



HOW GEOGRAPHICAL ORIGIN AND VINEYARD MANAGEMENT INFLUENCE CV. CABERNET SAUVIGNON IN CHILE – MACHINE LEARNING BASED QUALITY PREDICTION

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Abstract

Aims: The aims of this study were to i) characterize the impact of geographical origin and viticulture treatments on Chilean Cabernet Sauvignon, and ii) develop machine learning models to predict its quality.

Methods and Results: 100 vineyard plots representing the typical percentage distribution of geographical and viticulture impact factors on Chilean Cabernet Sauvignon were monitored across two seasons, 2018 and 2019. Chemical analysis of grapes and wines included the quantification of phenolic compounds by liquid chromatography and UV-vis spectral measurements, aroma compounds by gas chromatography mass spectrometry (GC/MS), and maturity parameters. Spearman correlation and Principal component analysis (PCA) identified correlations of several non-volatile and volatile compounds with quality, mainly by means of their anthocyanins, flavonols, flavan-3-ols, total tannins and hydroxycinnamic acids. Furthermore by trans-2-hexenol, trans-3-hexenol, hexanal, 2-isobutyl-3-methoxypyrazine (IBMP), yeast assimilable nitrogen (YAN), total soluble solids and acidity. Experimental winemaking of 600 kg per plot followed a standardized procedure, and the wines were analyzed by an expert quality rating. A sensory quality profiling for the wines was performed through a Napping Ultra Flash Profile (UFP). It revealed the distinction of three different quality levels by mainly mouthfeel attributes, and fruity and green aromas. However, neither the observed correlations of chemical analysis and sensory quality ratings, nor origin or viticulture treatment could fully explain quality. Different clustering methods, namely k-means, k-medoids and spectral clustering were evaluated in order to find categories given by the chemical analysis data itself as unsupervised machine learning. Spectral clustering led to optimum results, and independently of sample origin and viticulture traits, quality ratings were characterized to be significantly different across the clusters allowing their interpretation as quality categories.

Conclusions: Chilean Cabernet Sauvignon quality is associated with chemical quality markers known for this variety in Australia and California, including phenolic compounds, C₆ alcohols and aldehydes, IBMP, maturity parameters and YAN. However, evaluation of sensory quality is fairly subjective and viticulture treatments in practical application contain interdependency, therefore it is challenging to establish supervised models involving this data. The application of unsupervised spectral clustering is proposed as an objective quality classification approach, which can be trained using supervised models for predictive purposes.

Significance and Impact of the Study: There is a high industrial need for objective quality classification. For the first time chemical quality markers for Chilean Cabernet Sauvignon were determined, and an unsupervised machine learning approach based on these markers could be proposed for objective quality classification.

Keywords: Cabernet Sauvignon, spectral clustering, quality, terroir, vineyard management

Introduction

Wine quality and style are associated with geographical origin, climate and viticulture management, also understood as the concept of terroir (Leeuwen and Seguin, 2006). The understanding of wine quality, however, is complex and it highly depends on personal conception and experience (Charters and Pettigrew, 2007; Hopfer *et al.*, 2015; Hopfer and Heymann, 2014).

Wide parts of the Chilean Central Valley, located between the Andes and the Coastal Ranges, are used for winegrowing purposes. Chile can be divided into 18 main valleys, where Cabernet Sauvignon is typically cultivated in eight of these valleys between 30°41' SL in Limarí valley in the north, and 36°39' SL Itata valley in the south. The single valleys within the Central Valley are influenced by their location according to longitude which impacts temperature and radiation, and also by latitude that provides differences in precipitation and temperature by the impact of the Pacific Ocean and the Andes Cordillera (Rojas and Ugarte, 2016). Within these given environmental conditions, vineyard management is an important impact factor. In its entirety it can influence yield, photosynthesis, and total productivity of plant primary and secondary metabolites. Plant material including rootstock and scion, and their interactions, determine the exchange between environment, soil and the vine, and therein can influence vine physiology like shoot density, vigor, fruit yield and fruit composition (Sabbatini and Howell, 2013). Rootstock and nutrition uptake, depending on both factors, are also highly related (Lambert *et al.*, 2008). Trellis system and its management manipulate the appearance of the vine, which is an important influencing factor on the leaf area index, total light interception, vine balance, cluster light interception and total cluster microclimate, among others (Reynolds and Vanden Heuvel, 2009).

