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Differentiation of mangoes (*Magnifera indica* L.) conventional and organically cultivated according to their mineral content by using support vector machines

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ABSTRACT

Mangoes of uniform genetics (Lippens variety) cultivated in the Gomera Island (Canary Islands) by conventional and organic farming were used to analyze the mineral content in order to differentiate crops cultivated in the same geographic area by the cultivation practices. Farming differences as well as soil differences may be reflected in the mineral content of the mangoes cultivated in these extensions. Concentration metal profiles consisting of the content of Ca, Co, Cu, Fe, K, Mg, Mn, Na, Ni and Zn in mangoes were obtained by using atomic absorption spectrometry (AAS). Pattern recognition classification procedures were applied for discriminating purposes. Linear discriminant analysis (LDA) allows to a classification performance of about 73% and support vector machines (SVM) found up to a 93% of prediction ability. The classification success when applying support vector machines techniques is due to their ability for modeling non-linear class boundaries.

1. Introduction

The mango (*Magnifera indica* L.) belongs to the *Anacardiaceae* family, originated in the Indo-Malaysian region, described as the most favoured and valuable fruit along the tropics, is of major economic concern [1]. This fruit currently ranks fifth in total production among major fruit crops worldwide, and the third in the tropics, after banana and pineapple. Mango is produced in about 90 countries in the world. In the case of Spain, cultivation is feasible primarily in the provinces of Granada and Malaga in Andalusia region and Canary Islands. Specifically a total of 451 Ha in the islands, produce 8784 t of mangoes and profits of 10.921.000 euros [2,3].

The chemical composition of mango pulp varies with the location of cultivation, variety, and stage of maturity. The major constituents of the pulp are water ($>80\%$), carbohydrates, organic acids, fats, minerals, pigments, tannins, vitamins, and flavor compounds [4].

Environment, pollution, atmosphere, soil, harvesting and handling are some of the factors, which play an important role in contamination of crops by metals in different tissues. Macro and trace elements play a significant role for maintaining health in humans. It is therefore of interest to establish the levels of some inorganic ions in these crops because, at elevated levels, these minerals can also be dangerous and toxic [5,6]. However, it is also possible to characterize some food products with regard to their geographic origin by comparison of the elemental concentration profiles by chemometric classification procedures [7,8]. In the same geographical area there is only a little variation in the climate but the variation in soil character from site to site may be considerable. Other parameters affecting the environment are very much related to the cultivation practice [9].

Organic farming holds an increasingly important position in current agriculture. Organic vegetables are associated by the general public with healthier and more flavorsome food, as well as to noncontaminating sustainable agricultural practice [10,11]. In organic farming, with the use of farmyard manure and frequent rotation of crops but no use of pesticides, the biological attacks from fungi and insect may be very different from those in conventional farming, with an intensive use of fertilizers and pesticides [9].

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In the present work, mangoes of uniform genetics (Lippens variety) cultivated in the Gomera Island (Canary Islands) by conventional and organic farming were used to analyze the mineral content in order to differentiate crops cultivated in the same geographic area by the cultivation practices. With respect to the growing areas, the production regions are located in Chejelipes (San Sebastian de la Gomera) at the east side of the island, reaching from the sea 255.4 m. Soil from this location is permeable, rich in minerals nutrients and with a slightly acid pH because of its volcanic origin. The texture of the surface soil is composed by 20–45% of silt and 15–25% of clay, typical from this location called "medianías". The cultivation practices include application of farmyard manure for the last 10 years in organic farming and the employ of fertilizers and fungicides in the conventional farming.

San Sebastián de la Gomera has a subtropical-semi-arid climate, with warm dry summers and moderately warm winters. The east coast of the island is protected from the African winds and influenced by the September winds causes a mild and a pleasant climate which is steady and has almost no notable thermal differences. Its average annual temperature is 18 °C. In the coastal area there is almost no rainfall but in the inland, the valleys accumulate the muggy winds that come from the sea and the rainfall is higher (with an atmospheric average relative humidity of 61%).

Accordingly, farming differences (conventional vs organic) and in minor extent, soil differences could be reflected in the mineral content of the mangoes cultivated in these extensions. The aim of the present paper is the determination of the content of Ca, Co, Cu, Fe, K, Mg, Mn, Na, Ni and Zn by using atomic absorption spectrometry (AAS) in mangoes to differentiate between the two ways of cultivating (conventional and organic).

