension of 1×2. This equation defines a line in the **U**-space corresponding to the known spectrum in the **V**-space. Knowledge about the known spectrum can be applied as the equality constraint too. Therefor unique solution of the concentration profile for the second component would be obtained [4]. The complementarity theorem represents the mathematical relationship between **t** and it's complementary column of **Z**, or **z**:

$$\mathbf{tz} = 0 \quad (6)$$

This theorem resembles the duality concept. Based on the knowledge in one abstract space, both of them provide information of the remained components on the other abstract space.

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