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Relationship between astringency and phenolic composition of commercial Uruguayan Tannat wines: Application of boosted regression trees

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ABSTRACT

Phenolic compounds play a major role in the intensity and characteristics of wine astringency. However, studies involving commercial wine samples are still scarce. The aim of the present work was to study the relationship between astringency and phenolic composition of commercial Uruguayan Tannat wines using boosted regression trees (BRT), a novel predictive method. Forty commercial Tannat wines were evaluated by a trained sensory panel (9 members), who assessed their total astringency intensity using time-intensity (TI) and described their astringency sub-qualities using a check-all-that-apply (CATA) question composed of sixteen terms. The polyphenolic profiles of the wines were determined by HPLC-MS and conventional oenological parameters were also obtained. Fifty BRT models with different partitions of the data in training and test sets were built for astringency maximum intensity (Imax) and for the frequency of use of the 16 astringency sub-qualities considered in the CATA question. As predictor variables, 84 phenolic compounds and oenological parameters were considered for all BRT models. Both strong and weak predictive models were obtained for each response variable. Predictive accuracy was much higher for astringency intensity than for the frequency of mention of astringency sub-qualities. Still, the BRT models allowed to point out to some compositional variables most likely involved in wine astringency perception. Total tannin concentration (chemically determined) was the most relevant explanatory variable for sensory astringency, while flavan-3-ols were the individual phenolic compounds with the highest contribution to astringency, particularly some dimers, trimers and the sum of non-galloylated tetramers. However, the effect of these predictors differed according to the astringency sub-quality considered as response. As expected, non-linear relationships between phenolic compounds and astringency were found. These results contribute to the understanding of the influence of phenolic composition on wine astringency and stress the potential of BRT models for identifying the compounds responsible for this complex sensory characteristic.

1. Introduction

Red wine astringency has been reported to have a strong influence on wine's quality, complexity and persistence, which has placed it as one of the most relevant sensory characteristics of this product (Cheynier & Sarni-Manchado, 2010; Gawel, 1998; Peynaud, 1987). This sensory characteristic comprises a complex set of sensations related to drying, roughing and puckering of the mouth epithelium (ASTM, 2004).

Wine astringency has been mainly related to the presence of non-volatile phenolic compounds (Cheynier & Sarni-Manchado, 2010; Kennedy, Saucier, & Glories, 2006) and their ability to interact with salivary proteins. However, the mechanisms of astringency perception have not been fully unveiled yet (Ferrer-Gallego, Hernández-Hierro, Rivas-Gonzalo, & Escribano-Bailón, 2014; Ma et al., 2014).

Wine phenolics comprise a huge and heterogeneous family of compounds such as anthocyanins, phenolic acids, flavonols, flavanols and tannins, as well as a vast number of compounds derived from them through different chemical reactions (Garrido & Borges, 2013). For this reason, one of the foremost challenges of identifying the key individual or groups of compounds that contribute to astringency is the wide

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diversity of chemical structures (Ferrer-Gallego et al., 2014). Phenolic compounds range from simple low-molecular-weight compounds to large polymers with diverse substituents, and can be classified based on their number and arrangement of carbon atoms into flavonoids and non-flavonoids (Cozier, Jaganath, & Clifford, 2006; Garrido & Borges, 2013). Non-flavonoid phenolic compounds found in grapes and wine are phenolic acids, which can be divided into hydroxybenzoic acids (e.g. gallic acid) and hydroxycinnamic acids (e.g. *p*-coumaric acid) (Ribéreau-Gayon, Glories, Maujean, & Dubourdieu, 2006). On the other hand, relevant families of flavonoids for grape and wine are flavonols (e.g. quercetin), flavan-3-ols (e.g. (+)-catechin) and anthocyanins (e.g. malvidin-3-O-glucoside), among others (Garrido & Borges, 2013). Flavan-3-ols are the most diverse family of flavonoids, with compounds ranging from simple monomers to large and complex polymers (Cozier et al., 2006). Tannins are by definition substances capable of binding with proteins and other polymers, and correspond to polymers of simpler monomeric phenolic compounds (Ribéreau-Gayon et al., 2006). Usually, they are classified into hydrolyzable and non-hydrolyzable or condensed tannins. Hydrolyzable tannins are polymers of gallic acid and hexahydroxydiphenoyl acid, and as their name suggest, they can be degraded though pH changes and through enzymatic or non-enzymatic hydrolysis into smaller fragments (Cozier et al., 2006; Garrido & Borges, 2013). On the other hand, condensed tannins are oligomers and polymers of flavan-3-ols, and are also known as proanthocyanidins (Ribéreau-Gayon et al., 2006). Tannins that are naturally present in grapes and wine are predominantly of the condensed type (Garrido & Borges, 2013).

Proanthocyanidins have been pointed out by several authors as the major contributors of astringency intensity (Brossaud, Cheynier, & Noble, 2001; Lesschaeve & Noble, 2005). Besides its total concentration, individual characteristics of proanthocyanidins, such as their mean degree of polymerization and their subunit composition and distribution, have been reported to largely influence astringency perception (Chira, Jourdes, & Teissedre, 2012; Chira, Pacella, Jourdes, & Teissedre, 2011; Preys et al., 2006; Quijada-Morín et al., 2012; Vidal et al., 2003). However, recent research has demonstrated that low molecular weight non-volatile molecules, including flavan-3-ol and flavonol monomers and dimers, hydroxycinnamic and hydroxybenzoic acids, are also implied with red wine astringency (Ferrer-Gallego et al., 2014; Ferrer-Gallego et al., 2016; Gonzalo-Diago, Dizy, & Fernández-Zurbano, 2014; Hufnagel & Hofmann, 2008; Sáenz-Navajas, Avizcuri, Ferreira, & Fernández-Zurbano, 2012; Sáenz-Navajas, Tao, Dizy, Ferreira, & Fernández-Zurbano, 2010).

