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Review

Measuring Wine Quality and Typicity

Marianthi Basalekou *, Panagiotis Tataridis, Konstantinos Georgakis and Christos Tsintonis

Department of Wine, Vine and Beverage Sciences, School of Food Science, University of West Attica, 12243 Athens, Greece
* Correspondence: mbasalekou@uniwa.gr

Abstract: Wine quality and typicity are complex concepts that can be hard to define. Wine is a product destined to not only be consumed and appreciated but also marketed, and its distinctiveness, quality and typicity are important characteristics that describe a wine's sensory profile and, ultimately, add value to the finished product. Even though both quality and typicity are mostly assessed using a sensory evaluation, many studies have examined the feasibility of using chemical analysis methods in order to increase the objectivity of assessments. Today, the use of chemometrics facilitates the handling of big data, and outcomes from various analytical techniques can be integrated to produce more accurate results. This study discusses the existing sensory and analytical approaches, implications and future prospects for an objective measurement of quality and typicity as well as methods for the selection of appropriate data for predictive model development.

Keywords: wine; quality; typicity

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1. Introduction

Wine can be considered both a convenience product and a capital-preserving asset. For this reason, its quality is critical not only for its appreciation but also for its marketing. As an alcoholic beverage obtained exclusively from the total or partial alcoholic fermentation of fresh grapes (Reg. (EU) 1308/2013) [1], wine quality is greatly influenced by the raw material from which it derives most of the key compounds of its matrix. The diversity of grape varieties and terroirs, i.e., the collective effect that geographical origin, climatic conditions and the vinification technique have on the finished product, results in various wine profiles and styles. Geographic origin, in particular, has long been considered an important factor, and, for this reason, many countries have formed guidelines, such as the Protected Denomination of Origin (PDO) set by the European Union, that protect not only specific viticultural sites but also winemaking traditions. PDO labels add value to the wines, which are required to meet certain criteria regarding grape varieties and winemaking techniques and are expected to present similar sensory characteristics considered to be typical of their origin.

Quality and typicity are mostly recognized via sensory evaluation; however, both their evaluation and definition present difficulties. Wine appreciation involves a combination of the main senses and is considered a multisensory experience. Due to its complexity and the various factors affecting how the human brain perceives the multitude of olfactory and gustatory cues, tasting is prone to environmental and psychological variations. As a process with inherent subjectivity, there have been several techniques to increase the repeatability and objectivity of tasting scores and judgments, and many studies investigate the feasibility of using analytical chemistry methods either as an assistive or even a predictive tool. In this study, analytical techniques used for quality and typicity evaluation are discussed, and the possibility of developing prediction models is analyzed.

2. Wine Quality

Quality is generally defined as the degree of excellence of something when measured against other things of a similar kind [2]. To set an objective basis for comparisons, a technically flawless, free-from-faults wine presents a very appealing prototype as its quality can be easily defined with the absence of specific traits. A technically correct wine is expected to be free from microbiological/bacterial contaminations, have SO_2 and volatile acidity levels within the limits set by legislation [3] and should not show any signs of color (pinking or browning in white wines or brownish hues in red wines as a result of anthocyanin and tannin oxidation) or aroma oxidation (mainly acetaldehyde formation) [4]. Defining quality by the absence of flaws/faults may be an appropriate prototype of what is acceptable; however, this is not appropriate for measuring excellence as establishing the "degree of excellence" between acceptable samples requires an evaluation of all aspects involved in a wine sensory profile. Furthermore, to determine which wines are considered to be "similar samples", the vast number of grape varieties derived from different geographical origins and produced with various winemaking protocols should be considered. This task requires knowledge of wine styles and all of the aspects that form wine's olfactory and gustatory profile.

2.1. Aspects of Wine Quality

To evaluate wine quality, all the elements that elicit sensory responses must be assessed. Aroma, taste and mouthfeel are expressed differently in the diverse wine styles, and the multitude of sensory stimuli may be described using a vast descriptive vocabulary. According to Charters, wine quality is evaluated on the basis of taste, smoothness, body, drinkability, balance (the extent of an equilibrium across all olfactory and gustatory cues), concentration and the interest assessment of a wine [5]. Other aspects that may be taken into account include development, i.e., the detection of changes in the aromatic character of the wine as they occur during the tasting; the duration of the retainment of not only aromatic characters but also power and potential, i.e., how the wine is expected to age; complexity (an integrated evaluation of all of its aromatic elements); memorableness; and elegance [6]. Regional standards may also be considered [6].

The words Charters proposes for quality evaluation are abstract, or even aesthetic, driven descriptors, which may translate differently according to each evaluator's personal interpretation. However, the use of more straightforward attributes (which would include a vast number of different descriptors to cover the multitude of wine sensory profiles) would potentially produce rankings based on one-dimensional attributes, while wine perception is multidimensional [7]. Language is based on experience, and successive tasting experiences facilitate the verbalization of sensory patterns. Wine experts (professionals such as producers, winemakers, sommeliers and enologists) [8] develop specific terms for the description of various sensory cues [7] and demonstrate a consensus when evaluating wines based on these terms, however vague they may be.

Even though wine experts base their evaluation on cognitive rather than perceptual sensory spaces (mental representations formed by organoleptic characteristics) [9,10], specific guidelines have to be followed during wine tastings regarding the tasting room, the type and amount of information provided regarding the wines to be tasted, the preparation of the wine (decanting and temperature), the type of glasses to be used [11], the number of samples, the palate cleansing method [12] and the training of the tasters [6] in order to ensure repeatability and minimize error.