For classification and discrimination between mangoes coming from locations where different cultivation methods were employed, supervised pattern recognition techniques such as linear discriminant analysis (LDA) [12] and support vector machines [13–15] were applied. LDA is used to find the linear combination of features which best separate two or more classes of object or event. This method maximizes the ratio of between-class variance to the within-class variance in any particular data set thereby guaranteeing maximal separability [16]. SVM provide a clear intuition of what learning from examples is all about. An SVM corresponds to a linear method in a very high dimensional space that is nonlinearly related to the input space [16,17].

2. Experimental

2.1. Apparatus

Mineral content were determined using a Perkin-Elmer atomic absorption spectrophotometer, model 2100 equipped with hollow-cathode lamps. Determinations were carried out in triplicate. Table 1 shows the instrumental conditions used for each element. The fuel employed was acetylene and the air was the oxidant gas.

Table 1
2100 flame-AAS parameters used for analysis of each element in mangoes from conventional and organic crops.

Metal	Detection limits (mg/L)	Wave-length (nm)	Slit width (nm)	Acetylene flow (L/min)	Air flow (L/min)
Ca	0.020	589.0	0.4	2.5	8.0
Co	0.002	240.7	0.2	2.5	8.0
Cu	0.010	324.8	0.7	2.5	8.0
Fe	0.002	248.2	0.2	2.5	8.0
K	0.100	766.5	0.2	2.5	8.0
Mg	0.020	285.2	0.7	2.5	8.0
Mn	0.010	279.5	0.2	2.5	8.0
Na	0.020	589.0	0.4	2.5	8.0
Ni	0.001	232.0	0.2	2.5	8.0
Zn	0.005	213.9	0.7	2.5	8.0

2.2. Chemical and reagents

Panreac (Barcelona, España) standard solutions of about 1000 mg L^{-1} were used as stock solution of each element for calibration. Other reagents used where of analytical grade. Milli-Q treated water was used throughout.

2.3. Samples

A total of 130 samples of mangoes (Lippens variety) collected in 2 different crops in the island of La Gomera (Canary Island, Spain) were analyzed. Sixty of these mangoes were cultivated in an organic crop where different types of farmyard manure were used (code O) and the other 70 samples were cultivated with use of pesticides and fertilizers, as the conventional way (C).

The plastic containers used for storing and treating the samples were cleaned to avoid contamination of the samples with traces of any metal. Containers were treated with 5% nitric acid during 24 h followed with two washes with milli-Q water.

The dry ashing method has been considered more adequate to our purposes because with this method neither acid mixture is added to the sample that could produce high blank values sometimes [18]. All samples were handled with nitrile gloves. Each flesh mango was quartered and homogenized. In previously weighed porcelain capsules, 30 g of each homogenized samples flesh was weighed in triplicate. The capsules were oven-dried at 60–80 °C for 24 h. The crucibles with samples were introduced into a muffle furnace, gradually raising the temperature (50 °C every hour or so) to 450 ± 15 °C for 18–24 h to destroy any organic matter present in the sample. The white ash obtained by this procedure was dissolved in nitric acid 5% to a volume of 50 mL and once digested, were transferred to 100 mL polyethylene bottles.

2.4. Quality controls

Quality control of the analytical measurements was performed using blank samples and the following reference materials: SRM 1515 Apple Leaves and BCR 414 Plancton from the National Institute for Standards and Technology (NIST). The recoveries obtained with the reference materials were upper than 95% (Table 2). During all of the analytical procedures, each batch of 20 samples was analyzed together with at least a blank and a reference sample. Calibration was performed using the calibration curve method.

2.5. Data analysis

The content of each mineral element was considered as chemical descriptor. Pattern recognition methods were applied to the data matrix, composed of 10 columns (the analyzed elements) and 130 rows (mangoes samples). LDA and SVM were applied for differentiation between class C and O ways of mangoes' cultivation. The statistical package, STATISTICA 7 from Statsoft [19] was used for all the chemometric calculations.

3. Results and discussion

3.1. Mineral content in mangoes samples

The mineral content of the two different conventionally and organically grown mangoes was determined and carefully scrutinized.

