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Digital image-based tracing of geographic origin, winemaker, and grape type for red wine authentication

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ABSTRACT

This work proposes the development of a simple, fast, and inexpensive methodology based on color histograms (obtained from digital images), and supervised pattern recognition techniques to classify red wines produced in the São Francisco Valley (SFV) region to trace geographic origin, winemaker, and grape variety. PCA-LDA coupled with HSI histograms correctly differentiated all of the SFV samples from the other geographic regions in the test set; SPA-LDA selecting just 10 variables in the Grayscale + HSI histogram achieved 100% accuracy in the test set when classifying three different SFV winemakers. Regarding the three grape varieties, SPA-LDA selected 15 variables in the RGB histogram to obtain the best result, misclassifying only 2 samples in the test set. Pairwise grape variety classification was also performed with only 1 misclassification. Besides following the principles of Green Chemistry, the proposed methodology is a suitable analytical tool; for tracing origins, grape type, and even (SFV) winemakers.

1. Introduction

Production of foods and beverages occupies an important place in the economies of the world; this makes identification of fraudulent practices an issue of primary importance in quality control and safety (Council of the European Union, 1999; Arvanitoyannis, Katsota, Psarra, Soufleros, & Kallithraka, 1999; Versari, Laurie, Ricci, Laghi, & Parpinello, 2014). In the case of wines, fraud is most frequently related to falsification, adulteration and mislabeling, which taken together constitute an extensive problem inflicting serious financial damage to producers, regulatory agencies and consumers, as well as (depending on the type of adulterant added) augmenting consumer health risks (Arvanitoyannis et al., 1999; Cozzolino, 2012).

Wine production has been traditionally practiced in temperate regions; in the Northern Hemisphere between the 30th and 50th parallels, and in the Southern Hemisphere, between 30 and 45°; production outside of these regions was unlikely to be considered (Pereira, Vanderlinde, & Lima, 2011; Amarante, 2015). For fine wines from regions with tropical climates, Brazil is considered a pioneer for having started production about 30 years ago in the São Francisco Valley. Located between 8° and 10° latitude south, on the banks of the São Francisco River in Bahia and Pernambuco, principally between the cities of Remanso-BA and Sobradinho-BA; the region is tropical and semi-arid with an average annual precipitation (350 to 800 mm) that occurs mostly from December through March. With an average annual temperature of around 27 °C, the valley presents an approximate annual wine production of 7 million liters, making it the second largest wine-producing region in Brazil (Tonietto & Carbonneau, 2004; Tonietto & Teixeira, 2004; Versari et al., 2014; da Bacia, 2015).

The term 'tropical wines', such as wines produced in the San Francisco Valley, is used to identify wines produced in regions where natural conditions permit more than one vegetative cycle and more than one harvest per year, (Tonietto & Teixeira, 2004; Pereira et al., 2011). However, as to geographical indication of origin, São Francisco Valley wines are not yet certified. However, Brazilian research institutions, such as the Brazilian Farming Research Corporation (EMBRAPA), Bahia State University of (UNEB), Pernambuco Federal University of (UFPE), Rio Grande do Sul Federal University (UFRGS), São

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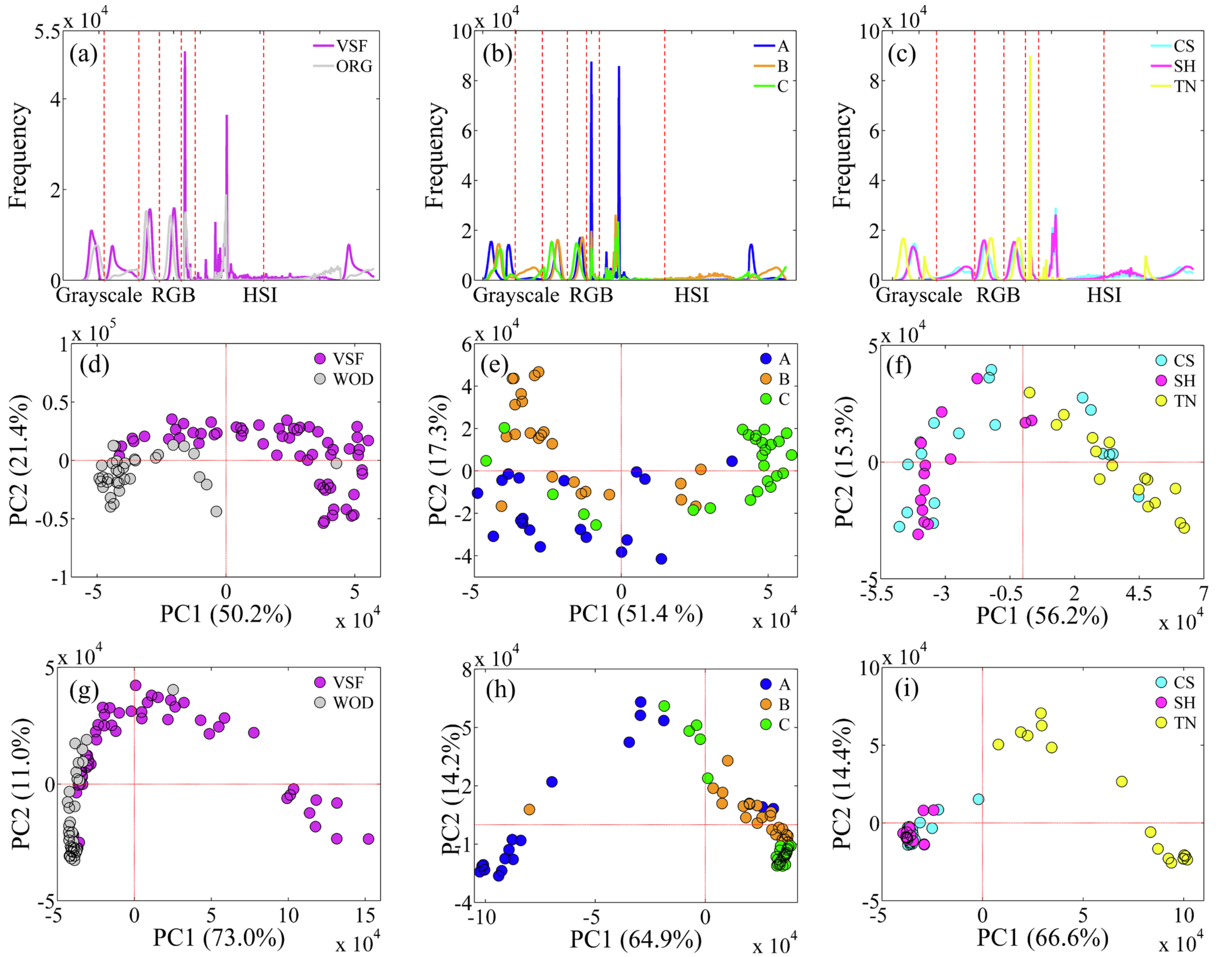