The sum and interactions of these cultivation conditions, associated with the concept of terroir, result in certain optimum or non-optimum conditions for the vine, which impact the chemical grape composition, and the sensorial properties of the later produced wines (Forde *et al.*, 2011; Leeuwen and Seguin, 2006; Robinson *et al.*, 2014). This raises two main questions: i) the characterization of representative geographical and viticulture data to understand these complex and interacting factors, and ii) the evaluation of grape and wine chemical composition to find the link between chemical composition and sensory properties, and also to translate this information into wine quality prediction based on grape composition. Cabernet Sauvignon composition is generally complex, and among all these compounds previous research has identified a variety of chemical compounds as quality discriminant chemical markers for Cabernet Sauvignon in Australia (Bindon *et al.*, 2020; Niimi *et al.*, 2020) and California, USA (Cleary *et al.*, 2015). These markers included pH, nitrogen compounds, polyphenols including anthocyanins and polymeric tannins, various volatiles including C₆ alcohols and aldehydes, 2-isobutyl-3-methoxypyrazine (IBMP), and terpenoids and their precursors. In the previously cited studies, these compounds were significantly correlated with a positive or negative contribution to wine aroma quality, noting these could still not to a full extent explain sensory wine quality classification, and the interactions are still not completely understood.

The aim of this work therefore was to first study the impact of geographical origin and viticulture on Chilean Cabernet Sauvignon chemical composition and quality. Second, machine learning models were investigated with the purpose of an objective quality classification. As a new approach, spectral clustering was applied on the chemical data as an unsupervised approach aiming the interpretation as quality categories.

Materials and Methods

Cabernet Sauvignon from 100 vineyard plots owned by Viña Concha y Toro (VCT) in Chile was sampled during the 2018 and 2019 seasons with annual duplicates for 90% of the samples. Included parameters were geographical origin (valley, climate), plant material and vineyard management at the level of rootstocks, scion, trellis system, and yield. Grapes were assigned according to their commercial classification (Table 1).

At harvest, yield was determined for each plot, and for grape analysis 50 bunches were randomly picked and bunch weight, number of berries per bunch and berry weight were measured. The berries were crushed and a sample was stored at -20 °C till further analysis. Before analysis, grapes were thawed overnight in the fridge, and samples were ground for 30 seconds with an Ultra Turrax T25 (Ika, Staufen, Germany). Winemaking took place in the CRI experimental winery, with a standardized procedure using approx. 600 kg of grapes. All samples were adjusted to 23.5 °Brix, and pH 3.5, maceration time was five days, alcoholic fermentation (AF) was terminated at residual sugar of < 2 g, malolactic fermentation (MF) at < 0.2 g/L malic acid, and SO₂ was adjusted to 35 mg/L. Wines were filtered (Nexis A, Pall, New York, USA), controlled for nephelometric turbidity units (NTU, < 20, turbidity meter 2100Qis, Hach, Loveland, USA), O₂ (< 1mg/L, multimetro HQ30d, Hach, Loveland, USA) and CO₂

(< 800 mg/L, decarbonisation, equipment LMS, Brigachtal, Germany), bottled in 0.75L green glass bottles (sanitized with ozone, inert N₂) with screw caps, and stored at 12 °C.

Table 1: Geographical origin and viticulture impact factors, with number of samples for harvest year 2018/2019, or ^b determined range in 2018-2019. ^a Reference Giraldo Olmos, 2017.

