

Original papers

Element selection and concentration analysis for classifying South America wine samples according to the country of origin



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ARTICLE INFO

Keywords:

Elemental content
Wine samples
Geographical origin
South America
Feature selection

ABSTRACT

This paper proposes an approach for feature selection aimed at classifying wines samples according to place of origin. The method relies on Kruskal-Wallis non-parametric test to remove non significant features, and Linear Discriminant Analysis to derive a feature importance index. The ranked features according that index are iteratively added and classification performance is assessed after each insertion. The number of selected features is chosen according the maximum accuracy in a repeated 10-fold cross-validation. Aiming at improving categorization accuracy, different classification techniques are tested. When applied to a wine dataset comprised of 53 samples from four South America countries (Argentina, Brazil, Chile, and Uruguay) and 45 chemical elements concentrations determined by ICP-OES and ICP-MS, the proposed framework yielded average 99.9% accurate classifications in the testing set, and retained average 6.73 of the 45 original elements. Retained chemical elements were then qualitatively assessed.

1. Introduction

The growth in international trades and potential markets for food and beverage products have motivated producing regions to develop and apply regulations to ensure product traceability (Zhao et al., 2013). In trading markets, the association of brands with their places of origin tends to boost product acceptance, leading to premium prices and commercial advantages (Diniz et al., 2014; Karoui and De Baerdemaeker, 2007). Thus, food and beverage manufacturers have displayed increasing interest in ensuring precise categorization of products into proper classes according to their place of origin, as well as in improving mechanisms for confirming products' authenticity (Borràs et al., 2015; Marcelo et al., 2014).

Wine attributes and quality strongly depend on grapes' features, soil properties and climate conditions, among other variables; such aspects, when combined with specific cultivation, production and preservation techniques become fundamental for product promotion and distinction (Marini et al., 2006). Wines cultivated in specific geographical regions and subjected to strict regulations are certified by a Controlled Denomination of Origin (CDO) distinction, which ensures their superior quality and adherence to best practices (Gómez-Meire et al., 2014). Thus, the development of reliable, fast and straightforward techniques

aimed at precisely recognizing wines' authenticity regarding their origin becomes a relevant issue to preserve the reputation of a CDO distinction (Marini et al., 2006).

An analytical approach to trace the origin of food and beverage products consists of assessing their elemental composition and chemical concentration (Drivelos and Georgiou, 2012). The analysis of elements' concentrations determined by inductively coupled plasma optical emission spectrometry (ICP-OES) and/or inductively coupled plasma mass spectrometry (ICP-MS) has been widely used to determine the quality of products such as organic coffee (Barbosa et al., 2014a), eggs (Barbosa et al., 2014b), rice (Maione et al., 2016), and tea (Diniz et al., 2014; Moreda-Pineiro et al., 2003). Due to its high sensitivity and ability to measure isotopes, ICP-MS is deemed one of the most appropriate techniques for the determination of trace elements in wine (González et al., 2009). Such technique quantifies the presence of several chemical elements (e.g. Cu, Fe, Mn, Sn and Zn) which may affect wine stability in terms of color, taste, and organoleptic aspects. The concentration of those elements may be determined by geochemistry features, as well as by variations on winemaking procedures. Thus, the assessment of elements' concentrations becomes a valuable resource to corroborate the authenticity of a wine. With that in view, focusing on chemical elements with higher discriminant ability becomes a crucial

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<https://doi.org/10.1016/j.compag.2018.03.027>

Received 17 August 2017; Received in revised form 7 March 2018; Accepted 22 March 2018

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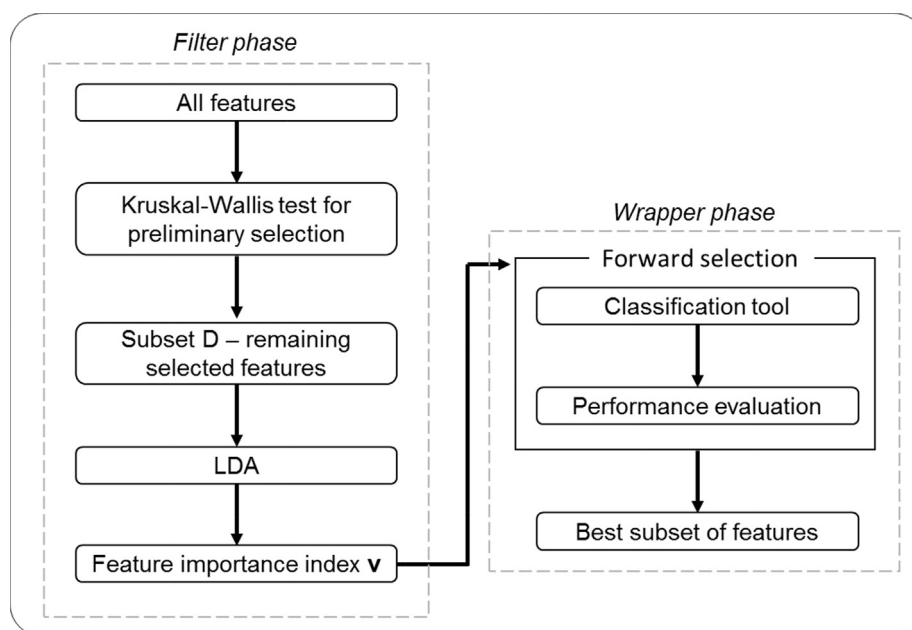