Fig. 1. Average color histograms in Grayscale, RGB and HSI channels according to three different classification approaches: (a) geographic origin, (b) winemaker (label), and (c) grape variety. PC1 × PC2 score plots for the red wines according to their geographic origin (d, g), winemaker (e, h), and grape variety (f, i) produced in the São Francisco Valley; respectively using RGB and HSI histograms. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Francisco Valley Federal University (UNIVASF), and the Federal Institute of the Pernambucano Sertão (IF Sertão-PE) have all concentrated their efforts to conduct qualitative and quantitative vineyard studies; adjusting the best vine varieties and production processes to soil and climate characteristics, and improving the quality of the wines produced in the region (Pereira et al., 2011).

A great number of grapevine varieties are cultivated in this terroir; such as Syrah, Cabernet Sauvignon, Alicante Bouschet, Tannat, Ruby Cabernet, Touriga Nacional, Chenin Blanc, Moscato Canelli, and Sauvignon Blanc, all properly adapted to the specific conditions of the North Eastern Brazilian *Sertão* (Tonietto & Teixeira, 2004; Tonietto & Carbonneau, 2004; Pereira et al., 2011; Amarante, 2015). However, since the region has only recently begun grape cultivation for fine wines, development of analytical methodologies to characterize the wines produced is thus necessary; taking into account each trademarked profile (and its unique congeners) associated with raw materials, climatic factors, fermentation methods, production, and maturation processes (Coelho et al., 2018; de Oliveira et al., 2019).

In this scenario, the use of geographical indications is an attempt by governments and producers to reduce fraud in foods and beverages (Brasil, 1996; Council of the European Union. (2006) (2006), 2006; OIV-International Organisation of Vine and Wine International. (2015), 2015). As consumers look to product labels for exclusive products or as a reference of quality, geographical indication increases the value-added to the product (van der Lans, van Ittersum, de Cicco, & Loseby, 2001; Holmberg, 2010). In Brazil, geographical indication is authorized by the National Institute of Industrial Property (INPI), through Indication of Provenance (IP) and Denomination of Origin (DO) (Brasil, 1996). Currently, Brazil has seven certified geographic winemaking regions with indications, six regions labeled by IP and one region labeled by DO; all are located in temperate climates.

Since wines with such labels are generally more expensive, fraudulent activities have often been associated with them. Other ways of defrauding wines can be found, such as those related to aging and the type of grapes used during production. Such practices can fool the consumer who lacks the expertise of a skilled taster (oenologist) to detect them. Thus, various studies using instrumental analytical techniques involving chemometrics have been developed (Versari et al., 2014). Satisfactory identification of authenticity and geographic origin of wines has been achieved using: Flame Atomic Absorption Spectrometry (Fabani et al., 2010), High Performance Liquid Chromatography coupled with Diode Array Detector and Mass Spectrometry (HPLC-DAD-MS) (Fraige, Pereira-Filho, & Carrilho, 2014), HPLC-Polymerase Chain Reaction (PCR) with Spectrophotometry (Muccillo et al., 2014),

Table 1
Classification results for red wine samples according to geographic origin using color histograms and pattern recognition techniques.

	PCA-LDA				PLS-DA				SPA-LDA			
	Training		Test		Training		Test		Training		Test	
	VSF	OGR	VSF	OGR	VSF	OGR	VSF	OGR	VSF	OGR	VSF	OGR
	Grayscale (2)				Grayscale (2)				Grayscale (16)			
VSF	36	6	14	4	35	7	14	4	40	2	14	4
OGR	6	17	6	4	6	17	6	4	7	16	6	4
Sn (%)	85.7		77.8		83.3		77.8		95.2		77.8	
Sp (%)	73.9		40.0		80.0		57.1		69.6		40.0	
Acc (%)	81.5		64.3		80.0		64.3		86.1		64.3	
	RGB (6)				RGB (10)				RGB (8)			
VSF	41	1	18	-	39	3	17	1	40	2	18	-
OGR	4	19	2	8	1	22	-	10	3	20	1	9
Sn (%)	97.6		100		97.5		94.4		95.2		100	
Sp (%)	82.6		80.0		96.1		100		90.0		90.0	
Acc (%)	92.3		92.9		93.8		96.4		92.3		96.4	
	HSI (14)				HSI (6)				HSI (8)			
VSF	42	-	18	-	39	3	18	-	39	3	17	1
OGR	1	22	-	10	1	22	-	10	1	22	-	10
Sn (%)	100		100		92.8		100		92.9		94.4	
Sp (%)	95.6		100		96.1		100		95.6		100	
Acc (%)	98.5		100		93.8		100		93.8		96.4	
	Grayscale + RGB (9)				Grayscale + RGB (2)				Grayscale + RGB (8)			
VSF	41	1	18	-	39	3	18	-	41	1	18	-
OGR	4	19	1	9	3	20	1	9	3	20	1	9
Sn (%)	97.6		100		92.9		100		97.6		100	
Sp (%)	82.6		90.0		88.5		90.0		90.0		90.0	
Acc (%)	92.3		96.4		90.7		96.4		93.8		96.4	
	Grayscale + HSI (14)				Grayscale + HSI (10)				Grayscale + HSI (9)			
VSF	41	1	18	-	40	2	17	1	39	3	16	2
OGR	1	22	1	9	-	23	-	10	1	22	-	10
Sn (%)	97.6		100		95.2		94.4		92.9		89.0	
Sp (%)	95.6		90.0		100		100		95.6		100	
Acc (%)	96.9		96.4		96.9		96.4		93.8		92.8	
	Grayscale + RGB +HSI (8)				Grayscale + RGB + HSI (8)				Grayscale + RGB + HSI (11)			
VSF	41	1	18	-	41	1	18	-	42	-	18	-
OGR	3	20	1	9	1	22	-	10	2	21	-	10
Sn (%)	97.6		100		97.6		100		100		100	
Sp (%)	86.9		90.0		95.8		100		91.3		100	
Acc (%)	93.8		96.4		96.9		100		96.9		100	