Table 2
Certified concentration values and concentration values obtained in this work.

Element	Material	Certified concentration[a]	Measured concentration[b]	Recovery (%)
Macroelements				
Na	SRM 1515[d]	24.00 ± 1.20	23.50 ± 1.10	97.92
K	SRM 1515	1.61 ± 0.02	1.58 ± 0.01	98.14
Ca	SRM 1515	1.53 ± 0.015	1.51 ± 0.013	98.69
Mg	SRM 1515	0.27 ± 0.008	0.27 ± 0.009	99.63
Microelements				
Fe[c]		80	82	102.50
Cu	SRM 1515	5.64 ± 0.24	5.61 ± 0.23	99.47
Zn	SRM 1515	12.50 ± 0.30	12.30 ± 0.31	98.40
Mn	SRM 1515	54.00 ± 3.00	54.60 ± 2.80	101.11
Co[c]		0.09	0.09	100.00
Ni	BCR-414[e]	18.80 ± 0.80	19.00 ± 0.70	101.06

[a] Confidence interval: 95%.
[b] Mean ± standard deviation.
[c] Non certified value. Given only with orientative purpose.
[d] NIST (National Institute of Standards and Technology) No 1515 (Apple Leave).
[e] NIST (National Institute of Standards and Technology No 414 (Plancton).

The results, expressed in mg/100 g were obtained from triplicate measurements and rounded up to the last significant figure associated with random error. Table 3 shows these results. The corresponding descriptive basic statistic for mangoes samples from both cultivation methods can be seen in Table 4. Looking at these values, K was the element with a major content in all samples. The mean concentration of K was higher in Conventional crops than in Organic ones, with average concentrations of 146.6 and 112.0 mg 100 g^{-1}, respectively. Ca was the second predominant element with similar values in samples from cultivation methods, 47.3 mg 100 g^{-1} in conventional crops, and 44.5 mg 100 g^{-1} in organic crops. Mg and Na presented lower and similar contents, with average values of 18.08 and 11.44 mg 100 g^{-1}, respectively, in conventional farming samples and 17.96, and 15.26 mg 100 g^{-1} in organic farming ones. Fe was present with lower values in both crops being almost twice higher in organic than in conventional farming (2.76 and 1.97 1 mg 100 g^{-1}, respectively). The other analyzed metals mostly appeared with values lower than 1 mg 100 g^{-1} such as Zn (0.20 mg 100 g^{-1} in conventional and 0.13 mg 100 g^{-1} in organic cultivation) and even lower, being Co, Cu, Ni and Mn the minerals with the lowest concentrations in both classes (C and O). These concentrations were close to 0.1 mg 100 g^{-1} in both crops (0.07; 0.07; 0.07 and 0.09 mg 100 g^{-1} in conventional cultivated mangoes and 0.07; 0.08; 0.05 and 0.07 in organic ones). All the values obtained for both classes were similar with the exception of K, Fe and Zn. The higher K content observed in conventional cultivated mangoes compared with organic ones coul be attributed to increasing K uptake by plants as a result of synthetic K fertilization supply (such as KNO_3) [20]. Significantly higher levels of iron have been detected in organic foods in comparison to conventionally produced foods [21]. This fact is in agreement with our results when comparing Fe levels in organic (+40%) versus conventional mangoes. The plants absorb zinc from the ground in small quantities. The zinc content in plants increases when zinc containing pesticides are used in conventional farming [22]. In the present study Zn concentration was slightly higher in conventional than in organic cultivation.

3.2. Statistical procedures for classification

Using the mineral content found in the analyzed mangoes samples as chemical descriptors; statistical methods were applied in order to establish differences between both types of agricultural crops.

In order to visualize some trends in the data, they were subjected to a Principal Component Analysis (PCA). Nevertheless, the suitable number of principal components (PCs) for explaining about 85% of data variance were 7, leading to communalities higher than 0.7 for the original descriptors. The corresponding scores plot by using the first two and three PCs did not show any discrimination between the samples belonging to the two classes. Thus, methods devoted to supervised learning pattern recognition for classification purposes have to be used. Anyway, data eigenanalysis is based in the maximization of data variance that cannot enhance discrimination between classes. Instead, a maximization of the ratio of between-class/within-class variance may lead to suitably discriminate them, for instance with LDA.