Fig. 1. Schematic view of the proposed method.

step to ensure proper classification of wine samples according to producing country or region. Although some studies have applied statistical and data mining-based techniques for classifying wines according to organoleptic features and geographical origin (e.g. Marini et al., 2006; Coetzee et al., 2014 and Azcarate et al., 2015), few have focused on the selection of relevant features (i.e. chemical elements) that enable accurate discrimination and classification of wine samples.

This paper proposes a novel framework for feature selection aimed at categorizing wines samples into classes according to place of origin. The method combines filter and wrapper-based feature selection procedures, and relies on two operational steps. In the first step, the method applies the Kruskal-Wallis (KW) non-parametric test to each feature; features presenting a p -value higher than a given threshold h are removed from the analysis. The aim here is to discard features with no significant ability to discriminate wine samples regarding their place of origin, reducing computational effort and potentially increasing the classifier's performance. Next, a Linear Discriminant Analysis (LDA) is applied to the remaining features, and a feature importance index is derived from LDA parameters; such index guides the selection process carried out in the next step of the proposed method. In the second step, a forward procedure based on the ranking of features given by the LDA importance index is employed. Best-ranked features are inserted one by one into the subset of features used for classification; after each insertion, classification performance is assessed. The number of selected features is chosen according to the maximum accuracy in the repeated cross-validation. Aiming at improving categorization accuracy, different classification techniques are tested.

2. Materials and method

2.1. Samples, materials and sample preparation

Fifty three (53) samples of red wine from four wine-producing countries in South America were purchased in local markets: 13 from Argentina, 15 from Brazil, 13 from Chile, and 12 from Uruguay. The cultivars (mostly *Vitis vinifera* species) and geographical origin were labeled on the wine bottles. The number of samples from each producing country was not the same, as some cultivars were not found in local markets.

For sample preparation and dilution, nitric acid (Merck) was used.

High-purity water (resistivity of 18.2 M Ω cm) obtained from a Milli-Q system (Millipore) was used for the preparation of all samples and solutions. Calibration solutions were prepared (in 5% v/v HNO₃) from serial dilutions of 10 mg L⁻¹ multielemental stock solutions (SPEX). The calibration solutions of P were prepared from a 1000 mg L⁻¹ P stock solution (Titrisol/Merck).

Wine samples were decomposed according to the following procedure: 1 mL of wine was transferred to polytetrafluoroethylene (PTFE) flasks to which 3 mL of HNO₃ were added; the mixture was left to stand for 15 h. Vessels were then closed and heated in a metal block in three steps: 50 °C during 1 h, 100 °C during 1 h, and 150 °C during 3 h. After cooling, the solution was transferred to a graduated-polypropylene vial, and the volume was completed with water up to 25 mL. This solution was tenfold diluted with 5% v/v HNO₃ for ICP OES analyses, and twofold diluted with 5% v/v HNO₃ for ICP-MS analyses. All samples were analyzed in triplicate. In order to assess the sample preparation procedure, a red wine sample was diluted with nitric acid solution (to obtain 5% v/v HNO₃) or left in contact with HNO₃ (1 mL of wine + 3 mL of HNO₃). The recovery results with closed vessel decomposition as sample preparation method were deemed better and used in this work.

2.2. Instrumentation

An Optima 2000 DV ICP OES spectrometer (PerkinElmer, Shelton, CT, USA) was used to determine the following 13 major and minor elements (Al, Ba, Ca, Fe, K, Mg, Mn, Na, P, Rb, Sr, Ti, and Zn). For that matter, Al (396.153), Ba (233.527), Ca (317.933), Fe (238.204), K (766.490), Mg (285.213), Mn (257.610), Na (589.592), P (213.617), Rb (780.023), Sr (407.771), Ti (334.940), and Zn (206.200) spectra lines (wavelength in nm) were monitored. The sample solution was introduced into the plasma by means of a pneumatic nebulizer fitted to a cyclonic spray chamber. The conditions in the ICP OES were the same used by Bentin et al. (2011): RF power (W), plasma gas flow rate (L min⁻¹), auxiliary gas flow rate (L min⁻¹), nebulizer gas flow rate (L min⁻¹) and sample uptake (mL min⁻¹) were set to 1500, 15, 0.2, 0.75 and 0.75, respectively.

Minor and trace elements were determined using an ELAN DRC II instrument (from PerkinElmer/SCIEX, Thornhill, Canada). 7Li, 9Be, 51V, 53Cr, 58Ni, 59Co, 65Cu, 75As, 82Se, 98Mo, 107Ag, 111Cd,

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