VSF: São Francisco Valley; **OGR**: Other geographical regions; **Acc**: Accuracy; **Sn**: Sensitivity; **Sp**: Specificity. The optimal number of PCs, latent variables or selected variables are indicated in parenthesis.

Fluorescence (Elcoroaristizabal et al., 2016), Inductively Coupled Plasma Mass Spectrometry (ICP-MS) (Rodrigues et al., 2011; Coetzee, van Jaarsveld, & Vanhaecke, 2014; Pérez-Álvarez et al., 2019) and ICP-MS with Cavity Ring-Down Spectroscopy (Orellana, Johansen, & Gazis, 2019). However, such techniques are laborious and expensive, which limits their use to more sophisticated laboratories and to large producers, and therefore they are not yet being used for low-price commercial wines.

We point out that multivariate classification using color histograms from digital images has already been successfully applied in food analysis for geographic origin classification in teas (Diniz et al., 2012), honey (Dominguez, Diniz, Di Nezio, Araújo, and Centurión (2014), and propolis (Pierini et al., 2016). In the case of wines, this analytical approach has also been used to identify adulterations in Spanish red wines, employing Tempranillo grapes with the *Rioja* Protected Designation of Origin (PDO) (Herrero-Latorre, Barciela-García, García-Martín, & Peña-Crecente, 2019). For this, PCA coupled with RGB histograms was employed considering two classes: one containing 6 samples of high-quality *Gran Reserva* GR wines; and one sample containing 72 synthetic adulterated GR samples prepared by mixing the 6 genuine GR wines with differing *Crianza* and *Joven* wines (which are cheaper and younger wines of the same grape variety, being 3 and 5 samples, respectively) at three different adulteration levels (10, 20, and 30%) in triplicate.

Given the above, this study proposes the development of a fast and low-cost methodology based on digital images and supervised pattern recognition to classify red wines (from the São Francisco Valley region) according to geographic origin, winemaker, and grape variety. Color

