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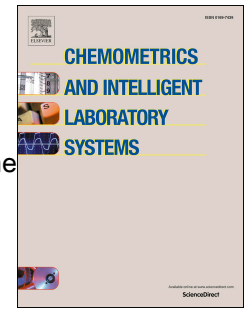

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Kernel-Partial Least Squares regression coupled to pseudo-sample trajectories for the analysis of mixture designs of experiments

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Abstract

This article explores the potential of Kernel-Partial Least Squares (K-PLS) regression for the analysis of data proceeding from mixture designs of experiments. Gower's idea of pseudo-sample trajectories is exploited for interpretation purposes. The results show that, when the datasets under study are affected by severe non-linearities and comprise few observations, the proposed approach can represent a feasible alternative to classical methodologies (i.e. Scheffé polynomial fitting by means of Ordinary Least Squares - OLS - and Cox polynomial fitting by means of Partial Least Squares - PLS). Furthermore, a way of recovering the parameters of a Scheffé model (provided that it holds and has the same complexity as the K-PLS one) from the trend of the aforementioned pseudo-sample trajectories is illustrated via a simulated case-study.

Keywords: mixture designs of experiments, Kernel-Partial Least Squares (K-PLS), pseudo-sample trajectories, Scheffé and Cox polynomials, Partial Least Squares (PLS), Ordinary Least Squares (OLS)

1. Introduction

A wide range of products currently used in daily life result from processing blends of two or more ingredients. Hence, the physicochemical properties of these products mainly depend on the raw materials being mixed and on the proportions in which they are added. Alloys, as well as drugs and foodstuffs, are just some of the numerous examples where this applies, and their

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