## Accepted Manuscript

Sparse N-way partial least squares with R package sNPLS

D. Hervás, J.M. Prats-Montalbán, A. Lahoz, A. Ferrer

PII: S0169-7439(18)30238-7

DOI: 10.1016/j.chemolab.2018.06.005

Reference: CHEMOM 3641

To appear in: Chemometrics and Intelligent Laboratory Systems

Received Date: 18 April 2018

Revised Date: 11 June 2018

Accepted Date: 16 June 2018

Please cite this article as: D. Hervás, J.M. Prats-Montalbán, A. Lahoz, A. Ferrer, Sparse N-way partial least squares with R package sNPLS, *Chemometrics and Intelligent Laboratory Systems* (2018), doi: 10.1016/j.chemolab.2018.06.005.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



## Sparse N-way Partial Least Squares with R Package sNPLS

Hervás, D.<sup>a</sup>; Prats-Montalbán, J.M.<sup>b\*</sup>, Lahoz A.<sup>c\*</sup> and Ferrer, A.<sup>b</sup>

a) Biostatistics Unit, Health Research Institute La Fe, Valencia, Spain
b) Multivariate Statistical Engineering Group, Universitat Politècnica de València, Valencia, Spain
c) Biomarkers and Precision Medicine Unit, Health Research Institute La Fe, Valencia,

Spain

\* Corresponding author: José M. Prats-Montalbán. Departamento de Estadística e IO Aplicadas y Calidad. Universidad Politécnica de Valencia. Cno. De Vera s/n, Edificio 7A, 46022, Valencia, Spain. Tlf: +34.96.387.70.07 ext. 74949, Fax: +34.96.387.74.99. E-mail: jopramon@eio.upv.es

\* Corresponding author: Agustín Lahoz. Biomarkers and Precision Medicine Unit, Analytical Unit (Metabolomics). Health Research Institute La Fe, Torre A-6-19. Avda. Fernando Abril Martorell, 106. 46026, Valencia, Spain. Tlf +34.96.124.66.52, Fax +34.96.124.66.20. E-mail: agustin.lahoz@uv.es

## Abstract

We introduce the **R** package **sNPLS** that performs *N*-way partial least squares (*N*-PLS) regression and Sparse (L1-penalized) *N*-PLS regression in three-way arrays. *N*-PLS regression is superior to other methods for three-way data based in unfolding, thanks to a better stabilization of the decomposition. This provides better interpretability and improves predictions. The sparse version also adds variable selection through L1 penalization. The sparse version of *N*-PLS is able to provide lower prediction errors and to further improve interpretability and usability of the *N*-PLS results. After a short introduction to both methods, the different functions of the package are presented by displaying their use in simulated and a real dataset.

Keywords: N-PLS, LASSO, Sparse matrices

Download English Version:

## https://daneshyari.com/en/article/7561842

Download Persian Version:

https://daneshyari.com/article/7561842

Daneshyari.com