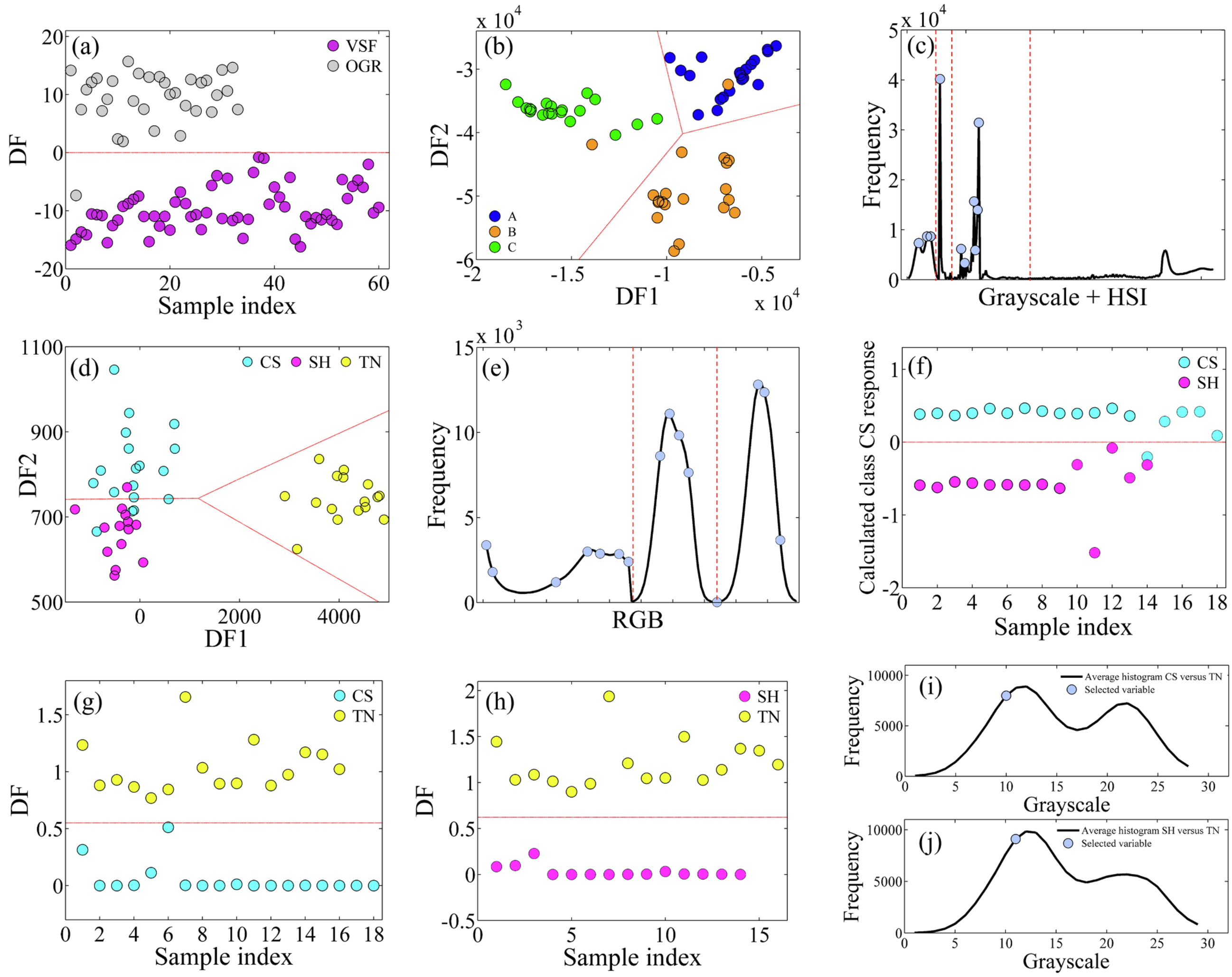

Fig. 2. São Francisco Valley red wine classification results: (a) Fisher's discriminant function plot for geographic origin classification using the PCA-LDA/HSI model; (b) Fisher's discriminant function plot and (c) its selected variables for winemaker classification using the SPA-LDA/Grayscale + HSI model; (d) Fisher's discriminant function plot and (e) its selected variables for grape variety classification using the SPA-LDA/RGB model; (f) response plot for Cabernet Sauvignon versus Syrah classification using the PLS-DA/HSI model; (g, h) Fisher's discriminant function plots and (i, j) its selected variables for the Cabernet Sauvignon versus Touriga Nacional, and Syrah versus Touriga Nacional classifications using the SPA-LDA/Grayscale model. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

histograms were obtained from digital images captured from commercial red wine samples without sample preparation, and used as input data for construction of multivariate classification models based on Partial Least Squares-Discriminant Analysis (PLS-DA) and Linear Discriminant Analysis coupled with Principal Component Analysis (PCA-LDA) and the Successive Projection Algorithm (SPA-LDA). The performance of these multivariate classifiers was compared in terms of accuracy, sensitivity, and specificity (Massart, Vandeginste, Buydens, Lewi, & Smeyers-Verbeke, 1998; Lavine, 2009).

2. Materials and methods

2.1. Samples

A total of 93 commercial red wine samples were collected for this study, being 53 purchased in the period between 2015 and 2017 in supermarkets located in Brazilian cities: Natal (Rio Grande do Norte) and João Pessoa (Paraíba), while another 40 samples were donated by winemakers of the São Francisco Valley and the IF Sertão-PE; at 20 samples each. All of the samples were duly coded, stored horizontally in a closed cabinet, and maintained at room temperature (23 ± 1 °C) until analysis.

To study geographic origins, 60 samples from the São Francisco Valley (SFV), and 33 samples from other geographic regions (OGR), including 7 from Rio Grande do Sul (Brazil), 5 from Argentina, 11 from Chile, 1 from France, 1 from Portugal, 1 from South Africa, 6 from Spain and 1 from Uruguay were analyzed. To classify by winemaker (label), the 60 samples from the São Francisco Valley were analyzed separately, being 20 samples for each producer (denominated as A, B, and C). For classification according to grape variety (São Francisco Valley red wines), three classes were analyzed: Cabernet Sauvignon (CS); 18 samples, Syrah (SH); 14 samples, and Touriga Nacional (TN); 16 samples. The remaining 12 samples, being seven different grape varieties were excluded from study since the sample number was insufficient to constitute individual classes.

For image acquisition (see section 2.2), the samples were conditioned in a glass cuvette with a 5 mm optical path to maintain visual uniformity at the sample surface, and a 1.5 ml internal volume.

2.2. Instrumentation and software

In this study, a simple and low-cost device for colorimetric measurements based on digital images was designed and built for acquisition of digital images. The apparatus consisted of a box built in wood

Table 2
Classification results for red wines samples from the São Francisco Valley as to winemaker (label) using color histograms and pattern recognition techniques.