Valley	Aconcagua (1/1), Cachapoal (14/12), Colchagua (26/32), Curicó (8/7), Itata (1/1), Limarí (2/2), Maipo (16/18), Maule (32/31)
Climatic indices ^a (accumulated)	photometric index (iftta), Richardson cold units (uRa), cold hours (hfa), cold stress hours (efa, <10°C), photosynthetic active hours (hepa, 10-30°C), heat stress hours (sta, >30°C), precipitation total (pac), degrees total (dga)
Scion	169 (1/1), 170 (0/1), 191 (4/3), 337 (11/13), 341 (6/6), 412 (0/1), 685 (0/1), 46C (2/8), massal selection 1 (2/2), massal selection 2 (72/66), R5 (2/2)
Rootstock	101-14 (6/7), 110R (1/3), 3309C (4/4), 5BB (2/2), Own-rooted (80/82), gravesac (1/0), Paulsen (1/1), SO4 (5/5)
Trellis system	Cruceta (3/2), Geneva doble curtain, GDC (1/1), Lyre (1/0), Minimal pruning (10/8), Pergola (26/30), Vertical shoot position, VSP (59/63)
Yield (t/ha)	0 ≥ 10 (19/28), 10 ≥ 20 (37/38), 20 ≥ 30 (27/22), 30 ≥ 40 (12/9), ≥ 40 (5/7)
Berry weight (g) ^b	0.38 - 1.59
Year of planting ^b	1904-2015
Commercial classification	Standard (low to high): S3 (30/28), S2 (20/23), S1 (0/0) Premium (low to high): P3 (36/38), P2 (10/11), P1 (4/4)

Grapes and wines were subjected to chemical analysis (Table 2). Basic analyses were measured enzymatically with Analyzer Y15 (Biosystems, Food Quality, Barcelona, Spain). Total phenolic compounds were analyzed by UV-vis spectroscopy (Cary 60, Agilent Technologies Santa Clara, USA). Anthocyanins, flavan-3-ols, flavonols and hydroxycinnamic acids were analyzed by HPLC-DAD (1290 Infinitely Series, oven 1290 TCC G1316C, 1260 DAD G4212B, Agilent Technologies Santa Clara, USA). Grape derived volatiles were analyzed by GC-MS (7890B GC oven, 7000C Triple Quad, 7693 ALS CombiPal 7697A, Agilent Technologies Santa Clara, USA).

Sensory quality profiling with a subset of 10 experimental wines of 2019 was done in replication with a panel of enologists of VCT (2 female, 14 male, 27-60 years) by Napping UFP based on Pagès, 2005. Napping was for global quality, and UFP asked to provide the assignation to quality level low, medium or high, and up to five descriptive attributes. Quality evaluation of all wines was independent ratings of overall quality, mouthfeel quality and aromatic quality on a structured scale between 1 (low) to 9 (high) by the same panel.

Data analyses were done using Add-in XLSTAT (version 2020. 3.17, Addinsoft, Paris, France) in Excel 2010 (Microsoft, Redmond, USA), and with the software R (R, 2013) which was used with different packages including FactoMineR package (Le *et al.*, 2008), SensomineR package (Le and Husson, 2008), cluster packages by Maechler *et al.* (2019) and by Kawa (2018).

Table 2: Chemical measurements of grapes and wines, partially only measured in ^a grape or ^b wine. Abbreviations: Gl: glycosid/glycosylated, Ac: acetylated, Cum: cumarylated, Gal: galactoside, Ac: acid.

Basic analysis	Total acidity, pH, Malic acid ^a , Total Soluble Solids (°Brix) ^a , Yeast Assimilable Nitrogen (YAN) ^a , °Ethanol ^b , volatile acidity ^b , residual sugar ^b
Phenolic compounds	Total Phenols Index (OD280), Color Index (OD420+OD520+OD620), Tannins (methyl cellulose precipitable, MCP), Anthocyanins (Decoloration SO ₂), Polymeric Pigments, Tannins, Phenols, Non Tannin Phenols, Anthocyanins (all Adams-Harbertson method)
Anthocyanins	Delphinidin-3-O-Gl, Cyanidin-3-O-Gl, Petunidin-3-O-Gl, Peonidin-3-O-Gl, Mavidin-3-O-Gl, Peonidin-3-O-Ac-Gl, Malvidin-3-O-Ac-Gl, Peonidin-3-O-Cum-Gl, Malvidin-3-O-Cum-Gl
Flavan-3-ols	Catechin, Epicatechin, Epicatechin-Gallate
Flavonols	Myricetin 3-O-Gal, Myricetin 3-O-Gl, Myricetin, Rutin, Hyperoside, Quercetin 3-O-Gl, Quercetin, Laricitin Hex., Siringin 3-Gal, Siringin 3-Gl, Kaempferol
Hydroxycinnamic acids	Caftaric Ac., Caffeic Ac., Coumaric Ac.
Grape derived volatile compounds	Hexanal, Trans-2-Hexenol, Cis-3-Hexenol, Trans-3-Hexenol, 1,4-Cineole, 1,8-Cineole, Linalol, α-Terpeneol, Citronellol, Nerol, Geraniol, β-Damascenone β-Ionone, 3-Isobutyl-2-methoxy-pyrazine (IBMP)