Recent efforts on differentiation/classification of food products and other chemical systems by linear discriminant analysis (LDA) and support vector machines (SVM) have been made by other authors [16–17,23–25]. In this case, our research starts from the priori knowledge of class membership of the samples to be processed and hence, typical supervised learning pattern recognition (PR) methods have to be applied. Two classes were considered, conventional (C) and organic (O) mangoes' crops. First of all, the method of LDA was applied for building linear frontiers between the two classes. Because of possible non-linear natural of class distribution, SVM was also applied.

The classification procedure is validated by randomly dividing the data set into training and validation sets containing about 75% and 25% samples of every class, respectively. The randomly generation of training and validation sets is repeated five times, and the classification performance is computed in average. The prediction ability is the usual measurement of classification performance, as the rate of evaluation samples correctly classified.

3.2.1. LDA

Linear discriminant analysis is a typical discriminating method, belonging to the first level of PR, where objects are classified into either of a number of defined classes [26]. Discriminant functions are obtained as linear combination of metal descriptors to maximize the F-ratio of between class sum of squares and within class sum of squares. If we have p descriptors and g classes, the number of uncorrelated discriminant functions are p or g-1 whichever is smaller; and so, in our case only one discriminant function can be obtained. The parameter called Wilks' lambda is the ratio between the within class sum of squares and the total sum of squares, calculated for each descriptor. The discrimination power of a given descriptor is better when its Wilks' lambda is lesser [27,28].

However, after application of standard LDA, the different descriptors exhibit very similar values of Wilks' lambda, and in consequence we cannot disregard any of them. Thus, all descriptors, namely Ca, Co, Cu, Fe, K, Mg, Mn, Na, Ni and Zn were used for distinguishing between class C and O samples. Evaluation samples are classified from the estimation of an a posteriori probability of class membership using the Bayes' theorem. The classification performance, expressed as prediction ability is 73.2%. This result, albeit fairly good, could be improved by using

Table 3
Experimental results for determination of elements (mg/100 g) in mangoes from conventional (C) and organic (O) agricultural crops.