2.2. Excellence

Times and palates change, and this is reflected on the new wine styles that emerge constantly. This affects whether a compound is considered an appreciated attribute that adds complexity or perceived as a fault/flaw, which is influenced not only by the current wine trends but also by the culture of the taster. Today, wines with prominent oxidation, orange wines and wines without filtration [13] are opening new markets, and flaws such as protein-related turbidity or the presence of tartrate crystals sediments are forgiven. The need for sulfur-free and "clean" wines has led to the use of natural additives, such as grapevine shoot, almond skin or eucalyptus extracts, and the application of high hydrostatic pressure (HHP), pulsed electric fields (PEF) or high-power ultrasound (HPU), among other techniques. Most of these efforts either have an immediate impact on the volatile composition of wines by altering the perception of fruity characters and freshness or lead to an increase in oxidation compounds during storage [14–16]. In some cases, new odorant compounds may be added to the volatile profile, while in red wines a decrease in the anthocyanin content has been documented when SO_2 was replaced by grape stems or their extracts [17,18]. Moreover, wines today are completely different from those savored years ago. The reason is not only the emergence of new winemaking technologies but also the advance of analytical methods. Before 1982, for example, "brett" was thought to be a characteristic of the aroma of wines from Burgundy, until Anthony Hanson found the nose of stable and farmyard to be objectionable and linked these odors to Brettanomyces contamination [19]. Additionally, typical wine faults such as volatile acidity or acetaldehyde may be perceived as acceptable in wines even though they exceed the sensory perception thresholds or even the limits set by legislation [3]. Indeed, volatile acidity is thought to add complexity to certain wines [20], while acetaldehyde is an important part of the sensory profile of fortified wines such as sherry [21]. A characteristic example in which faults become virtues is the case of a 1947 Château Cheval Blanc wine from Saint–Émilion, which has been described by some critics as the "greatest wine of all time" even though its volatile acidity levels were extremely high and it had 5 g of residual sugar as a result of a stuck fermentation [20]. This wine today would probably not have been marketed.

2.3. Typicity as a Quality Dimension

Another example in which flaws are regarded as part of the sensory profile is the case of mature Riesling wines characterized by kerosene or petrol odors, which are associated with the presence of TDN (1,1,6-trimethyl-1,2-dihydronapthtalene), a C13-norisoprenoid [20]. Even though it is largely considered a favorable attribute of the Riesling aroma, there has been great debate whether it should be labeled a fault/flaw. TDN is mostly present in Rieslings originating from warm climates or vintages, and, for this reason, it is more acceptable from European winemakers than from winemakers from Australia and New Zealand [20].

Thus, to better define quality, it is necessary to take into account the expected or the considered when assessing the typical profile of a wine. It is important to notice that typicality or typicity presupposes quality, in the sense that faults/flaws are incidental and unwanted taints. Typicity assessment normally aids quality evaluation as it provides context for comparisons and can be considered a quality dimension.

3. Typicity

Typicity (or typicality) may be generally defined as "the ability to express a combination of traits characteristic of a distinctive group" [22]. In wine, these traits are connected to the terroir, i.e., the geographical origin of the grapes, the type of the cultivar and the vitivinicultural style, and the techniques applied for its production. Typicity derives from the word "typicité", which is used in the French wine world to describe the connection of a wine to its terroir. For this reason, in many studies, the word "typicality" is used when assessing distinctive components of terroir such as variety or origin. However, most researchers do not differentiate between the two words [23] and may use, for example, both "varietal typicity" and "varietal typicality".

3.1. Typicity and Consumer Expectation

In wine marketing, typicity is connected to expectation. A wine may present varietal typicity, brand typicity or be typical of its origin. For example, as mentioned earlier, a mature Riesling is expected to smell of kerosene because this smell is considered typical of the variety (varietal typicity). Similarly, it is typical for a Chablis, i.e., a Chardonnay from the Chablis Protected Designation of Origin (PDO), to be mineral and chalky or for an Asyrtiko from Santorini to be mineral and with a sharp acidity [24], and this is what wine experts or experienced consumers expect to taste. However, minerality is not necessarily present in Chardonnays from outside Chablis or in Asyrtikos from outside Santorini as wines made from the same grape variety in different geographical regions may express different characteristics [25]. It is evident that typicity may be recognized by experienced tasters who are familiar with the wines that collectively form a group of typical sensory characteristics; however, the evaluation outcome is predicated on the existence of a common recognized prototype [26]. As typicity is linked to the reputation of wines, it consequently influences their position in the market. For this reason, in 1991, the European Commission launched the EU wine databank (actual regulation issued in 2008) containing the isotopic composition of EU wines, which—with a series of reforms—aims not only to highlight the importance of origin but also to minimize malpractice and fraud [27].

3.2. Typicity in a Changing World Scenario

Today, globalization and climate change add an extra level of diversity in wine profiles within the same category. Climate change, in particular, is already influencing grape maturation, and research [28] has shown that grape quality at harvest is linked to typicity as wines made from riper grapes receive higher typicity scores from experts. Changing climatic conditions are expected to alter some aspects of typicity, and a reconsideration of wine classifications may be necessary [29]. The results of climate change are already evident in wines with higher alcohol levels or decreased tartaric acid, and viticultural and winemaking readjustments will be required in order to maintain a uniform sensory profile.

4. Evaluating Wine Quality and Typicity

Both quality and typicity are evaluated via sensory analysis by a panel of wine experts. Sensory assessment includes the identification of a wine's sensory space, its perceptual evaluation and its sensory description [10].

The identification of the sensory space is essentially the affirmation of the appropriate words that best describe it and that ensure a consensus between tasters regarding the extent to which their mental representations of a term are in agreement (e.g., what words tasters mostly associate with the term "elegance" in wine).

The perceptual evaluation of the sensory space is achieved via the categorization of wines based on their similarities. Clusters formed may be created either freely or according to directions provided. Categorization techniques include projective mapping, and unstructured scales may be used in which left and right ends represent "bad" and "good" examples of a wine regarding how well it belongs to a group of a given "prototype" [10].