	PCA-LDA						PLS-DA						SPA-LDA					
	Training			Test			Training			Test			Training			Test		
	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C	A	B	C
	Grayscale (3)						Grayscale (2)						Grayscale (20)					
A	12	3	-	5	-	-	12	3	-	5	-	-	12	2	1	4	1	-
B	2	8	5	-	2	3	3	7	5	-	2	3	2	12	1	1	3	1
C	3	5	7	1	2	2	3	5	7	1	2	2	2	3	10	1	3	1
Sn (%)	80.0	53.3	46.7	100	40.0	40.0	80.0	46.7	46.7	100	40.0	40.0	80.0	80.0	66.7	80.0	60.0	20.0
Sp (%)	83.3	73.3	83.3	90.0	80.0	70.0	81.8	78.9	86.8	90.0	84.6	76.9	86.7	83.3	93.3	80.0	60.0	90.0
Acc (%)	60.0			60.0			57.8			60.0			75.6			53.3		
	RGB (3)						RGB (3)						RGB (20)					
A	12	2	1	5	-	-	12	2	1	5	-	-	14	1	-	5	-	-
B	3	12	-	-	5	-	2	13	-	-	5	-	2	13	-	-	5	-
C	4	-	11	-	-	5	4	-	11	-	-	5	1	-	14	-	-	5
Sn (%)	80.0	80.0	73.3	100	100	100	80.0	86.7	73.3	100	100	100	93.3	86.7	93.3	100	100	100
Sp (%)	76.7	93.3	96.7	100	100	100	81.8	93.7	97.1	100	100	100	90.0	96.7	100	100	100	100
Acc (%)	77.8			100			80.0			100			91.1			100		
	HSI (6)						HSI (4)						HSI (9)					
A	12	3	-	5	-	-	13	2	-	5	-	-	14	-	1	5	-	-
B	1	13	1	-	5	-	1	13	1	-	5	-	1	14	-	-	5	-
C	1	-	14	-	-	5	1	-	14	-	-	5	1	-	14	-	-	5
Sn (%)	80.0	86.7	93.3	100	100	100	86.7	86.7	93.3	100	100	100	93.3	93.3	93.3	100	100	100
Sp (%)	93.3	90.0	96.7	100	100	100	93.7	93.7	96.7	100	100	100	93.3	100	96.7	100	100	100
Acc (%)	86.7			100			88.9			100			93.3			100		
	Grayscale + RGB (3)						Grayscale + RGB (3)						Grayscale + RGB (15)					
A	12	2	1	5	-	-	12	2	1	5	-	-	13	2	-	5	-	-
B	3	12	-	-	5	-	3	12	-	-	5	-	2	13	-	-	5	-
C	3	-	12	1	-	4	3	-	12	1	-	4	1	-	14	-	-	5
Sn (%)	80.0	80.0	80.0	100	100	80.0	80.0	80.0	80.0	100	100	80.0	86.7	86.7	93.3	100	100	100
Sp (%)	80.0	93.3	96.7	90.0	100	100	80.0	93.3	96.7	90.0	100	100	90.0	93.3	100	100	100	100
Acc (%)	80.0			93.3			80.0			93.3			88.9			100		
	Grayscale + HSI (8)						Grayscale + HSI (5)						Grayscale + HSI (10)					
A	12	2	1	5	-	-	14	1	-	5	-	-	15	-	-	5	-	-
B	1	13	1	-	5	-	1	13	1	-	5	-	1	13	1	-	5	-
C	1	-	14	-	-	5	1	-	14	-	-	5	-	-	15	-	-	5
Sn (%)	80.0	86.7	93.3	100	100	100	93.3	86.7	93.3	100	100	100	100	86.7	100	100	100	100
Sp (%)	93.3	93.3	93.3	100	100	100	93.3	96.7	96.7	100	100	100	96.7	100	96.7	100	100	100
Acc (%)	86.7			100			91.1			100			95.6			100		
	Grayscale + RGB + HSI (3)						Grayscale + RGB + HSI (6)						Grayscale + RGB + HSI (6)					
A	11	2	2	5	-	-	14	1	-	5	-	-	12	3	-	4	-	1
B	1	12	2	-	5	-	2	12	1	-	5	-	1	13	1	-	5	-
C	1	-	14	-	-	5	-	-	15	-	-	5	-	-	15	-	-	5
Sn (%)	73.3	80.0	93.3	100	100	100	93.3	80.0	100	100	100	100	80.0	86.7	100	80.0	100	100
Sp (%)	93.3	93.3	86.7	100	100	100	93.3	96.7	96.7	100	100	100	96.7	90.0	96.7	100	100	90.0
Acc (%)	82.2			100			91.1			100.0			88.9			93.3		

VSF: São Francisco Valley; **OGR**: Other geographical regions; **Acc**: Accuracy; **Sn**: Sensitivity; **Sp**: Specificity. The optimal number of PCs, latent variables or selected variables are indicated in parenthesis.

cut by laser, with dimensions of 16 cm × 7 cm × 7 cm and internally covered with white acrylic paint. A Nokia Lumia 710 smartphone, with the Windows Phone 7.5 operating system was attached to the apparatus, and kept frontally fixed to the cuvette holder at a constant distance of 3.5 cm. To maintain the internal illumination constant, a lighting system composed of six white LED lamps was positioned for the sample holder (on the lateral sides and above), being electrically powered by a 9 V battery. All images were recorded at room temperature.

The sample images were sequentially captured in triplicate in JPEG format (16.7 million colors with a resolution of 1944 × 2592 pixels); capturing a region of interest (ROI) corresponding to 26% of the total image as delineated from the center of each image and decomposed into color histograms, and which described the frequency distribution of the pixels as a function of the color component recorded (Diniz et al., 2012). Histograms in the Grayscale, Red-Green-Blue (RGB), and Hue-Saturation-Intensity (HSI) color spaces were obtained using the free software "Images_gui" available at http://laqa.quimica.ufpb.br/index.php/downloads. For each sample, the average of three histograms was calculated and used as an instrumental response for construction of the classification models.

Table 3
Classification results for red wine samples from the São Francisco Valley as to grape variety using color histograms and pattern recognition techniques.