Results and Discussion

Origin and Viticulture Impact on Chemical Composition

Harvest year impacted all chemical measurements, as pairwise RV coefficients were below 0.3 for all compounds including harvest parameters. This could be aligned by normalization of the results; Robert and Escoufier, 1976). PCA of the 2018 and 2019 normalized grape data revealed a negative correlation of polyphenolic compounds including flavan-3-ols, flavonols, hydroxycinnamic acids, anthocyanins and tannins (by HPLC and UV-vis), °Brix and pH against volatile compounds including IBMP, trans-2-hexenol, trans-3-hexenol, hexanal, acidity and YAN by principal component (PC) 1 for grapes (figure 1, 30.2%). By PC 2 (8.5%), few individual samples were furthermore separated due to terpenoids including alpha-terpeneol, beta-damascenone, and cineole. The results for wines were consistent with these findings, only ethanol added to the correlation on the polyphenols side, furthermore the impact of volatiles was increasing, while it was decreasing for hydroxycinnamic acids (not shown). The commercial quality classification was associated with the chemical measurements, and premium samples were to a large extent projected with the phenolic compounds, and standard samples vice versa. However, especially the medium part was characterized by superposition of premium and standard classification, and considerable numbers of outliers were observed. As the decision about commercial classification is made based on viticulture data and experience of agricultural engineers, an objective classification based on chemical measurements is considered to improve the results. However, the observed association of measurements and quality was in accordance with previous investigations that had aimed to define quality markers for Cabernet Sauvignon in Australia and California (Bindon *et al.*, 2020; Niimi *et al.*, 2020, Cleary *et al.*, 2015). The discussed chemical compounds were hereupon considered as representative for Chilean Cabernet Sauvignon.

Regarding geographical and viticulture determinants, coldness (hfa, efa, uRa) and precipitation (pac) were associated with valleys located more in the south, that are naturally characterized by colder and rainier climate compared to other wine producing regions. This included Maule, Itata, and Curico (Figure 1). Consequently these valleys were also correlated with more photosynthesis productive hours between 10-30°C (hepa). Heat (dga, sta) vice versa, was associated with valleys of the north that overpass 30 °C regularly, including Maipo, Aconcagua and Colchagua. Regarding the geographic influence on the chemical measurements, C₆ alcohols and aldehydes, and IBMP were associated with the colder regions, and terpenoids and polyphenolic compounds with warmer regions. However, the existing interdependence with viticulture impact factors complicated the interpretation. Maule valley, as an example, was completely committed to the application of trellis system VSP, aiming to produce high quality wines. VSP, due to its application, is associated with low yield, and smaller grape berries, which has an impact on chemical composition (Forde *et al.*, 2011). Furthermore, viticulture factors were difficult to assess. VSP and pergola were widely used, and could be associated with yield and berry size (low for VSP, high for pergola), but due to its particular distribution no further conclusions could be drawn from the plant material.

Sensory Quality and Correlation with Chemical Measurements

Napping UFP revealed diverse and partially very subjective attributes associated with quality by the enologist panel, which had been expected as quality evaluation underlies subjectivity even for experts (Hopfer and Heymann, 2014). However, filtering attributes by three or more panelists, mainly very personal descriptions (usable, green touch, good potential, etc.), synonyms and redundancy were removed. A Spearman correlation revealed distinction correlations of the quality levels low, medium and high, in which the panelists did have a consensus. Positively correlated were red, black, ripe and fresh fruits (fruity aromas) together with mouthfeel descriptors including full body, juiciness, fat, concentrated and softness, while attributes expressing vegetal, bell pepper, grassy (green aromas) and dryness, tannins, bitterness or watery were negatively correlated (not shown).