Finally, the description of the sensory space is based on the qualitative and quantitative characterization of a wine, using words considered to be the most appropriate for the description of the samples' sensory attributes. The words (descriptors) are produced by the tasting panel and are subsequently ranked based on their importance, either statistically, by calculating the frequency of citation, or by the panel itself, in which case the results depend on taster selection [10]. Quantitative characterization is achieved by the ranking of attributes. Various scales have been developed for this purpose and by the type of evaluation (analysis of consumer preference, competitions, etc.), including the Chebnikowski Winespider evaluation system, the Amerine and Roessler (1983) rating system and the Robert Parker wine rating scale [30].

Sensory evaluation results depend on the method, the taster selection, the ranking scale and the statistical technique utilized for the analysis of the results. The most famous sensory evaluation known as the "Judgement of Paris", which introduced California wines to the world after a blind assessment ranked them higher than French wines, has been the focus of many studies that either scrutinize the criteria used for the selection of tasters or reevaluate the results using different statistical approaches in a bid to improve them [31,32].

4.1. Quality Sensory Evaluation

The most intuitive method for quality sensory evaluation is based on the categorization of samples in quality levels (very low, low and very high) [33] and can be followed by the intensity ranking of specific characteristics to provide insight on the most important drivers behind taster evaluations.

Sáenz-Navajas et al. (2013) [34] used the categorization method to group six wines from the Spanish appellation of DOCa Rioja and six French wines from AOC Côtes du Rhône according to their quality and performed ANOVA on quality scores, followed by a pairwise comparison test. The study resulted in specific sensory descriptors used by the expert panel that correlated with quality: "red fruits" for high quality wines and "vegetal" and "animal" terms for low quality wines.

García-Muñoz et al. (2014) used sensory descriptive analysis to evaluate the quality of wines from 18 minor grape varieties [35]. Expert tasters were presented with a questionnaire consisting of sensory, visual and olfactory descriptors along with a body and flavor quality evaluation and were instructed to give an overall quality score as well. Descriptors were rated based on a scale from zero (not perceivable) to ten (very strong). PCA was used to produce a preference map for grouping wines, and clusters formed were used to correlate sensory attributes with taster preference and agronomical parameters in order to explore their influence on quality.

Caissie et al. (2021) studied the factors involved in red wine quality assessments and the extent to which a consensus was reached between tasters regarding the individual aspects of wine matrix factors [36]. The results showed that the strongest decisional consensus between tasters was vision, while individual differences were noted in smell assessment. The consensus was affected by the taster's degree of expertise and the knowledge of the descriptor words [36].

4.2. Typicity Sensory Evaluation

A typicity evaluation is conducted based on conformance with prerequisites, and, for this reason, the tasters require familiarity and knowledge of a specific variety, wine style or geographic origin. According to the type of focus, i.e., variety, PDO category, brand, vintage and geographical origin, tasting samples are selected in such a manner as to increase variability. A typicity evaluation includes two parts, one conceptual, which is in essence the organoleptic evaluation of the wine, and one perceptual, which takes into account terroir-related aspects such as geography, history, climate and the winemaking processes [37].

In the case of PDO wines, the official tool for sensory evaluation is the competition sheet developed by the International Organization of Vine and Wine; however, there are no details or specific definitions for a quality scale of sensory parameters [38]. The only accredited method has been set by Etaio et al. (2010) [39] and is used to evaluate typicity from young red wines from Rioja Alavesa. This method recommends using decision trees to grade the quality of different parameters and uses specifically developed odors, tastes and mouthfeel references to enhance taster consensus.

Correlations between typicity groupings with sensory attributes depend on the selection of wines considered to be typical. Wine experts that perform the selection need to be familiar with the wines to be tasted, and their mental constructs of what they perceive as typical or prototypical should be developed by habitual exposure to the wines. Otherwise, there is the risk of basing correlations on a "caricature" [40], i.e., a prototype exhibiting extreme sensory characters from attributes that are most frequently referred to in wine reviews. In a study assessing the typicity of wines from the appellation of Savennières [41], no consensus on which wines were considered typical was reached between the panels performing the sensory evaluation, and the knowledge of the panel was called into question as experts from the further Anjou area were selected instead of professionals working daily in the Savennières POD only [42].

The most frequently used method for typicity evaluation is the method developed by Ballester et al. [43], in which tasters are instructed to simply answer whether the wine tasted is a good or bad example of its category using an 110 mm unstructured scale in which the left side corresponded to a "very bad example" and the right to a "very good example". A data analysis is performed using marks converted to 1–10 scores and results are analyzed via principal component analysis (PCA). This approach depends heavily on the selection of the tasters and their collective consensus on what they consider a "typical" example.

In an effort to understand the sensory attributes most connected to the typicity of Australian Cabernet Sauvignon, Gonzaga et al. (2019) applied a content analysis on the tasting results of wines from three Australian regions from both online reviews and an expert panel [44]. The correspondence analysis (CA) of online reviews revealed that Margaret River samples were characterized more as "leafy", "complex" and "floral"; Coonawarra samples as "minty", "astringent", "sweet" and "earthy"; and Yarra Valley samples as "herbal", "green" and "medium bodied". The CA of the expert panel assessment also showed a higher use of attributes such as "brett", "mineral" and "savoury" for Cabernet Sauvignon wines originating from Bordeaux, while descriptors correlating with wines from Australian regions were "ripe fruits" and "high acidity". Gonzaga et al. [45] also evaluated the addition of descriptive and rate-all-that-apply (RATA) analysis coupled with PCA and canonical variate analysis (CVA) of the results for the representation of Cabernet Sauvignon in the sensory space.

Parr et al. (2010) [46] also used descriptive profiling to assess the typicity of Sauvignon blanc wines from New Zealand and explore the perceived differences with Sauvignon blanc wines from France. The results showed that principal component analysis (PCA) could separate NZ and French wines, and NZ wines were found to exhibit higher levels of green and fruity notes, as opposed to French wines that were characterized to have a higher dry herbaceous character and mineral notes.

