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Descriptor Fingerprints and Their Application to Red Wine Clustering and Discrimination.

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Abstract*: The investigation was performed to test the potentials of the fingerprint clustering algorithm for a set of 1599 red wines in relation to some wine properties, comprised in the notion 'wine quality". We have obtained a distribution of the wines into different clusters as a result. Each cluster was composed of wine objects with similar values of laboratory parameters and with a wine quality certificate. A correlation between the quality of wines (a sensory taste factor) and the phisicochemical descriptors (laboratory analytical test results data) was observed and analyzed.*

Key words*: similarity search, descriptor fingerprints, red wine clustering*

Introduction

In recent years, the interest in wine consuming has increased, leading to growth of the wine industry. As a consequence, companies are investing in new technologies to improve wine production and selling. Quality certification is a crucial step for both processes and is currently largely dependent on wine tasting by human experts. This work aims at the prediction of wine preferences from objective analytical tests that are available at the certification step.

The investigation was performed to test the potentials of a fingerprint clustering algorithm for a set of 1599 red wines in relation to some wine properties, comprised in the notion '*wine quality*".

Wine certification is generally estimated by physicochemical and sensory tests [1]. Routine laboratory tests used to evaluate wine quality include analytical determination of some physicochemical wine descriptors such as sugar content, density, alcohol, pH values, while sensory tests rely mainly by experts. The sensory tests are usually carried out by human senses such as flavor and taste and they require extremely experienced persons. The relationships between the physicochemical and sensory analysis are too much complex and still poorly understood [2], thus wine classification becomes a serious problem. Our investigation aimed to check and expose the possibility of the descriptor fingerprints procedure to rank and distinguish different classes of red wines.

Experimental

A large dataset of laboratory analytical test values (11 items) for a group of 1599 red wines (vinho verde samples from Northen regions of Portugal) was taken from literature [3] and used for descriptor fingerprints creation. Descriptor fingerprints were generated on the basis of physicochemical laboratory data routinely used for wine characterization (fixed and volatile acidity; residual sugar, total and free sulfur dioxide, citric acid, chlorides, sulfates, density, pH and alcohol content). As a next step similarity search was carried out and followed with clustering procedure of Butina [4].

Results

We have obtained a distribution of 1299 wine objects into 12 different clusters as a result of similarity search based on descriptor fingerprints. Each cluster was composed of objects with similar values of laboratory parameters and with a wine quality certificate. The wine quality is characterized by a 10-point system (point 0 means very bad wine quality; point 10 is equal to excellent quality) and is perceived

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subjectively by a flavor and taste sense perception. The quality of the wine samples in our case varied between 4-7 points. In the end of similarity search some wines of the same quality has fallen into different clusters with different values of the laboratory descriptor parameters and vice verse the wines falling in the same cluster clearly show either the same or closely similar laboratory test parameters.

Discussion

A correlation between the quality of wines and the phisicochemical descriptors was observed.

The diagrams on Figures 1-8 illustrate the values varying (min, max and mean) for different laboratory wine quality tests specific for the cluster. Each of the 12 generated clusters unites the wines with equal taste quality (indicated on the x-axis as „q"). In order to check the quantitative relationships between the wine quality (Q) and the laboratory tests values we performed the correlation analyses and generated the multiple linear regressions MLR:

$$Q=133.4(\pm65.9) +0.18(\pm0.07)acid_{fix}. - 0.99(\pm0.28)acid_{volatile} -$$
$$-0.12(\pm0.05)sugar_{resid} -2.88(\pm1.03)Cl +1.5(\pm0.66).10^{-2}SO_{2(free)} -$$
$$- 2.2(\pm1.7).10^{-3}SO_{2(total)} -132.72(\pm67.31)dencity +$$
$$+0.54(\pm0.51)pH +1.01(\pm0.39)sulphates +0.125(\pm0.088)alcohol$$

($R = 0.68$; $R^2 = 0.462$; $s = 0.429$; $F = 11.2$)

The red wine quality (Q) was performed as a linear combination of routine laboratory test descriptors. All analytical descriptors used (except citric acid content) proved a significant effect on the red wine quality. According to oenological theory the citric acid and the residual sugar levels are more important in white wines, where the equilibrium between the freshness and sweet taste is more appreciated. In our equation the descriptor "residual sugar" enters with a negative sign and low significance (Fig.1).