	PCA-LDA						PLS-DA						SPA-LDA					
	Training			Test			Training			Test			Training			Test		
	CS	SH	TN	CS	SH	TN	CS	SH	TN	CS	SH	TN	CS	SH	TN	CS	SH	TN
	Grayscale (6)						Grayscale (1)						Grayscale (3)					
CS	8	5	-	4	1	-	10	-	3	5	-	-	9	4	-	4	1	-
SH	3	6	-	-	5	-	8	-	1	5	-	-	4	5	-	2	3	-
TN	-	-	11	-	-	5	-	-	11	-	-	5	-	-	11	-	-	5
Sn (%)	61.5	66.7	100	80.0	100	100	76.9	-	100	100	-	100	69.2	55.6	100	80.0	60.0	100
Sp (%)	85.0	79.2	100	100	90.0	100	60.0	100	81.8	50.0	100	100	80.0	83.3	100	80.0	90.0	100
Acc (%)		75.8			93.3			57.8			66.7			75.8			80.0	
	RGB (8)						RGB (3)						RGB (15)					
CS	9	4	-	3	2	-	7	6	-	2	3	-	12	1	-	3	2	-
SH	2	7	-	1	4	-	2	7	-	1	4	-	1	8	-	-	5	-
TN	-	-	11	-	-	5	-	-	11	-	-	5	-	-	11	-	-	5
Sn (%)	69.2	77.8	100	60.0	80.0	100	53.8	77.8	100	40.0	80.0	100	92.3	88.9	100	60.0	100	100
Sp (%)	90.0	83.3	100	90.0	80.0	100	90.0	75.0	100	90.0	70.0	100	95.0	95.8	100	100	80.0	100
Acc (%)		81.8			80.0			75.8			73.3			93.9			86.7	
	HSI (2)						HSI (3)						HSI (8)					
CS	8	4	1	2	3	-	7	5	1	2	3	-	9	4	-	3	2	-
SH	2	7	-	1	4	-	3	6	-	1	4	-	1	8	-	1	4	-
TN	-	-	11	-	-	5	-	-	11	-	-	5	-	-	11	-	-	5
Sn (%)	61.5	77.8	100	40.0	80.0	100	53.8	66.7	100	40.0	80.0	100	69.2	88.9	100	60.0	80.0	100
Sp (%)	90.0	83.3	95.4	90.0	70.0	100	85.0	79.2	95.4	90.0	70.0	100	95.0	83.3	100	90.0	80.0	100
Acc (%)		78.8			73.3			72.7			73.3			84.8			80.0	
	Grayscale + RGB (1)						Grayscale + RGB (17)						Grayscale + RGB (13)					
CS	4	6	3	2	2	1	13	-	-	3	2	-	10	3	-	3	2	-
SH	1	8	-	1	4	-	-	9	-	1	4	-	1	8	-	1	4	-
TN	1	-	10	-	-	5	-	-	11	-	-	5	-	-	11	-	-	5
Sn (%)	30.8	88.9	90.9	40.0	80.0	100	100	100	100	60.0	80.0	100	76.9	88.9	100	60.0	80.0	100
Sp (%)	90.0	75.0	86.4	90.0	80.0	90.0	100	100	100	90.0	80.0	100	95.0	87.5	100	90.0	80.0	100
Acc (%)		66.7			73.3			100			80.0			87.9			80.0	
	Grayscale + HSI (1)						Grayscale + HSI (1)						Grayscale + HSI (14)					
CS	4	9	-	-	5	-	12	0	1	5	0	0	11	2	-	5	-	-
SH	2	7	-	1	4	-	9	0	0	5	0	0	1	8	-	4	1	-
TN	-	-	11	-	-	5	0	0	11	0	0	5	-	-	11	-	-	5
Sn (%)	30.8	77.8	100	-	80.0	100	92.3	-	100	100	-	100	84.6	88.9	100	100	20.0	100
Sp (%)	90.0	62.5	100	90.0	50.0	100	55.0	100	95.4	50.0	100	100	95.0	91.7	100	60.0	100	100
Acc (%)		66.7			60.0			69.7			66.7			90.9			73.3	
	Grayscale + RGB + HSI (1)						Grayscale + RGB + HSI (2)						Grayscale + RGB + HSI (3)					
CS	7	5	1	2	3	-	7	6	0	3	2	0	11	1	1	3	2	-
SH	1	8	-	1	4	-	2	7	0	1	4	0	3	6	-	4	1	-
TN	-	-	11	-	-	5	0	0	11	0	0	5	-	-	11	-	-	5
Sn (%)	53.8	88.9	100	40.0	80.0	100	53.8	77.8	100	60.0	80.0	100	84.6	66.7	100	60.0	20.0	100
Sp (%)	95.0	79.2	95.4	90.0	70.0	100	90.0	75.0	100	90.0	80.0	100	85.0	95.8	95.4	60.0	80.0	100
Acc (%)		82.2			73.3			75.8			80.0			84.5			60.0	

VSF: São Francisco Valley; **OGR**: Other geographical regions; **Acc**: Accuracy; Sn: Sensitivity; **Sp**: Specificity. The optimal number of PCs, latent variables or selected variables are indicated in parenthesis.

2.3. Chemometric procedure

Initially, the exploratory analysis of data was performed using Principal Component Analysis (PCA). The dataset was divided into training (70%), and test (30%) sets (for all studied cases) using the Kennard-Stone (KS) algorithm (Kennard & Stone, 1969). These sets were used to construct supervised pattern recognition models applying PLS-DA, PCA-LDA and SPA-LDA. The performance of the multivariate classifiers was evaluated in terms of precision, sensitivity, and specificity for both training and test sets. Accuracy was calculated as the number of correct classifications divided by the total number of samples in the set under consideration. Sensitivity was calculated as the number of correct positive decisions divided by the total number of known positive cases, while specificity was calculated as the number of negative decisions divided by the total number of known negative cases (Fernandes et al., 2019). All calculations were run using the software Matlab® 2011b (Mathworks Inc).

3. Results and discussion

3.1. Exploratory analysis

Red wines present a characteristic color containing the blues, purples, and all shades of red which come from anthocyanins. These are pigments of the flavonoid class presenting differing structures whose red tones may vary depending on temperature, inter-molecular copigmentation, and pH; being this last the most important. Moreover, several factors, including grape variety, climate, fermentation, and maturation processes, etc., can provoke differences in the wine's color due to the differing anthocyanin chemical structures in the medium. Anthocyanins absorb electromagnetic radiation in the entire visible region; predominately red in an acid medium (Bridle & Timberlake, 1997; Cabrita, Fossen, & Andersen, 2000; Košir et al., 2004; Tôrres et al., 2011). Because of this, when taking color RGB histograms from digital images of studied wine samples (Fig. 1a–c), one can verify that

Table 4
Classification results for red wine samples from the São Francisco Valley; Cabernet Sauvignon versus Syrah using color histograms and pattern recognition techniques.