Recently, Lerice et al. (2020) [37] developed a methodology for a typicity evaluation of PDO wines by combining several other methodologies and evaluating conceptual and perceptual typicity. In this study, professionals familiar with the evaluated terroirs identified conceptual typicity using factors such as soil, location and grape variety, and professionals unfamiliar with the terroirs based their evaluation on their assumptions formed by the reputation of the wines or their sensory characters. All descriptors used in the study were chosen by consensus from the tasters of each group (experts from within or from outside the terroir). The descriptors most helpful for categorization as good examples of a terroir included the terms "length", "strength", "minerality", "roundness", "tannins", "woody" and "red fruits", among many others, while descriptors for bad examples were related to the absence of these attributes along with excessive freshness.

5. Measuring Wine Quality and Typicity

Chemical methods are very appealing as they are objective and can produce reproducible and accurate results. However, even though most compounds included in the wine matrix can be qualitatively or quantitatively estimated, chemical analyses rarely manage to describe quality or typicity and usually provide only a synopsis of its manifestation. Moreover, the extensive set of analyses linked with sensory attributes produces another disadvantage as instrumental methods should be practical, rapid and cost-effective.

Analytical methods approach the wine matrix as a set consisting of color, aroma and flavor compounds as these compounds are more likely to have an impact on the wine's sensory properties. Classical analyses such as alcohol, acidity, pH residual sugars and the phenolic index provide information about a wine's "skeleton" and are necessary for the categorization of samples to a specific wine style [3]. Several chemical groups have been found to qualify as quality discriminators, and attributes that generally positively correlate with quality include high color, fruitiness and an astringent, full-bodied mouthfeel [47]; however, no value range exists for the evaluation of results. Moreover, interactions between compounds and synergistic effects in wine aromas are also difficult not only to estimate but also to comprehend. The vintage effect is another factor adding difficulty to evaluations as each year makes its mark on the wine's profile. These implications are being addressed with the use of profiling methods, metabolomics and chemometrics, while machine learning techniques that also aim to predict both quality and typicity are showing encouraging results. Analytical methods aim to simulate a taster's evaluation, and, for this reason, understanding sensory techniques is essential for the optimum utilization of their results as quality and typicity sensory evaluation methods not only lead to wine rankings but also produce important findings and give insight on the potential implications and drivers behind preference evaluation. It should be noted that typicity differs from authenticity as typicity also takes into account the aesthetic aspect of the wine. Authenticity ensures the geographical origin or the variety of the grapes used to make the wine; however, whether the results will correlate with taster typicity perception depends on the data analyzed. For example, the analysis of isotopes provides accurate results on geographical origin but cannot be correlated with tasting scores as isotopes do not correlate with sensory cues.

Chemical methods may be categorized into two groups. One group is descriptive as it deals with the revelation of the compounds that are responsible for categorizations produced by sensory evaluation, and one is predictive as it aims to reproduce taster evaluation with the developed models. Due to the extensive knowledge required to review statistical techniques and because of these techniques' dependance on the type of analytical and sensory data to be correlated, the statistical analysis of results is outside of the aim of this study and will not be discussed.

5.1. Chemical Characterization of Wine's Sensory Space

Many analytical methods have focused on the aromatic profile of wines as it is one of the most important factors influencing consumer acceptance [48], and taster evaluation has been shown to present higher agreement regarding the mental representation of olfactory and visual cues [49]. However, mouthfeel and color have also been found to be useful. This section discusses the analyses that have been employed to chemically translate wine sensory spaces that offer insight on quality and typicity evaluations.

Olfactometry is one of the most appealing methods for aroma description as it is capable of assigning specific compounds to aroma characteristics. In essence, it bears some resemblance to winetasting as it requires a trained panel of judges and follows a standardized methodology [50]. It can be associated with gas chromatography (one-dimensional or multidimensional) and has been extensively used for the determination of molecules that explain the particular nuances of different grape varieties. Even though this approach does not seem to apply to all varieties, its ability to differentiate among wines based on their origin, grape variety and aging is undisputable [51,52]. Apart from the description and evaluation of the intensity and duration of odors of volatile compounds, coupling olfactometry with a sensory evaluation can lead to more information with greater accuracy on the overall wine aroma [52]. Gas chromatography–olfactometry was employed to model the quality of premium red wines from 11 different denominations of origin in Spain [53]. Aromatic compounds from 25 wine samples were quantitated and subsequently correlated to quality scores obtained by an expert panel that evaluated wines and grouped them to 5 quality categories (exceptional, good/very good, right/approved, poor/disappointing and defective/rejectable). This study showed that quality did not correlate positively with a single odor or olfactometric vector but with the summation of odorants presenting similar odors, while negative quality correlated positively with the summation of defective odorants represented by olfactometric scores. PLS regression revealed that defective odorants and negative aroma nuances along with the olfactory vector representing fruity notes produced a satisfying quality model (79% of the variance explained). It is interesting to note that few studies focus on the correlation of sensory attributes with quality without considering typicity as well. GC–Olfactometry has also been successfully used to establish the aroma profile of wines relating to their typicity perception. Detection frequency analysis was employed in a study conducted by Falcão et al. (2008) [54], and the aroma profile of Brazilian Cabernet Sauvignon wines from five different vineyards was established.

Gas chromatography alone, without olfactometry, has also produced significant results. Delgado et al. (2022) used GC-MS and Quantitative Descriptive analysis (QDA) to assess the sensory aroma typicity of Petit Verdot wines from La Mancha from five vintages [48]. To evaluate the volatile compound contribution to the aroma according to their threshold of perception, the odor activity value (OAV) was determined. The results were analyzed by ANOVA (analysis of variance) and revealed that the wine aromatic profile was characterized by high concentrations of C6 and benzene compounds along with terpenes and C13 norisoprenoid compounds. Partial least squares regression (PLS) was further applied on results and "prune" and "sweet" tasting descriptors were positively correlated with ethyl octanoate and isoamyl acetate, while "red fruit" and "liquorice" correlated positively with beta-damascenone, ethyl butyrate, decanoic acid, citronellol and 4-vinylguaiacol [48].

