Multivariate statistical approaches for wine classification based on low molecular weight phenolic compounds

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A short running title: Multivariate statistical for wine classification

Abstract

Background and Aims: Phenolic compounds influence the colour, flavour and astringency of wines. These compounds are extracted into the wine during grape fermentation and maceration and thus the winemaking process is the main factor affecting the phenolic content of wines, besides the varietal factor. In this work, we aimed to apply self organizing maps to investigate the relationships between the profile of phenolic compounds and grape variety of wines, as well as the changes in the phenolic profile resulting from the malolactic fermentation. The results are compared with principal component analysis, and variation partitioning.

Methods and Results: A reversed phase liquid chromatography/DAD method was used for the analysis of major non-flavonoid phenolic compounds in wines. The method employed allowed to evaluate the impact of malolactic fermentation in low molecular phenolic compounds in different wine varieties: Trincadeira, Aragonez, Cabernet Sauvignon, Alfrocheiro, Castelão and Touriga Nacional. The malolactic fermentation process was also study in Trincadeira variety using indigenous bacteria and two different commercial lactic bacteria. The impact of malolactic fermentation and grape varieties on the phenolic profile was evaluated by different multivariate statistical approaches: principal component analysis, variation partitioning analysis and artificial neural network.

Conclusions: Principal component analysis allowed to explain 86.5% of the total variance among samples, without any additional information. Artificial neural network showed a significant clustering of samples according to grape variety, and confirmed that malolactic fermentation has a minor effect on wines phenolic profile. Variance partitioning enable to extract more information about the data since it allow to identify explanatory variables responsible for variability among samples. In this study, it was

possible to identify grape variety as the main responsible factor for explaining total variability (63.6%) being malolactic fermentation responsible only for 4.0%

Significance of Study: The results obtained from each of the three multivariate statistical approaches showed clearly ways of analyzing and handling large chemistry experimental data sets. When explained variables are available in the data set, the variance partitioning method could be considered as a step forward in the data analysis, providing a more solid and complete information concerning the variability on the sample system allowing a more objective result not possible by PCA and neural networks alone.

Key Words

Wine; Phenolic compounds; Principal component analysis; Variance partitioning; Artificial Neural Networks