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Abstract:

Progress made in the design of spectrometric equipment but also in the processing of associated spectral data has democratized the use of spectrometry for experimental acquisitions. In agronomy, spectral data has thus demonstrated its value for disease detection *(Mahlein et al., 2012)* or even for crops monitoring *(Ecarnot et al., 2013; Mahajan et al., 2016; Vigneau et al., 2011)*. Consequently, spectral data are expected to increasingly be associated with experimental designs. An experimental design is designed to study the variables involved, called factors. In agronomy, these factors can be genotype, treatment or time. An experimental design allows as well, to separate and evaluate the effects of these factors on variance *(Kirk, 1982)* with a minimum of experiments. Especially for multivariate data where all sources of variability may affect conclusions *(Massart, 1997)*.

Lately, chemometrics methods have been developed to analyze multivariate data fully integrated to an experimental design *(Brereton et al., 2017)*. Initially used in metabolomics as NMR spectroscopy and chromatography, ANOVA-Simultaneous component analysis (ASCA) *(Smilde et al., 2005)* and ANOVA-Target-Projection (ANOVA-TP) *(Marini et al., 2015)* provide statistical significance of every factor and information about their effect on the variability of the data. We are interested here in the use of these techniques for the study of vegetation spectra associated with an appropriate experimental design.

In this presentation, we first discuss the assumptions involved in ASCA and ANOVA-TP. Then, we compare these methods to analyze a dataset of 480 vegetation spectra where 10 genotypes of maize are confronted to 2 irrigation treatments. Spectra are acquired above the crops with a high-spectral resolution (256 bands) in the range of 310 nm – 1100 nm. The obtained results confirm that both methods, with their own specificities, are relevant to describe the influences of factors on the variance. ASCA and ANOVA-TP share many similarities and provide the same conclusions concerning the significance of each factor. However some differences are highlighted in terms of scores and loadings. Indeed, ASCA provides orthogonal loadings whereas ANOVA-TP gives accurate estimation of between and within-class variance.

References

Brereton, R.G., Jansen, J., Lopes, J., Marini, F., Pomerantsev, A., Rodionova, O., Roger, J.M., Walczak, B., Tauler, R., 2017. Chemometrics in analytical chemistry—part I: history, experimental design and data analysis tools. Anal. Bioanal. Chem. 409, 5891–5899.

Ecarnot, M., Compan, F., Roumet, P., 2013. Assessing leaf nitrogen content and leaf mass per unit area of wheat in the field throughout plant cycle with a portable spectrometer. Field Crops Res. 140, 44–50. https://doi.org/10.1016/j.fcr.2012.10.013

Harrington, P. de B., Vieira, N.E., Espinoza, J., Nien, J.K., Romero, R., Yergey, A.L., 2005. Analysis of variance–principal component analysis: A soft tool for proteomic discovery. Anal. Chim. Acta 544, 118–127. https://doi.org/10.1016/j.aca.2005.02.042

Kirk, R.E., 1982. Experimental design. Wiley Online Library.

Mahajan, G.R., Pandey, R.N., Sahoo, R.N., Gupta, V.K., Datta, S.C., Kumar, D., 2016. Monitoring nitrogen, phosphorus and sulphur in hybrid rice (Oryza sativa L.) using hyperspectral remote sensing. Precis. Agric. https://doi.org/10.1007/s11119-016-9485-2

Mahlein, A.-K., Steiner, U., Hillnhütter, C., Dehne, H.-W., Oerke, E.-C., 2012. Hyperspectral imaging for small-scale analysis of symptoms caused by different sugar beet diseases. Plant Methods 8, 1.

Marini, F., de Beer, D., Joubert, E., Walczak, B., 2015. Analysis of variance of designed chromatographic data sets: The analysis of variance-target projection approach. J. Chromatogr. A 1405, 94–102. https://doi.org/10.1016/j.chroma.2015.05.060

Massart, D.L. (Ed.), 1997. Handbook of chemometrics and qualimetrics, Data handling in science and technology. Elsevier, Amsterdam ; New York.

Smilde, A.K., Jansen, J.J., Hoefsloot, H.C.J., Lamers, R.-J.A.N., van der Greef, J., Timmerman, M.E., 2005. ANOVA-simultaneous component analysis (ASCA): a new tool for analyzing designed metabolomics data. Bioinformatics 21, 3043–3048. https://doi.org/10.1093/bioinformatics/bti476

Vigneau, N., Ecarnot, M., Rabatel, G., Roumet, P., 2011. Potential of field hyperspectral imaging as a non destructive method to assess leaf nitrogen content in Wheat. Field Crops Res. 122, 25–31. https://doi.org/10.1016/j.fcr.2011.02.003