The ratings of global, mouthfeel and aromatic quality were then correlated (Spearman) with the chemical measurements (Figure 2). From the grape data, the highest correlations with wine global quality were found for maturity parameters °Brix (0.42), pH (0.42), and acidity (-0.52). IBMP negatively influenced global and aromatic quality (-0.41, and -0.55, respectively). Flavan-3-ols and tannins were positively correlated, including epicatechin (0.25). From the wine data, ethanol (0.41) and IBMP (-0.49) were found to have the greatest impact on global quality. Furthermore, flavonols were widely positively, and volatiles including hexenols and terpenoids negatively correlated. However, the observed correlations between sensorial data and the most chemical markers were fairly low, and less specific for individual compounds. This was presumably due to the sensory data, because although a certain consensus was found among the panelists the evaluation of quality is subjective, and the practical working environment of a winery is challenging for detailed analysis (high numbers of samples, lacking availability of panelists). Single sensory descriptors have been shown to highly correlate with chemical measurements (Niimi *et al.*, 2020), however, based on the actual dataset a classification on the chemical markers was aspired.

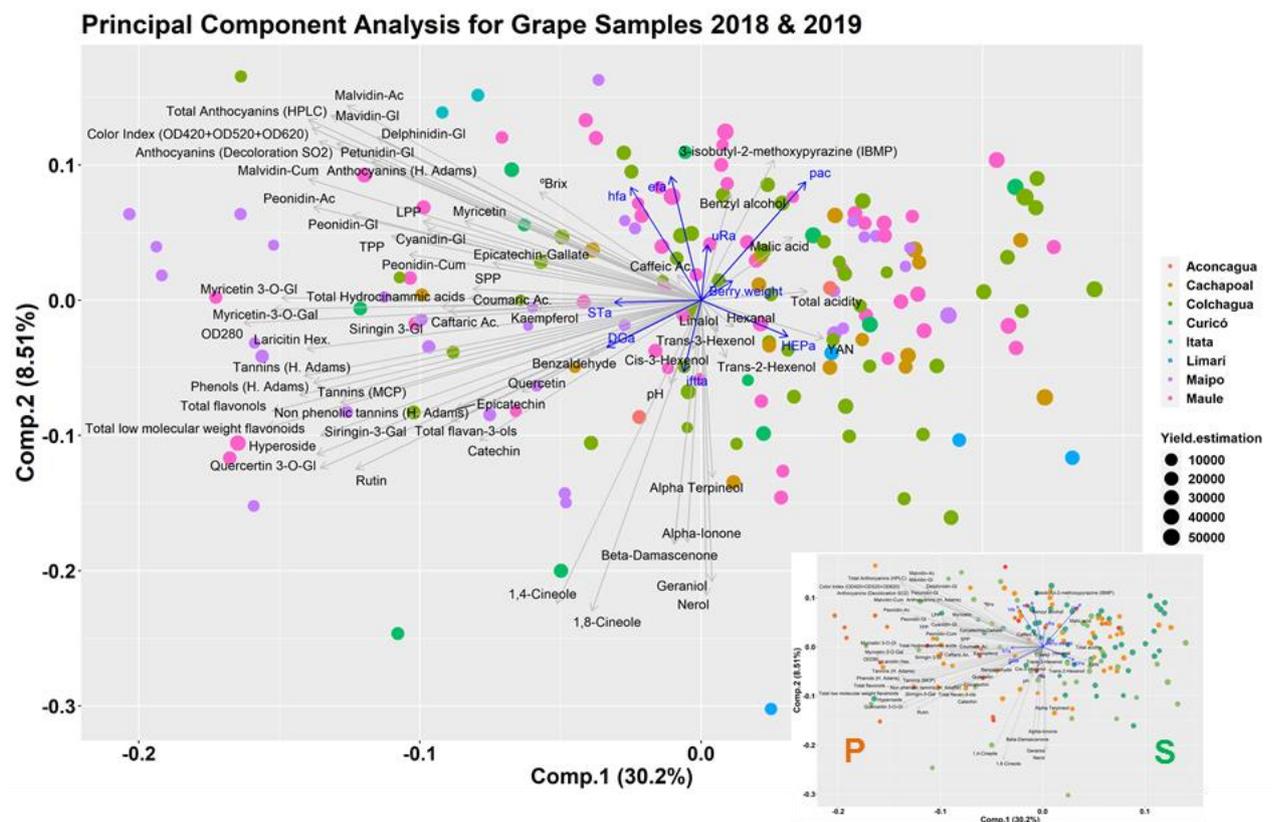


Figure 1: PCA projection of normalized grape chemical measurements, origin and viticulture data (2018 and 2019). Highlighted origin valley (large figure), and commercial classification (S standard, P premium, small figure).