In addition, it could be hypothesized that different astringent sensations may be related to specific polyphenolic structures that elicit astringency through different mechanisms. Although most studies on the relationship between phenolic composition and wine astringency have focused on its global intensity (Boulet et al., 2016; Gonzalo-Diago et al., 2014; Kallithraka, Kim, Tsakiris, Paraskevopoulos, & Soleas, 2011; Preys et al., 2006; Quijada-Morín et al., 2012; Quijada-Morín, Williams, Rivas-Gonzalo, Doco, & Escribano-Bailón, 2014), some advances have been recently made in identifying relationships between specific compounds and astringency sub-qualities (Ferrer-Gallego et al., 2014; Ferrer-Gallego et al., 2016; Gawell, Francis, & Waters, 2007; Hufnagel & Hofmann, 2008; Vidal et al., 2003; Vidal et al., 2004). For example, Hufnagel and Hofmann (2008) have reported that certain flavon-3-ol and dihydroflavon-3-ol glycosides elicit velvety astringency. However, there are still too few studies involving commercial wine samples (Sáenz-Navajas et al., 2010; Sáenz-Navajas et al., 2012; Sáenz-Navajas et al., 2015).

A vast number of regression methods are available both for prediction and to extract information about the mechanisms that associate response variables to a set of exploratory variables (Elith, Leathwick, & Hastie, 2008). Most research attempting to establish relationships between sensory characteristics and wine composition have relied on simple correlation tests and simple or multiple linear least square regressions (Boulet et al., 2016; Gonzalo-Diago et al., 2014; Kallithraka et al., 2011; Quijada-Morín et al., 2012; Sáenz-Navajas et al., 2015). Others have used more sophisticated multivariate statistical methods, such as Principal Component Analysis (PCA), Partial Least Square Regression (PLSR) and Common Components and Specific Weights Analysis (CCSWA) (Bindon et al., 2014; Preys et al., 2006; Sáenz-Navajas et al., 2010; Sáenz-Navajas et al., 2012). These approaches rely on statistical data modelling and therefore assume that the mechanism that generated the data can be described by an appropriate stochastic model. For this reason, they may not be appropriate to study complex phenomena, such as wine astringency.

On the contrary, algorithmic modelling assumes that the observed data is generated by an unknown and complex process, relying on an algorithm to learn patterns in the data and predict the response variable from the independent ones (Breiman, 2001). A vast number of these algorithmic methods, also known as machine learning methods, have been developed and popularized in the last decades (Hastie, Tibshirani, & Friedman, 2009). In the present work, a relatively new method called Boosted Regression Trees (BRT) was applied to build a predictive model for astringency intensity and astringency sub-qualities based on the polyphenolic profile of the wines.

BRT takes advantage of both statistics and machine learning techniques: it combines a large amount of simple regression trees to build a single model that optimizes the predictive performance (Elith et al., 2008). This approach has several advantages compared to other methods, such as the ability to include both categorical and continuous variables and to handle missing data, a high tolerance to outliers and invariance under transformations of the predictors (thus, scaling is not an issue). They also perform internal feature selection, so they are not affected by the inclusion of many irrelevant predictor variables (Hastie et al., 2009). Besides, they can model nonlinear responses, which are likely to be relevant for astringency perception. The application of BRT in food science is still scarce although some recent applications can be found in the literature, including predictive models for wine age (Rendall, Pereira, & Reis, 2017) and for antioxidant capacity of soluble coffee (Podio et al., 2015) and wheat (Podio, Baroni, & Wunderlin, 2017) based on their phenolic profile.

In this context, the aim of the present work was to study the relationship between astringency and phenolic composition of commercial Uruguayan Tannat wines using boosted regression trees. Tannat is a red variety of *Vitis vinífera* that has become Uruguay's emblematic wine variety (Carrau, 1997). Tannat wine is characterized by its high total content and differential composition of phenolic compounds, which are responsible for its intense colour and high astringency compared with other red wines (Alcalde-Eon, Boido, Carrau, Dellacassa, & Rivas-Gonzalo, 2006; Blanchard, 1999; Boidron et al., 1995; González-Neves, Gómez-Cordovés, & Barreiro, 2001). Research on the astringency characteristics of Tannat wine and their relationship with phenolic composition is relevant for the Uruguayan wine industry, as this type of information has been reported for other red wine varieties but not yet for Tannat. The present work focused on 40 commercial Tannat wines, which have been previously characterized by a sensory trained panel (Vidal et al., 2017).

2. Materials and methods

2.1. Wine samples

Forty commercial samples of Uruguayan varietal Tannat wine were obtained directly from the wineries. Samples were selected to represent high quality Uruguayan Tannat wines but providing different astringency characteristics. Samples from different wineries, vintages (2006 to 2014) and price segments were selected. Furthermore, 28 wines had been aged in oak barrels while the rest had not. Wines were bottled in 750 mL bottles and were conserved at 12 °C until their analysis.