	PCA-LDA				PLS-DA				SPA-LDA			
	Training		Test		Training		Test		Training		Test	
	CS	SH	CS	SH	CS	SH	CS	SH	CS	SH	CS	SH
	Grayscale (14)				Grayscale (15)				Grayscale (9)			
CS	13	-	2	3	13	-	1	4	9	4	3	2
SH	2	7	3	2	-	9	5	-	3	6	1	4
Sn (%)	77.8		40.0		83.3		20.0		69.2		60.0	
Sp (%)	100		40.0		80.0		0		66.7		80.0	
Acc (%)	90.9		40.0		80.0		10.0		68.2		70.0	
	RGB (1)				RGB (1)				RGB (10)			
CS	6	7	3	2	6	7	3	2	11	2	4	1
SH	2	7	1	4	2	7	1	4	-	9	1	4
Sn (%)	46.1		60.0		46.1		60.0		84.6		80.0	
Sp (%)	77.8		80.0		77.8		80.0		100		80.0	
Acc (%)	59.1		70.0		59.1		70.0		90.9		80.0	
	HSI (1)				HSI (16)				HSI (10)			
CS	7	6	3	2	13	-	4	1	10	3	4	1
SH	3	6	1	4	-	9	-	5	1	8	3	2
Sn (%)	53.8		60.0		100		80.0		76.9		80.0	
Sp (%)	66.7		80.0		100		100		88.9		40.0	
Acc (%)	59.1		70.0		100		90.0		81.8		60.0	
	Grayscale + RGB (1)				Grayscale + RGB (14)				Grayscale + RGB (9)			
CS	6	7	4	1	13	-	3	2	10	3	4	1
SH	3	6	1	4	-	9	2	3	1	8	2	3
Sn (%)	46.1		80.0		100		60.0		76.9		80.0	
Sp (%)	66.7		80.0		100		60.0		88.9		60.0	
Acc (%)	54.5		80.0		100		60.0		81.8		70.0	
	Grayscale + HSI (1)				Grayscale + HSI (1)				Grayscale + HSI (10)			
CS	7	6	3	2	7	6	3	2	10	3	5	-
SH	4	5	1	4	3	6	1	4	-	9	4	1
Sn (%)	53.8		60.0		53.8		60.0		76.9		100	
Sp (%)	55.6		80.0		66.7		80.0		100		20.0	
Acc (%)	54.5		70.0		59.1		70.0		86.4		60.0	
	Grayscale + RGB +HSI (1)				Grayscale + RGB + HSI (1)				Grayscale + RGB + HSI (2)			
CS	7	6	3	2	7	6	3	2	12	1	3	2
SH	3	6	1	4	1	8	1	4	3	6	4	1
Sn (%)	53.8		60.0		53.8		60.0		93.2		60.0	
Sp (%)	66.7		80.0		88.9		80.0		66.7		20.0	
Acc (%)	59.1		70.0		68.2		70.0		81.8		40.0	

VSF: São Francisco Valley; **OGR**: Other geographical regions; **Acc**: Accuracy; Sn: Sensitivity; **Sp**: Specificity. The optimal number of PCs, latent variables or selected variables are indicated in parenthesis.

the red channel exhibits the important differences between classes under consideration; the green and blue components remains virtually similar. Notably, the Hue and Intensity channels in the HSI histograms present the most pronounced difference between classes, while the Saturation channel presents overlapping low frequencies.

PCA (Fig. 1d–i) was initially used as an exploratory analysis tool to investigate similarities and differences; employing color histograms in the Grayscale, RGB, HSI channels (and their combinations) as analytical information concerning the natural behavior of the data according to the three different classification requirements: (*i*) geographic origin; (*ii*) winemaker (label); and (*iii*) grape variety. For illustration, the PCA score plots obtained for the red wine samples using the RGB and HSI color spaces are shown; respectively, for identification of the geographic origin (Fig. 1d and g), winemaker (Fig. 1e and h), and grape variety (Fig. 1f and i).

As can be seen in Fig. 1d and g, there is a good separation trend between the red wine classes from the São Francisco Valley (SFV) and other geographic regions (OGR), with the OGR samples being more closely grouped. There is greater dispersion in the scores of the SFV samples, which can be attributed to the greater varietal composition of the wines, since this wine class is composed of 10 varietals and 3 different assemblages. The OGR samples participate mostly as varietal Cabernet Sauvignon or as an assemblage. In Fig. 1e and h, the PCA scores reveal a subtle separation trend for the three winemaker classes studied (A, B, and C), with class C differentiating from the others (RGB histograms), and class A differentiating from the others when using HSI histograms. Additionally, the PCA scores in Fig. 1f and i do not show a separation trend for the samples produced with Cabernet Sauvignon

(CS) and Syrah (SH) grapes. However, when HSI histograms were used we noted that the Touriga Nacional (TN) samples were completely differentiated from the two other classes.

3.2. Classification

Table 1 presents the results for geographic origin classification using different color histogram combinations with PCA-LDA, PLS-DA and SPA-LDA in both training and test sets. As can be seen, several approaches using PCA-LDA/HSI, PLS-DA/HSI, PLS-DA/Grayscale + RGB + HSI and SPA-LDA/Grayscale + RGB + HSI correctly classified all of the samples in the test set. However, they also yielded training set classification errors, with respectively 1, 4, 2, and 2 misclassifications. The best overall performance was obtained using PCA-LDA coupled with HSI histograms, yielding a correct classification rate (accuracy) of 98.5 and 100% in the respective training and test sets. This model employed 14 PCs and reached 100% sensitivity for the red wine samples produced in the SFV region. Yet in a wine sample from another geographic region (in this case, a Tempranillo wine from Spain), the model erroneously classified it as a SFV. The geographic origin classification results for the red wines under study are illustrated in the Fisher's discriminant function plot in Fig. 2a.