C6 and benzenic compounds were also found to contribute to the free varietal aroma of red wines from minor grape varieties originating from the La Mancha region in Spain after GC-MS and sensory evaluation were conducted, followed by ANOVA for the statistical analysis of results [55].

Lukic et al. (2007) [56] subjected 30 samples of Malvazija young wines from the Istria region of Croatia to sensory evaluation, followed by GC-MS analysis, linear regression analysis and PCA. Wines were selected by wine experts as the most representative regarding their aroma, and the tasting was performed using the 100-point scale method of OIV. The attributes that correlations were based on included "aspect", "bouquet", "flavor" and "harmony", and in wines with higher scores, isoamyl acetate, ethyl decanoate, ethyl octanoate, ethyl hexanoate, hexanoic acid, decanoic acid and octanoic acid were found to be the most important, while wines with lower scores were characterized by the presence of isobutanol and isoamyl alcohol.

Thte varietal typicity of Sauvignon blanc from New Zealand was explored in a study conducted by Parr et al. (2007) [57]. Professional tasters were asked to evaluate wines using a 100 mm scale ranging from absent to extreme and, subsequently, to rate wines regarding how well they exemplified Marlborough Sauvignon blanc. Gas chromatography coupled with mass spectrometry was employed for the correlation with the sensory data. The results revealed that the most important characteristics involved in the sensory profile of wines were green capsicum, correlating with pyrazine compounds, and grapefruit from a wider category of ripe/fruity/tropical aromas found to correlate with volatile thiols and boxwood. The authors note that "green" aromas also correlate with ripening and vinification; however, this study did not aim to differentiate the origin of the aroma. The contribution of methoxypyrazines to the volatile profile of Sauvignon blancs produced by cool climate-grown grapes has been well documented in the literature [58].

Schüttler et al. (2015) [59] used volatile profiling and GC-MS analysis to characterize the aroma typicity of Riesling wines originating from Germany and France. A sensory evaluation was based on the method developed by Ballester et al. (2005), and a free comment profiling technique allowed judges to use their own vocabulary. The statistical analysis revealed that 3-Sulfanylhexan-1-ol concentrations highly correlated with typicity perception. Interestingly, TDN concentrations were found to mostly correlate with aging notes descriptors.

Kustos et al. (2020) [60] used a combination of sensory markers along with volatile profiles produced by GC-MS chromatography to evaluate the regional typicity of Chardonnay and Shiraz fine wines from Australia. The wines selected originated from various regions, and all were assigned a score higher than 90 from wine critic James Halliday. Tastings were performed by panels with previous descriptive analysis experience and, for ratings, a 15 cm scale ranging from low to high was used. The typicity was assessed by conducting a discriminant analysis on sensory and volatile attributes that were found to differ significantly and linked different sub-regions to specific compounds and sensory attributes. Cool-climate Chardonnays were found to present a more pronounced vegetal character, while warmer climate samples showed more fruit and oak-driven attributes. Shirazes did not present important differences, probably due to their similar climate. In this study, chemical analyses also included pH, titratable acidity, alcohol, residual sugar and phenolics (MCP tannin assay and modified Somer's assay) based on which a PCA revealed a strong impact of the wine style on the results.

Few studies have explored quality and typicity via correlations with the non-volatile profile, even though mouthfeel sensations such as astringency and acidity have been well studied and associated with specific chemical compounds [61,62]. The phenolic profile was employed for typicity correlation by Lukic et al. (2019), who used targeted ultra-performance liquid chromatography coupled with triple quadrupole mass spectrometric (UPLC-QqQ-MS/MS) to produce the phenolic profile of 173 wines from red and white varieties (4 red and 6 white) [63]. A panel consisting of experts familiar with the wines selected the appropriate descriptors for sensory evaluation, and representative samples were tasted audibly in order to standardize taster criteria. Typicity was assessed using a 10-point structured scale (from not typical to very typical). The results showed that the typical red color intensity of Teran red wines was linked to a high anthocyanin concentration, while deficiency, especially in acetylated forms of anthocyanins, correlated to the lower purple intensity of Plavac mali red wine. The accentuated astringency of Plavac mali wine did not sufficiently correlate with the phenolics analyzed, while the color evaluation of the sensory panel did not correlate with a particular or total anthocyanin concentration of monovarietal wines, possibly due to the significant role anthocyanin complexes play in color intensity.

Sophisticated instruments such as UPLC or multidimensional GC are used in order to increase the total number of compounds detected while facilitating their identification and quantification. The different characteristics that must be analyzed to develop a meaningful predictive model include the results from "routine" analyses that help characterize a wine. For their integration, chemometrics are employed. Today, untargeted approaches use all the compounds identified by both techniques, producing the volatilome and metabolome profile of the wine, thus increasing the amount of available information. The detection, identification and quantification of compounds may present difficulties due to coelutions, and, for this reason, many different approaches have been employed that allow the detection of as many compounds as possible while facilitating detection in a non-laborious or time-consuming way [52]. The data produced by omics platforms such as HPLC-MS, GC-MS or NMR-based techniques require particular handling due to their complexity and variability in terms of properties and orders of magnitude. For this reason, various processes exist for the conversion of raw data to processed and interpretable biological information and for their statistical analysis [64]. Recently, LC-MS and GC-MS were combined to acquire the metabolome of rosé wines differing in their fermentation process, and partial least squares discriminant analysis (PLS-DA) was employed for the revelation of potential fermentation markers [64]. Metabolites were found to correlate with sensory descriptors produced by a trained panel. The panel had previously agreed on five attributes for the olfactory phase assessment (red, black, citrus and tree fruit, and aroma intensity) and six attributes for the taste phase assessment (intensity, alcohol, acidity, persistence, balance and complexity). Interestingly, three taste attributes (balance, acidity and alcohol) and two aroma attributes (citrus and tree fruit) highly correlated with the same compound, namely, 3-isopropyl-1-pentanol, which is characterized as having a sweet, solvent-like scent [65]. Even though metabolomics, in essence, differ from simpler approaches, mainly in the number of data incorporated in the statistical analyses, few studies have focused on the relation between metabolites and sensory analysis. A reason for the limited use of metabolomics in studies that correlate results with sensory data is the particularities of untargeted methods, in which many of the metabolites cannot be quantified or even identified. For this reason, metabolomics are used as features rather than compounds [66]. It is obvious that unknown compounds cannot provide insight on sensory drivers; however, they can be used when performing a discriminant analysis regarding, e.g., geographical origin. An untargeted approach using ultra high-performance liquid chromatography (UPLC) has been useful in providing the metabolome profile of wines while also producing correlations between wine metabolome with quality scores produced by an expert panel [67]. The feasibility of applying nuclear magnetic resonance (NMR) spectroscopy-based methods for quality control has also been highlighted [68].