In the equation the red wine quality is favorably influenced with the presence of sulfur dioxide in the free form; presence of sulphate ions, alcohol content and acidity of the medium (pH and fixed acidity).

The most intriguing result is the high importance of sulphates (Fig.2).

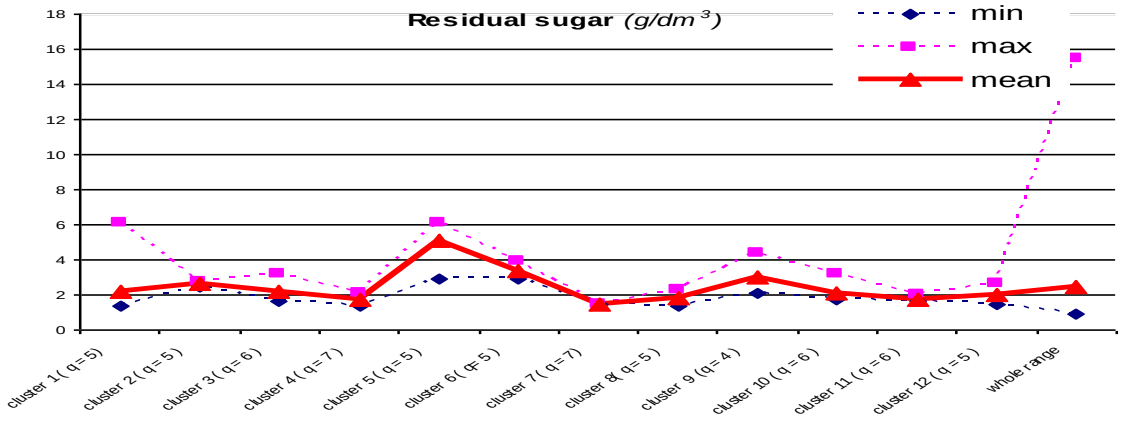

Figure 1.

Oenologically this result could be very interesting. An increase in sulphates might be related to the fermenting nutrition, which is very important to improve the wine aroma.

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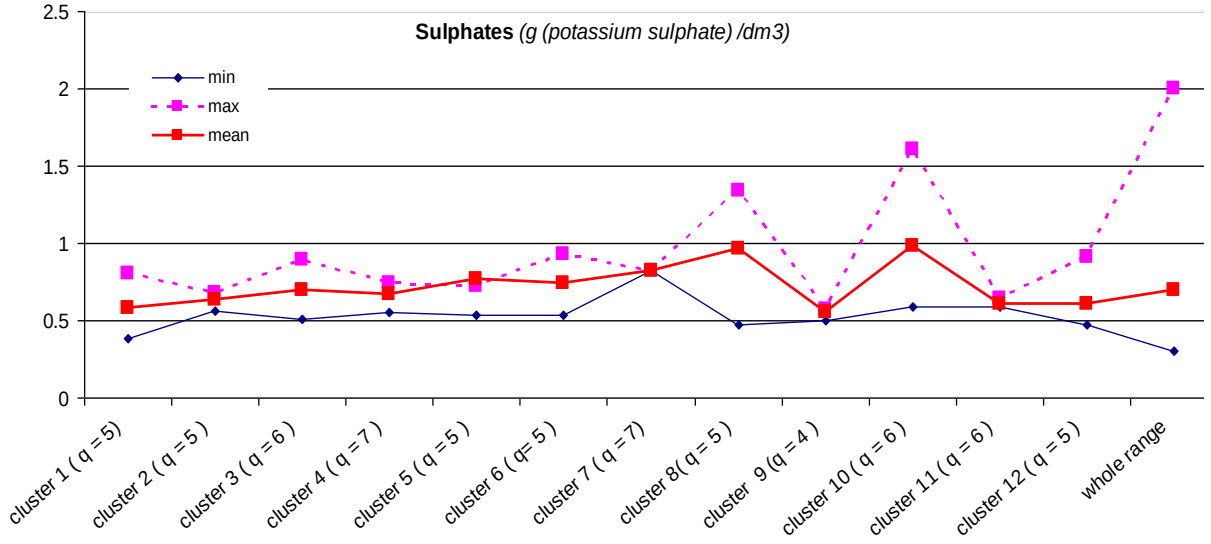

Figure 2.