Regarding classification according to label from the São Francisco Valley; Table 2 presents the confusion matrix, with the accuracy, sensitivity, and specificity of the results obtained using the PCA-LDA, PLS-DA and SPA-LDA models in the training and test sets with different histogram combinations in the Grayscale, RGB, and HSI color spaces.

Similar to classification by geographic origin, all of the test set samples were correctly classified using the various models: (a) PCA-LDA, PLS-DA and SPA-LDA models constructed with RGB, HSI and Grayscale + HSI histograms; (b) both PCA-LDA and PLS-DA models using the complete histogram (i.e. Grayscale + RGB + HSI); and (c) the SPA-LDA model employing the Grayscale + RGB histogram. However, of all constructed models, SPA-LDA employing the Grayscale + HSI histogram achieved the best result, reaching 100% accuracy, sensitivity, and specificity for the test set, and obtaining only two misclassifications in the training set. The errors occurred with two class B samples that were erroneously classified as A and C, respectively, as shown in Fig. 2b. For this result, the SPA selected only 10 variables (Fig. 2c), an elimination of 97.7%, leading to a more parsimonious model in relation to the others. We note that variable selection per SPA-LDA (as compared to PCA-LDA and PLS-DA) presented better classification results for all of the color histogram combinations, except Grayscale + RGB + HSI.

The classification results for the São Francisco Valley red wines according to grape variety are presented in Table 3. As can be seen, the models constructed by PLS-DA using the Grayscale + HSI histogram, and by SPA-LDA using the RGB histogram obtained the best respective mean accuracy rates at 90.0 and 90.3%. The first correctly classified all of the training set samples; the second obtained the lowest number of misclassifications in the test set, (2 for the SPA-LDA model, and 3 for the PLS-DA model). However, to obtain these results, the PLS-DA model employed 17 latent variables, while the SPA-LDA model selected only 15 variables, eliminating about 98% of them. Thus, for parsimony, the SPA-LDA/RGB histogram approach was the most suitable, for presenting better discriminative ability and employing a smaller number of variables. The Fisher's discriminant function plot, and the variables selected by the SPA-LDA model using the RGB histogram are shown in Fig. 2d and e. We noted that in both cases, classification errors stemmed from difficulties in discriminating Cabernet Sauvignon and Syrah samples. The Touriga Nacional samples were differentiated completely from the others. Such errors might be due to chemical similarities of the Cabernet Sauvignon and Syrah red grape (French) varieties; Touriga Nacional is Portuguese.

To better investigate classification by type of grape, multivariate classification models were constructed on a pairwise basis, in three approaches: (a) Cabernet Sauvignon versus Syrah; (b) Cabernet Sauvignon versus Touriga Nacional; and (c) Syrah versus Touriga Nacional. In the latter two, all of the models correctly classified all of the samples (i.e. 100% correct classification for both training and test sets), regardless of the color histogram employed. The classification results for Cabernet Sauvignon versus Syrah are presented in Table 4. As can be seen, PLS-DA coupled to HSI histograms achieved correct classifications of 100% for the training set and of 90.0% for the test set, with only a single sample of Cabernet Sauvignon misclassified as Syrah, as shown in Fig. 2f. In addition, we present the Fisher's discriminant function plots obtained by SPA-LDA using the Grayscale histogram for Cabernet Sauvignon versus Touriga Nacional (Fig. 2g), and for Syrah versus Touriga Nacional (Fig. 2h). The histogram was chosen selecting a single variable for construction of both the Cabernet Sauvignon versus Touriga Nacional, and the Syrah versus Touriga Nacional models (Fig. 2i and j, respectively), making these therefore the most parsimonious models, through elimination of 99.6% of the variables.

As mentioned before, there are two distinctive signs for geographical indication (GI) in Brazil: (*i*) the Indication of Provenance (IP), which refers to the name of the place that has become known for producing, extracting or manufacturing a particular product or providing a certain service; and (*ii*) the Designation of Origin (DO), which refers to the name of the place that has come to designate products or services, whose qualities or characteristics may be attributed to their geographical origin. This latter, in addition to the place of production, requires that a process be carried out *in situ* (Brasil, 1996; Wilkinson, Cerdan, & Dorigon, 2017). Therefore, the strategies proposed here can be very useful and promise for red wines authentication purposes in terms of geographic origin, winemaker, and grape variety, because this flexibility in Brazilian legislation also allows the recognition of GI strategies in the manufacturing and service sectors.

4. Conclusion

This paper demonstrates the feasibility of employing color histograms obtained from digital images for classification of red wine samples in the São Francisco Valley region; according to geographic origin, winemaker, and grape variety, and using chemometric modeling whether PCA-LDA, PLS-DA, or SPA-LDA. The methodology developed is simple, fast, and inexpensive, consumes very low sample volumes; requires no pre-treatments, chemical reagents, or toxic solvents, and is in accordance with the principles of Green Chemistry. Additionally, the proposed methodology may contribute as a suitable analytical tool to trace red wines produced in the São Francisco Valley region, providing an advantage towards future certified geographical indication labeling. However, to guarantee any generalization of the proposed methodology, a larger and more varied testing of red wine samples, using more varieties, wineries, harvest years and geographic origins must be implemented.

CRediT authorship contribution statement

Carlos Monteiro de Lima: Conceptualization, Methodology, Investigation, Formal analysis. **David Douglas Sousa Fernandes:** Software, Formal analysis, Validation, Writing - original draft. **Giuliano Elias Pereira:** Resources, Funding acquisition. **Adriano de Araújo Gomes:** Conceptualization, Methodology, Software, Supervision. **Mário César Ugulino de Araújo:** Conceptualization, Methodology, Resources, Writing - review & editing, Supervision, Project administration, Funding acquisition. **Paulo Henrique Gonçalves Dias Diniz:** Writing - original draft, Writing - review & editing, Data curation, Visualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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