Other interesting approaches include analytical techniques based on the use of Fourier transform infrared spectroscopy and NMR combined with chemometrics [69]. Infrared spectroscopy has been successfully used for authentication purposes, has shown potential for the prediction of several wine characteristics and sensory attributes, and is capable of producing the fingerprint of a wine. However, it has also been shown to potentially assess the volatile profile indirectly, but research is ongoing in this area [70–74].

5.2. Development of Predictive Models

As analyzed earlier, a chemical reproduction of the organoleptic "fingerprint" of a wine as the summation of specific compound concentrations cannot be used due to various interactions between compounds that have a non-negligible impact on its sensory profile. Even if this was feasible, the development of optimum compound concentration scales would be subject to exceptions, as illustrated in the case of the 1947 Cheval blanc, in which the volatile acidity exceeded limits thought to compromise wine quality.

Statistical analysis can provide algorithms that take into account variable—in the form of analytical data—interactions and can efficiently sort out which of the data do indeed have an impact on the parameters of interest. With this approach, analytical responses are grouped according to sensory evaluation results, incorporating into data handling the aesthetic aspect of a wine profile. Modeling follows two steps: the first step deals with the training of the model using samples belonging to known classes or with known scores, and the second allows the assignment of unknown samples to classes according to the algorithms produced based on the data used in model training.

Modeling can be achieved using several statistical techniques, and data can be drawn from several of the analytical techniques presented above or from artificial sensory evaluation and machine learning technologies. Machine learning technologies are a branch of artificial intelligence that aim to produce models predicting outcomes utilizing appropriate data and algorithms. Artificial sensory evaluation imitates the perception of human sensory systems by simulating the different human senses such as taste, aroma and vision, and intelligent sensory technologies include electronic noses (e-nose) and tongues and colorimetric techniques [75].

Early studies showed that wine quality rankings may be predicted by VIS-NIR spectroscopy with various levels of success, depending on the wine style, the type of variety and the wine color [76]. In an effort to mimic the human eye, Hernández et al. [77] found that hue measured by CIEL*a*b* coupled with a discriminant analysis was the most helpful color parameter for the reproduction of red wine categorization according to the taster's preference [77]. Advancements have also been made for the assessment of attributes fundamentally assessed via tasting, such as the foam quality of sparkling wines [78]. Due to poor calibration results or the inability to produce a scale of acceptability rankings, these types of predictive grading are considered useful only as a rapid assessment of wine, and a complementary tool for sensory analysis.

Electronic noses (EN) are multisensory systems that transform aroma to measurable electrical signals, which, through a pattern recognition system, can be identified and classified [79]. In wine, difficulties may occur as the extraction procedure used for aroma collection must represent the original without degrading or altering it, while water, ethanol and sulfur dioxide present in the wine matrix either influence sensor sensitivity or poison the sensors. The use of MS–EN (mass spectroscopy e-noses) instruments has allowed the fingerprinting of volatiles and has been found capable of providing information on complex aroma features such as quality grading [80]. E-noses have been found to correlate with sensory scores based on the selection of appropriate sensors. Tasting panels were, however, more efficient at aroma identification, but it should be noted that the e-nose correlated more closely with the taster panel scores than with the GC-MS results [81].

Similarly, electronic tongues (ET) using sensors that do not interfere with the wine matrix have been used for the assessment of taste. Recent research has shown the potential of corelating ET measurements with scores produced by a tasting panel with the employment of fast Fourier for data compression and genetic algorithms [82].

Further studies have employed machine learning following a more integrative approach using analytical data regarding attributes related to different senses. Machine learning with the use of the synthetic minority oversampling technique (SMOTE) algorithm was used for the classification of white wines from Portugal, categorizing them into high, normal and poor quality groups [83]. The variables used for the model development were fixed and included volatile acidity, citric acid, residual sugars, chlorides, free and total sulfur dioxide, density, pH, sulphates and alcohol. No aromatic compounds were analyzed. Wine data and quality scores were derived from the UCL machine learning repository, and SMOTE was used to handle imbalance occurring between classes of major and minor quality classes (4535 samples were of normal quality and 363 samples were of high or low quality). No data were given on the quality's method of evaluation. The classifying technique that was found to be more useful for prediction was the random forest technique. The results showed a 4.7% error rate with an ROC (true positive rate/false positive rate) value of 0.99. The study highlighted volatile acidity, free sulfur dioxide and alcohol as the most important variables in determining wine quality.

The UCL learning data repository was also used in a study by Dahal et al. (2021) for the prediction of the quality of red wines [84]. The variables used for model development were the same as those in the study conducted by Hu et al. (2016) [83]. The dataset contained results from 4898 wines, and the tasting results were acquired by several tasters that ranked the wines from 0 (poor) to 10 (excellent) during a blind tasting. The authors noted that the data were nonuniform and the variables with large values may have dominated over other quantities and highlighted the need for data standardization. For this reason, data were standardized, and the optimum model developed used the gradient boosting regression (GBR) algorithm. The variables most useful for prediction were identified to be alcohol, sulphates and volatile acidity.

