Chemometrics and Intelligent Laboratory Systems 152 (2016) 97–106

Contents lists available at ScienceDirect

Chemometrics and Intelligent Laboratory Systems

journal homepage: www.elsevier.com/locate/chemolab

Use of the common components and specific weights analysis to interpret supersaturated designs

M. Claeys-Bruno [a,*], A. Béal [a], D.N. Rutledge [b], M. Sergent [a]

[a] Aix Marseille Université, LISA EA4672, 13397, Marseille Cedex 20, France
[b] AgroParisTech, UMR1145 Ingénierie Procédés Aliments, 16, rue Claude Bernard, 75005 Paris, France

ARTICLE INFO

Article history:
Received 23 April 2015
Received in revised form 24 November 2015
Accepted 24 January 2016
Available online 29 January 2016

Keywords:
Supersaturated design
Multi-block analysis
Common Components and Specific Weights Analysis
ComDim

ABSTRACT

We propose a new method to treat supersaturated designs which relies on the multivariate CCSWA (Common Components and Specific Weights Analysis), or ComDim, method. This method can be applied through two approaches. The first considers this method as a novel procedure to analyse supersaturated designs. This can reveal influential factors, and correctly identify the active factors even when the results do not fully comply with the standard hypotheses (sparsity). The second approach extracts the information common to the results obtained using a wide range of methods to analyse the designs. This could make it possible to overcome the errors specific to each of these methods.

1. Introduction

A supersaturated design is a design for which there are fewer runs than effects to be estimated. First introduced by Satterthwaite in 1959 [1], two-level supersaturated designs are becoming increasingly popular and are very useful in many preliminary studies involving a large number of potentially relevant factors. In the literature, many construction methods have been developed since the new class of supersaturated designs based on half-fractions of Hadamard designs was published by Lin in 1993 [2], for example, augmented Hadamard designs where interaction columns are added [3], and many other construction methods [4–17]. More recently, some authors have proposed new classes of designs which can take into account two-factor interaction effects [18]. All these construction methods lead to different supersaturated designs regarding the optimality criterion. For example, Wu [16] proposed a method by augmenting Hadamard matrices by adding interaction columns, Tang et Wu [14] proposed a new construction using columnwise-pairwise algorithms. All these methods allow the construction of optimal and adapted matrices to the different problems. Today, the difficulties remain the procedure for solving them once experimentally applied.

However, even though the number of articles proposing construction methods is continuously growing, there are very few descriptions of applications. This lack of use stems from the fact that it is very difficult to conform to the utilisation hypotheses, i.e., a very low number of truly influential factors should be identified (around 10% of the factors studied). Another difficulty lies in data treatment. To identify the sparse active effects, interpretation methods are essential since classical strategies, such as least squares regression, can no longer be applied. In 2003, Li and Lin [19] proposed a comparative study of methods to analyse supersaturated designs. Stepwise variable selection may not be appropriate, and some traditional approaches such as selection of the best subset of variables may be difficult to use (long calculation time); Bayesian variable selection, boosting or Ridge regression, and non-convex penalised least squares regression were also tested. However, for the moment, none of these methods was found to provide risk-free analysis leading to reliable conclusions, even if the initial hypotheses are confirmed. The aim of this study is to explore a novel data treatment method, Common Components and Specific Weights Analysis (CCSWA or ComDim), which relies on the multivariate analysis of multiple tables.

In a first section we will review the principle of the method and its potential uses in the analysis of supersaturated designs; we will then present some applications.

2. The Common Components and Specific Weights Analysis, or ComDim

2.1. General presentation

The Common Components and Specific Weights Analysis method, or ComDim, was developed to simultaneously consider multiple line-paired tables to sequentially determine the components that are common to all the tables and the contribution of each of the tables to each of these components. Historically, this method was developed

* Corresponding author. Tel.: +33 491288186.
E-mail address: m.claeys-bruno@univ-amu.fr (M. Claeys-Bruno).