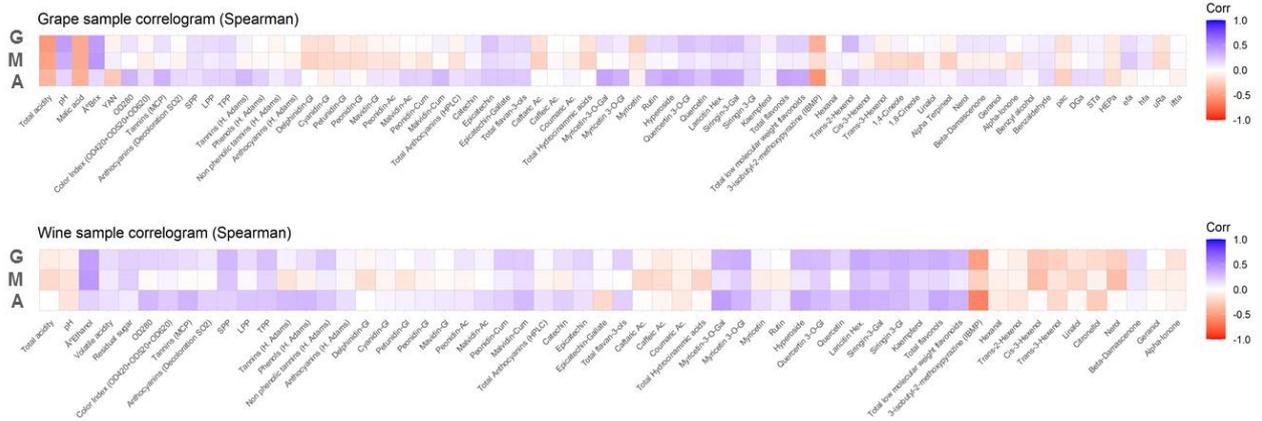


Figure 2: Spearman correlation of global (G), mouthfeel (M) and aromatic (a) quality ratings with markers (2019).

Unsupervised Machine Learning Clustering Models Based on Chemical Measurements

Spectral clustering consists of a graph-based clustering algorithm that calculates the eigen-value decomposition (EVD) on the normalized Laplacian matrix of the data. For the purposes of this study, eigenvector picking was settled to the corresponding eigen-vectors of the smallest two non-zero eigen-values ignoring the trivial constant eigen-vector (Hastie *et al.*, 2013). In order to get the optimal number of clusters, average silhouette method was applied (Charrad *et al.*, 2014). The spectral clustering of the 2018 and 2019 normalized grape and wine chemical measurements resulted in six and four clusters, respectively. ANOVA and Tukey's test of samples that belonged to each cluster revealed the significant drivers for the cluster formation. These were mainly non-volatile phenolic compounds, including anthocyanins, flavonols, flavanols, and hydroxycinnamic acids measured by HPLC, MCP tannins, °Brix, acids, YAN and IBMP for grapes. For wines they were again phenolic compounds, and additionally volatiles were seen to have a more significant impact on the cluster formation, including IBMP, trans-2-hexenol, trans-3-hexenol and hexenal, while monoterpenes and C₁₃-norisoprenoids were without significant impact (not shown). So far, the use of the shown main drivers for Cabernet Sauvignon quality was sufficient to cluster the datasets, and for future analysis it could be considered to include further compounds that have been shown to be markers like amino acids, or esters (Bindon *et al.*, 2020).

Subsequently, the obtained wine cluster model (four clusters) was interpreted with the sensory quality ratings. As a semi-supervised approach, the sensory data available for 2019 was applied on the normalized clusters of the 2018 and 2019 harvest. The clusters had been characterized by decreasing concentrations of phenolic compounds, and increasing concentrations of volatile C₆ compounds and IBMP across the clusters one to four (C1-C4, figure 3). Although the differences were fairly low, the quality ratings were consistently decreasing from cluster one to four, with the exception of mouthfeel which was found to be lowest in cluster two. Interestingly, apart from other phenolic compounds, cluster two had been characterized by outstanding concentrations of tannins and flavan-3-ols that might have led to the lower rating of mouthfeel quality. In general, polyphenolic compounds contribute to mouthfeel sensations, and have been shown to impact the perception of quality (Gawel *et al.*, 2007; Sáenz-Navajas *et al.*, 2011). Mouthfeel descriptors were furthermore highly correlated to quality in the Napping UFP, and volume and astringency were evaluated positively while dryness and tannins were negatively correlated. However, the decreasing rating of aroma quality was presumably associated with the increase of volatile compounds including trans-2-hexanol, trans-3-hexenol, hexenal and IBMP. These volatile compounds evoke the perception of green aromas (Francis and Newton, 2005; Noble *et al.*, 1995), and these green attributes had also been profiled to represent low quality. For this model, the clusters one and four could be applied as four quality categories. As an example, the currently used commercial classification leads to considerable numbers of misclassifications and an improvement can be expected from the spectral clustering prediction (Figure 1 and Figure 3).