A very promising approach for predictions is the use of metabolomics, which can integrate data from various analytical techniques describing wine sensory space. A recent study combined the metabolite profile from volatile and non-volatile compounds in order to predict the quality ratings of Pinot noirs [85]. PLS regression analysis was used for the evaluation of the predictive ability of each profile individually and in combination, highlighting the non-volatile profile of Pinot as the most successful for predictions. It should be noted that only Pinot noirs were used in the sensory evaluation. In this study, several compounds were found to negatively or positively correlate with quality. Despite their advantages, little research has been conducted on the use of metabolomics for quality score prediction. In the case of typicity, studies with metabolomics that approach it in terms of sensory expression and not as authentication are scarce. Authenticity, and its closely related concept of traceability, may incorporate the typicity expression of wines, not to examine or explain it, but to certify the absence of fraud or adulteration. Even though authenticity presupposes typicity, the opposite is not always true, as while origin and grape variety may be certified, the wine produced may not be typical of either. However, minimizing fraud is of high importance, and, for this reason, most studies focus on authentication and traceability instead of typicity.

5.3. Holistic Approaches: The Case of Pinot Noir

A holistic approach has been employed for the evaluation and prediction of New Zealand Pinot noir quality utilizing extensive research that has provided necessary insight for the evaluation of color, aroma, mouthfeel and other sensory attributes.

Pinot noir has been known to have a lighter color compared to other wines due to the lower concentrations of phenols (tannins and anthocyanins) in the grape berries [86]. To investigate the importance of its visual perception on wine tasters, Parr et al. (2016) analyzed the results produced by the sensory evaluation of two expert panels (one with French experts and one with experts from NZ) on French and NZ Pinot noirs. A statistical analysis revealed that "balance", rather than color (as hue, brightness and intensity), was an important driver for quality perception. A multiple regression analysis was further employed for the prediction of the tasting results with minimum success; however, the use of PCA revealed that varietal typicity, as expressed via the detection of attributes such as oak, structure and fruits (red, black, and ripe), enhanced the quality perception of Pinot noir.

Research on the attributes driving high-quality perception has revealed the most important descriptors to be expressiveness, varietal typicity, overall structure, fruity aromas, harmony and balance [87]. This study further supported the findings of Parr et al. (2016), showing that wine color was not found to significant influence Pinot noir quality perception, and revealed that, for tasters, varietal typicity was synonymous with quality. Complexity was found to negatively correlate with tannin harshness, astringency and bitterness and positively correlate with freshness, balanced acidity, expressiveness, elegance and overall structure. Interestingly, hue and color density were found to be involved in taster preference via phenomena involving the influence of visual cues to smell, mouthfeel and taste.

The mouth attributes of NZ Pinot noir and their importance in quality perception have also been investigated by Dias Araujo et al. (2021) [88]. This study linked volume, body, smoothness and viscosity with higher quality rankings, while tannin harshness and bitterness correlated with lower quality judgments, supporting the findings of Parr et al. (2020) [87]. Several sensory attributes were linked to phenolic compounds.

Drawing from the results of the studies presented above, recently (2022), a machine learning application was developed for the prediction of the wine quality of New Zealand Pinot noir from two vintages [89]. For the construction of the model, 54 different characteristics, including volatile compounds, total phenols and total anthocyanins, and the results from classical analyses, such as acidity and ethanol, were considered. Quality was evaluated by an expert panel following the method set by Parr et al. (2020) [87]. The study's low sample number (18) was addressed by the synthetic minority over sampling technique (SMOTE), which was used to produce sufficient samples for machine learning. Different feature selection techniques were also evaluated for the optimum identification of the most important features. Important characteristics were selected according to their relevance to the feature selection methods and were used for wine quality prediction. According to the results, six characteristics were found to be essential in at least three feature selection methods. Two compounds, ethyl octanoate and 4-ethyl-2-methoxyphenol, which are esters responsible for the fruity and sweet qualities of Pinot noir, were found to be the most significant. The remaining four were monoterpenes and esters related to flowers, caramel, apple notes and a rose-like varietal flavor, and one, β-Ionone, is responsible for the violet and black berry notes in Pinot noir [89]. The results showed that the Adaptive Boosting classifier (AdaBoost technique) provided the most accurate predictions (100% accuracy), utilizing features selected by the extreme gradient boosting XGB technique.

6. Discussion

Wine quality and typicity are essentially assessed only via sensory evaluation by expert tasters. Frequent issues involved in tastings such as taster bias and repeatability have been addressed with the development of several techniques; however, subjectivity as an inherent problem of sensory evaluation remains an important issue. The most straightforward tasting approaches instruct experts to group wines following a scale ranging from "low" to "high" quality or as "good" or "bad" to determine typicity, while a descriptive analysis may also be employed to give more insight on the criteria behind taster evaluation. In both cases, a consensus between tasters and a good knowledge of the assessed wine are required.

As an alternative to sensory evaluation, analytical approaches aim to chemically describe the wine matrix, and the integration of the results with the use of chemometrics can lead to a holistic reproduction of a wine's profile. However, the basis for model development is the existence of classes (quality levels or groups of good/bad examples of typicity) or scores, which are in turn produced by tasting panels. Even though this approach enhances repeatability and accuracy, these outcomes are essentially simulations of panel evaluations and are, therefore, again dependent on taster selection and performance. For example, in the case of Anjou Village, tasters failed to reach a consensus on what they considered as typical, and no typicity classes for correlation purposes were formed by the sensory evaluation.