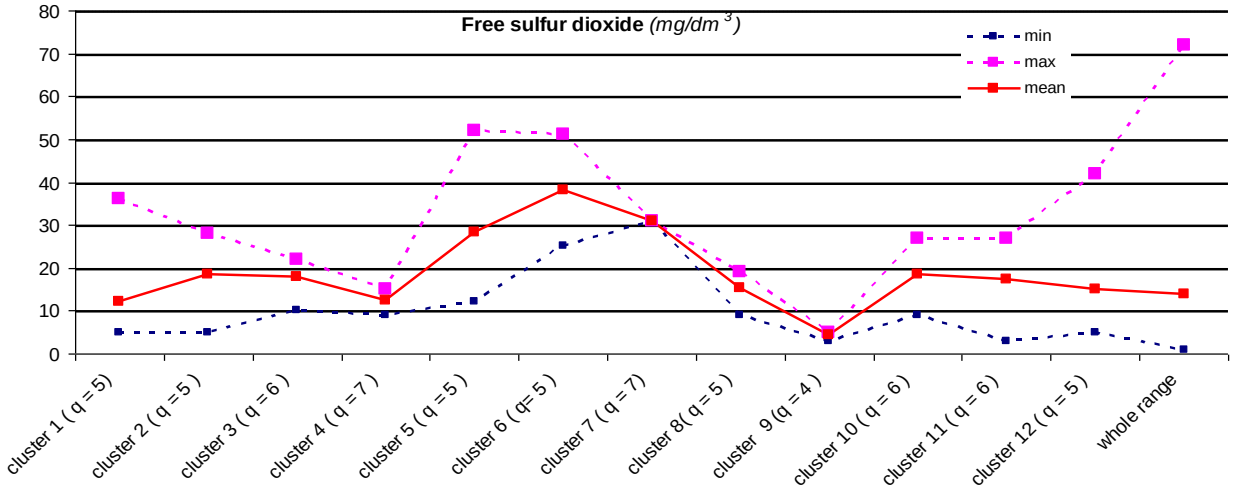

Figure 3.

It was interesting to see why the wine samples of equal quality has been combined in different clusters (for example wines with mediate quality q=5 fall into 1, 2, 5, 6, 8 and 9 cluster; with quality q=7 – into the forth and the seventh cluster; with q=6 - into cluster 3, 10 and 11). At 1-8 Figures can be compared quantitative laboratory test results for individual clusters.

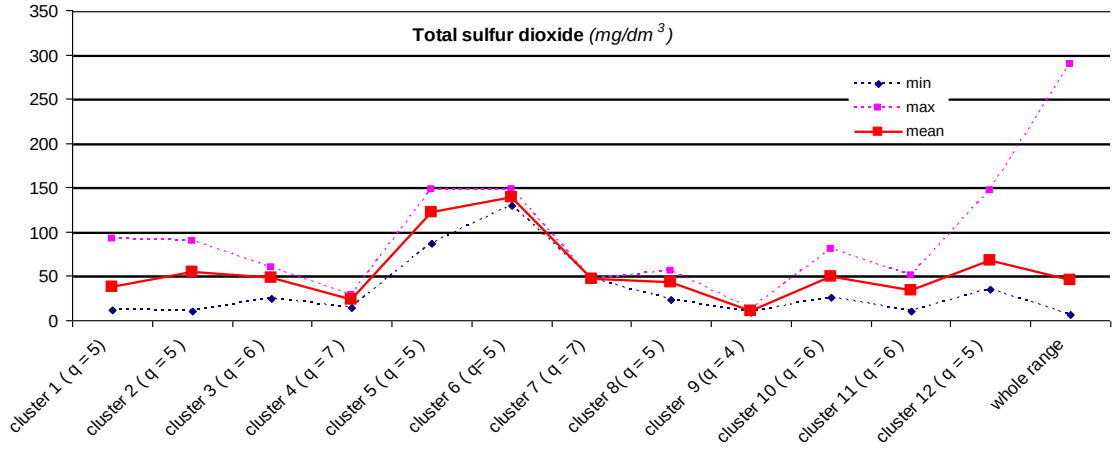

Figure 4.