http://dx.doi.org/10.1016/j.chemolab.2016.01.014
0169-7439/

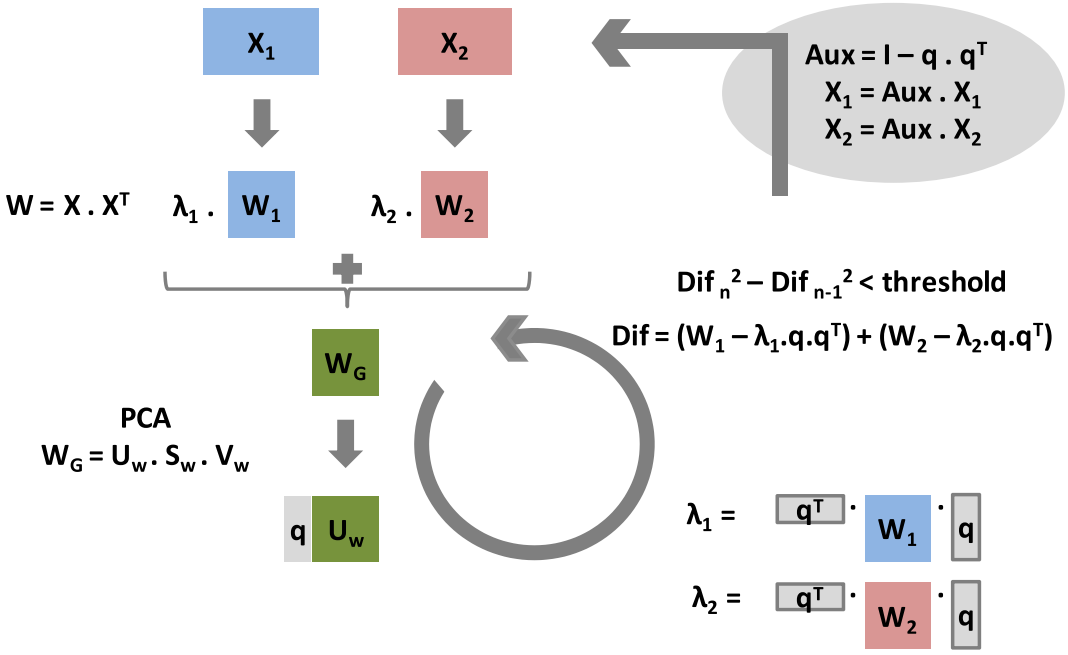

Fig. 1. Algorithm of the **C**ommon **C**omponents and **S**pecific **W**eights **A**nalysis or ComDim method [29].

to analyse tables as part of sensory assessment [20–23]. More recently it has been used to combine various analytical methods [24–26]. We will use an implementation of this method known as ComDim in the *SAISIR* toolbox [27,28] with which we can simultaneously explore several tables while seeking explanations for the common spatial dimensions defined by the tables. In other words, ComDim determines a common

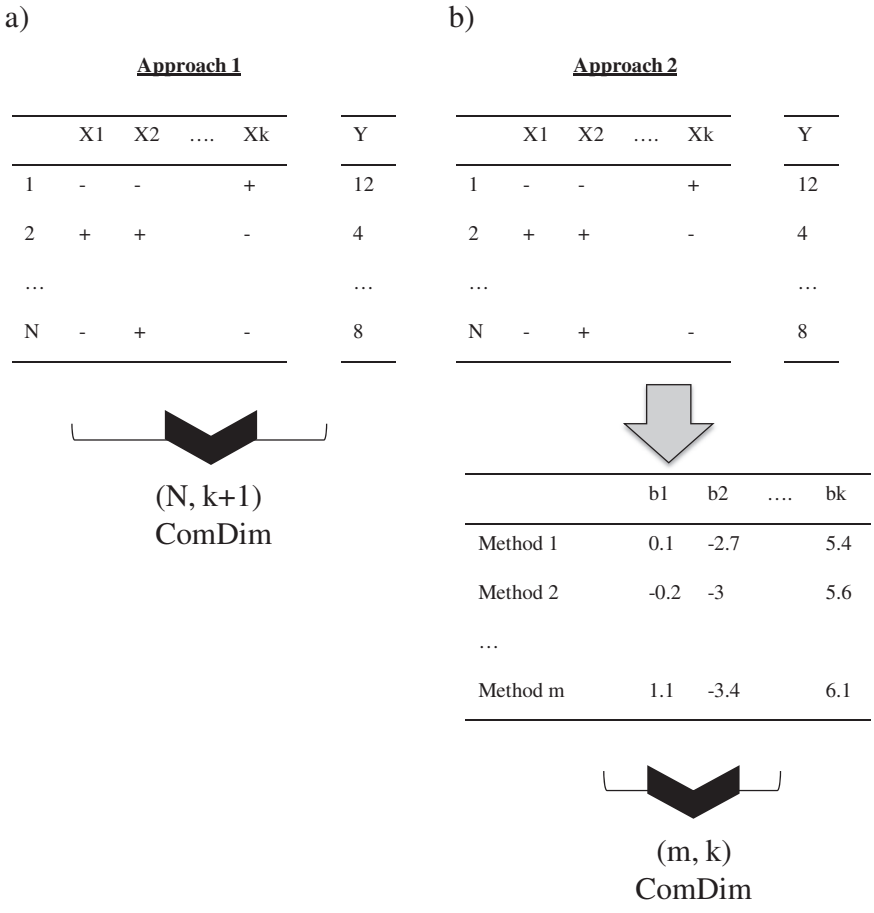

Fig. 2. The ComDim method can be used in two different ways to treat supersaturated designs.