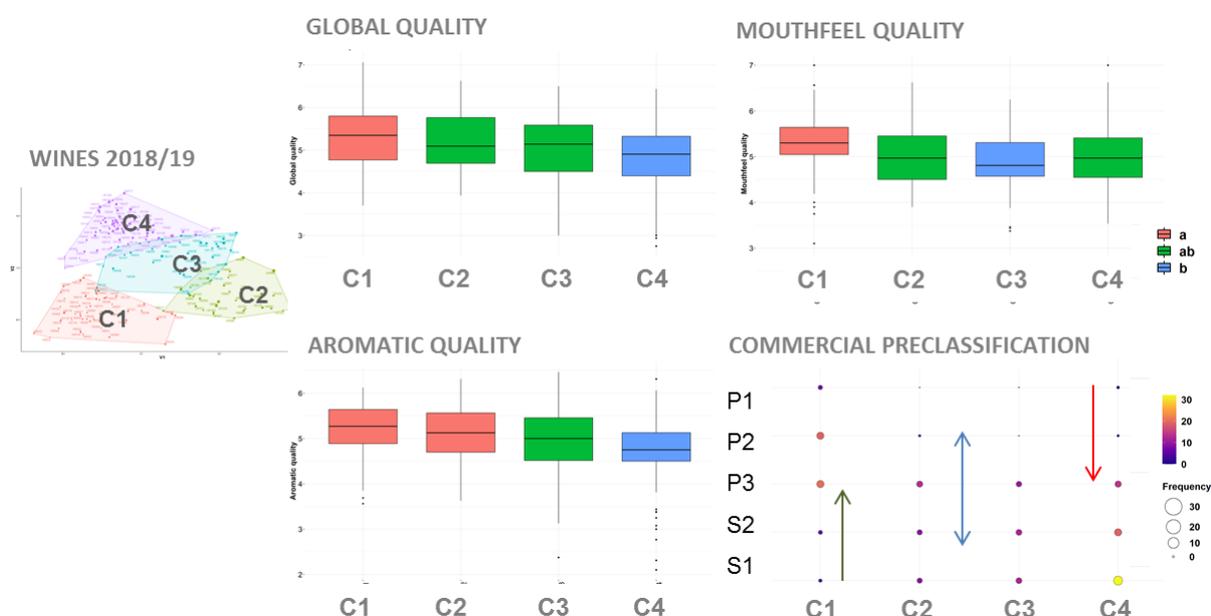


Figure 3: Spectral clustering of normalized wine chemical measurements 2018/2019, and characterization of the 4 obtained clusters sensory quality evaluation and commercial classification. C Cluster, S Standard, P Premium.

Conclusions

With this study and to the best of our knowledge for the first time chemical quality markers for Chilean Cabernet Sauvignon were determined. However, the complexity and interdependence of all external impact factors, associated with the terroir of a vineyard plot, complicate quality prediction of grapes to produce wines of a certain quality or style in the practical working environment of a winery. Sensory quality assessment, although profiled for a general consensus with the evaluating enologist panel, contains subjectivity. To enable objective quality assessment, spectral clustering was applied as unsupervised machine learning including only chemical measurements. The grapes and wines were clustered by the chemical markers known to be main drivers for Cabernet Sauvignon quality, but the advantage, and innovation of spectral clustering is that through the cluster formation the method provides fixed categories from chemical data. The use of the sensorial data to characterize the obtained clusters allows their interpretation as quality categories. In conclusion, spectral clustering is proposed as a powerful method for objective quality classification, suitable for practical application with complex entrance and output variables.

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