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Sulphurous acid is is widely used in winemaking thanks to its *antiseptic and antioxidant* property. It blocks some of the oxidative enzymes and also paralyzes the function of the yeast cell. Cultural yeast (Sacch.vini) also proved deficiency of oxygen. But they switch *to anaerobic metabolism* of the matter, i.e. to fermentation. The sulphurous acid may exist in wine wort either as an undissociated form, as a gas SO_2, or in the form of $(SO_3)^{-2}$ or $(HSO_3)^-$ anions.

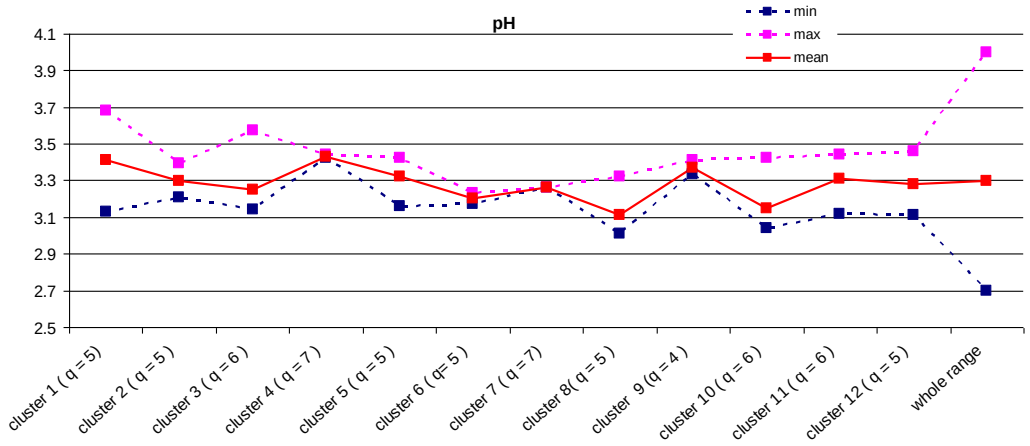

Figure 5.

Just the undissociated form of sulphurous acid has antiseptic properties. The concentration of the undissociated form in the wine solution is very low (Fig.3) and depends on pH (Fig.5) and on the temperature of the solution.

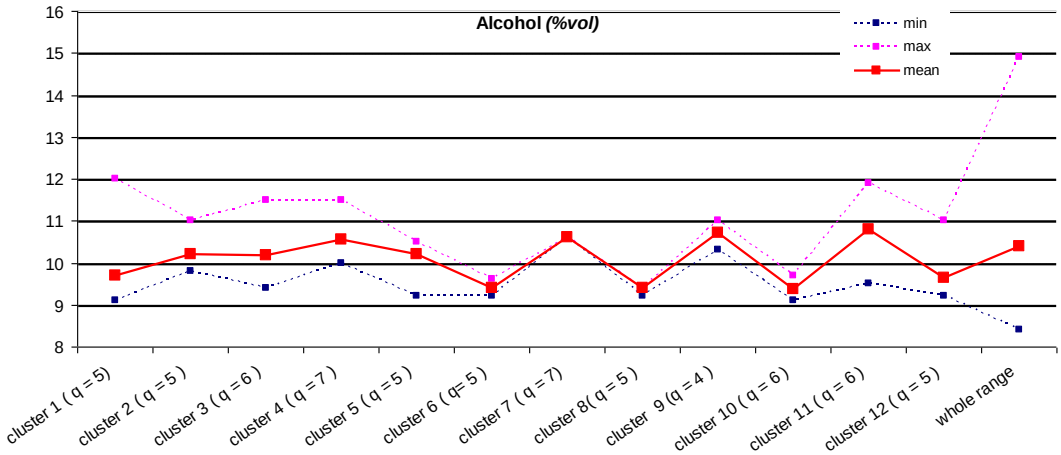

Figure 6.

The sulphurous acid stimulates the alcoholic fermentation. It acts as inhibitor and suppresses the oxidative activity of enzymes and prevents the formation of the oxidized products, spoiling the taste of wine bouquet. Sulphurous acid acts as an acceptor of oxygen and leads to a reduction of its quantity in the raw material and so stops the growth of *aerobic* microorganisms.