In sensory analysis, panel selection is based on specific criteria, and taster performance can be validated by repetitive tastings. In model development, validation is based on the analysis of samples derived from the known data pool, while an extra step of model testing is performed on unknown samples outside the dataset to evaluate the model's performance. Thus, it would be important to examine how well a model performs when a wine is evaluated in repetition. The study conducted by Cadot et al. (2020) [41] raises another interesting issue, which is the incorporation of outliers (wines outside the area examined) in the sensory evaluations of typicity. As shown earlier, the results from a descriptive analysis of wine profiles in different experiments do not always result in attributes correlating with unique compounds. For example, C6 compounds were found to be characteristic of the aromatic profile of Petit Verdot wines from La Mancha [48], but the same compounds also contributed to the free varietal aroma of red wines from minor grape varieties from the same area, showing a possible link with grape origin [55].To evaluate the varietal typicity of Petit Verdot, samples outside the La Mancha region are necessary, but to evaluate the overall typicity of La Mancha Petit Verdot, samples outside of this region are considered outliers and could be helpful to better evaluate the contribution of C6 compounds. Typicity has been shown to be included in the overall quality perception of tasters, and the success of developed models depends on the decisions made when selecting samples.

Another important factor of model development is the selection of appropriate analytical data. As discussed earlier, volatile profiling techniques have successfully been correlated with wine aroma attributes, while phenolic profiling has shown a good correlation with taste attributes. Several classical analyses are indirectly linked to quality as well, such as free sulfur dioxide, for example, since lower concentrations mean less protection from oxidation or microbial spoilages [4]. Modeling based on indirect parameters has been examined in studies using the UCL learning data repository and has resulted in successful predictive models. It has been well established that correlation alone does not imply causation, and, in this case, the models produced can only reflect the technical aspects of quality. For example, even though aroma evaluation contributed to the wines' quality score, no compounds correlating to the varietal or fermentative aroma of the wines were used in model development. For this reason, the authors proposed the use of their models as a tool for winemakers to employ the fast screenings of wines and not as a quality indicator.

Modeling based on quality scores alone, without incorporating typicity as a quality indicator or on wines from different varieties, present several implications. Sensory evaluations that produce scores using numerical scales (such as the Parker rating scale or 0–100 ranging scales used for medal awarding in competitions) can be performed blindly but are based on the comparison of samples belonging to the same category (i.e., variety, origin and wine style). Grades used out of context as an absolute number for the comparison of wines from different categories do not provide meaningful outcomes. In modelling, using scores without context may lead to groupings that do not reflect the attributes that the taster evaluation has been based on. For example, in the case of Malbec and Pinot noir, varieties with extreme differences in their sensory perception, Malbec (rich in anthocyanins) would be evaluated more highly for its visual appearance than Pinot noir (lower anthocyanin concentrations) in a blind tasting; inversely, however, feeding a model with high scores from tastings that evaluate each wine's quality based on its variety would confuse the algorithms with regard to how important anthocyanins are for the model that is being developed.

Wine style is chemically described using classical analyses, which should be incorporated to datasets along with data from profiling techniques. However, to simulate sensory evaluation, prediction models should consider compounds that influence the entire sensorial space of a wine, as perceived with all five senses. The case of Pinot noir is an interesting example of what can be achieved in this area. Pinot noir has been extensively studied, and key aspects of its sensory profile have been correlated to specific chemical compounds or groups of compounds. As a first step, groupings according to quality were provided, and descriptive analyses were employed to reveal suitable descriptors of the most important attributes of the wines. These descriptors were further used as the basis of chemical analyses from which the data used to train the model were produced. Similarly, the combination of the metabolite profiles formed by volatile and non-volatile data, which Sherman et al. (2020) [85] employed for the prediction of NZ Pinot noir quality, qualifies as a very promising approach, highlighting again the need for repetitions (the question of bias was raised regarding each taster's country of origin) and for test sets as at least one compound was not determinately assigned as a quality or origin predictor. The difficulty to identify compounds that appear to significantly correlate with the parameter examined (i.e., quality, in this case) shows the need for further research, while the identification of new or unexpected compounds that are strongly associated with sensory properties reveals the need for the further examination of their origin and sensory attributes.

Finally, expert tasters increase the accuracy of their assessments via repetitive tastings on a wide range of wine styles, vintages and origins and in various conditions. For example, the gustatory preferences of Robert Parker, one of the most known and respected wine critics, are well established due to an excessive number of evaluations, which the critic performed based on the "Robert Parker" rating scale. This has led to the term "Parkerization", which reflects the supposed shift of winemakers' effort towards the production of more powerful and fruit-driven wines that are expected to be graded higher by Parker [90]. In a similar manner, model calibration based on successive tasting outcomes could potentially benefit prediction accuracy. Yearly calibrations could also be used for typicity modeling, in which the importance of including "keepers of memory" [42] in tasting panels has been highlighted, e.g., in the French PDO guidelines, as a means to incorporate vintage effects on an overall perception of this concept.

7. Conclusions

Even though many efforts have been made to predict tasting scores, and emerging methodologies such as machine learning applications are able to efficiently handle outputs from various analytical techniques, few models have shown the potential to produce satisfactory results. Predictions heavily rely not only on the chemical analyses, the data selected and the statistical technique employed for correlation purposes but also on the group of tasters the model is calibrated on, the tasting method and the extent to which a consensus is reached regarding what is considered to be a prototype in the case of a typicity evaluation. Several analytical methods have shown good potential for correlating with sensory evaluation results and for the development of predictive models for quality and typicity evaluation, which can assist winemaking decisions in a changing wine world. Predictive models can also increase knowledge on wine attributes and the way tasters perceive them and could be used as educational tools in the same manner that the wine community has been able to produce a mental representation of Robert Parker's preferences. Incorporating the analysis of wines from various vintages or outliers, either in the pool of training data or as a form of validation, and performing repetitive evaluations would be necessary to better reflect the diverse and time-dependent sensory profile of wine and enhance model accuracy. Future research should focus on the use of more cost-effective and rapid analytical methods for the facilitation of data production.

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