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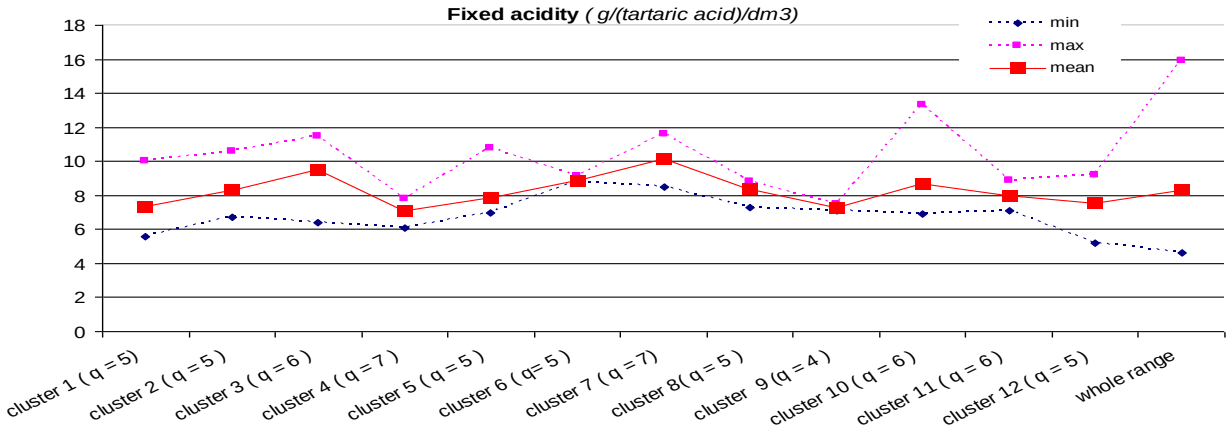

Figure 7.

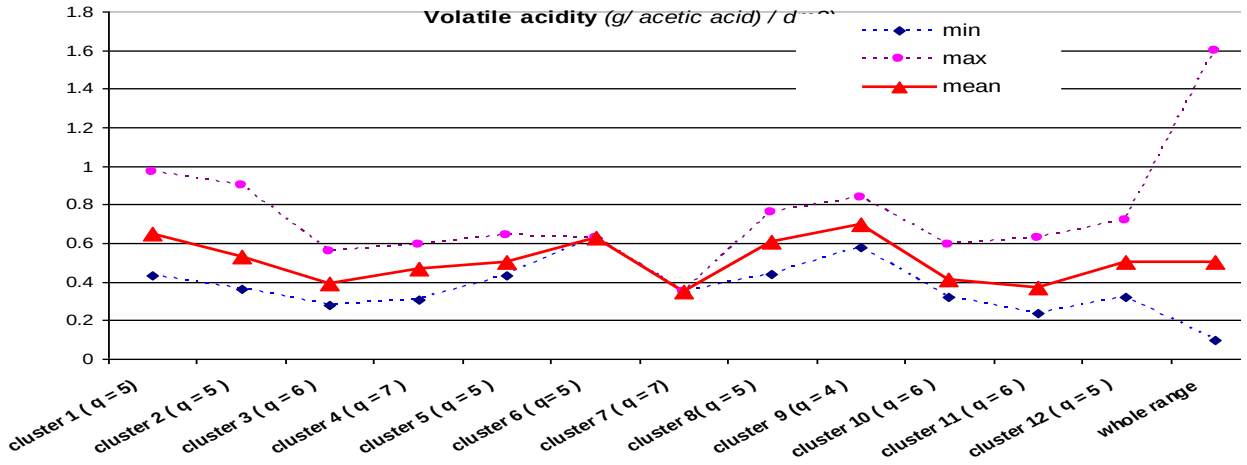

Figure 8.

An increase in the alcohol tends to result in a higher quality of the wine (Fig.6). Formation of alcohols occurs at the biochemical fermentation processes: in processing of grapes under *anaerobic conditions* to produce dry wines and champagne.

Conclusion

Using of descriptor fingerprints for similarity search groups the red wine samples into different clusters with similar certificate quality and comparable to sensory tests.

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