Sample	Code	Fe	Mn	Ni	Cu	Co	Zn	Ca	Mg	Na	K
1	C	1.21	0.03	0.02	0.02	0.11	0.13	65.97	10.51	31.72	102.36
2	C	2.17	0.09	0.09	0.02	0.03	0.15	22.54	11.66	0.97	132.15
3	C	3.04	0.04	0.08	0.02	0.03	0.07	83.20	41.42	1.37	117.89
4	C	2.32	0.24	0.06	0.05	0.11	0.40	37.78	23.15	1.17	98.84
5	C	2.80	0.20	0.03	0.03	0.11	0.04	32.36	13.33	0.80	59.16
6	C	0.15	0.08	0.05	0.03	0.11	0.21	4.75	28.53	0.88	56.17
7	C	1.42	0.03	0.02	0.02	0.03	0.13	27.48	18.43	0.69	56.48
8	C	1.13	0.03	0.06	0.04	0.11	0.15	7.52	10.35	0.62	70.62
9	C	1.87	0.11	0.06	0.05	0.03	0.23	4.20	4.38	0.81	53.87
10	C	2.54	0.10	0.10	0.04	0.03	0.22	13.38	11.38	1.16	88.96
11	C	1.88	0.09	0.03	0.02	0.09	0.31	41.77	30.84	1.04	92.94
12	C	2.15	0.08	0.08	0.04	0.03	0.10	12.91	18.17	3.36	96.54
13	C	0.69	0.07	0.05	0.01	0.03	0.23	20.68	24.85	6.98	500.74
14	C	2.36	0.07	0.09	0.02	0.03	0.21	15.10	14.12	3.01	98.94
15	C	0.16	0.14	0.07	0.06	0.11	0.14	17.77	19.31	2.76	45.76
16	C	0.09	0.30	0.03	0.01	0.11	0.07	42.81	7.97	38.96	47.99
17	C	1.28	0.24	0.10	0.02	0.11	0.14	77.47	13.93	6.41	51.00
18	C	1.19	0.05	0.07	0.03	0.10	0.10	20.77	12.31	5.99	61.20
19	C	0.67	0.07	0.06	0.02	0.03	0.10	23.84	7.30	28.52	72.61
20	C	0.94	0.08	0.07	0.10	0.03	0.16	5.67	5.67	4.27	56.68
21	C	1.50	0.05	0.03	0.02	0.11	0.13	9.61	8.31	4.88	146.59
22	C	3.21	0.11	0.12	0.16	0.04	0.23	68.82	11.95	4.74	68.96
23	C	1.86	0.04	0.10	0.06	0.03	0.28	36.56	11.72	4.33	56.69
24	C	1.33	0.09	0.07	0.02	0.03	0.10	129.76	5.61	3.07	354.58
25	C	2.79	0.22	0.10	0.04	0.05	0.50	20.00	11.49	15.64	114.46
26	C	0.91	0.25	0.10	0.06	0.05	0.07	42.25	22.09	16.09	137.60
27	C	4.55	0.20	0.09	0.03	0.05	0.08	63.00	3.00	16.80	140.20
28	C	0.02	0.04	0.09	0.03	0.05	0.01	19.69	36.45	17.54	215.20
29	C	1.06	0.09	0.12	0.05	0.05	0.16	20.45	19.32	17.26	180.11
30	C	2.69	0.09	0.12	0.12	0.05	0.16	41.28	21.12	17.44	24.81
31	C	6.41	0.04	0.10	0.04	0.06	0.60	21.09	28.52	15.23	56.05
32	C	4.39	0.03	0.11	0.07	0.05	0.07	17.66	33.53	10.71	372.82
33	C	4.52	0.03	0.10	0.02	0.05	0.08	15.17	27.54	14.57	113.37
34	C	1.08	0.07	0.09	0.03	0.06	0.08	21.50	17.55	16.96	116.77
35	C	0.94	0.10	0.09	0.05	0.05	0.49	15.97	15.77	10.78	151.70
36	C	3.32	0.04	0.12	0.03	0.06	0.46	11.38	14.77	7.19	138.72
37	C	4.71	0.04	0.12	0.16	0.05	0.07	15.55	3.94	12.99	268.70
38	C	3.16	0.10	0.10	0.04	0.05	0.16	25.65	15.23	13.43	182.36
39	C	3.18	0.03	0.10	0.17	0.05	0.16	61.34	3.16	13.41	26.23
40	C	4.71	0.05	0.11	0.05	0.05	0.10	43.51	2.59	14.17	59.08
41	C	2.46	0.03	0.10	0.08	0.05	0.18	70.27	15.91	13.07	124.43
42	C	3.04	0.07	0.10	0.04	0.12	0.04	43.17	16.24	13.47	57.43
43	C	3.48	0.04	0.12	0.08	0.06	0.15	165.13	68.79	8.86	356.45
44	C	2.65	0.04	0.12	0.10	0.17	0.19	241.72	20.96	9.38	197.60
45	C	0.88	0.15	0.11	0.33	0.17	1.31	50.99	13.69	9.13	433.33
46	C	1.26	0.02	0.07	0.03	0.11	0.12	61.25	30.58	7.87	111.00
47	C	0.70	0.05	0.03	0.04	0.03	0.05	94.07	27.19	7.14	24.21
48	C	2.38	0.06	0.03	0.04	0.04	0.05	179.18	13.63	7.41	138.88
49	C	1.92	0.14	0.03	0.27	0.11	0.44	58.04	36.07	6.00	195.07
50	C	0.18	0.04	0.05	0.14	0.11	0.17	86.20	11.19	7.05	197.55
51	C	1.57	0.13	0.04	0.13	0.11	0.16	110.49	34.46	7.03	196.18
52	C	0.22	0.27	0.06	0.12	0.11	0.16	104.32	15.99	5.55	202.77
53	C	5.43	0.03	0.01	0.02	0.11	0.12	86.77	10.55	5.69	196.80
54	C	0.10	0.07	0.04	0.01	0.11	0.23	55.02	21.93	5.88	121.80
55	C	0.14	0.09	0.05	0.11	0.11	0.12	20.66	12.25	7.49	193.86
56	C	0.12	0.07	0.04	0.12	0.11	0.18	19.27	10.80	51.01	177.35
57	C	0.14	0.20	0.04	0.04	0.11	0.16	38.47	21.65	6.59	193.35
58	C	1.33	0.09	0.08	0.02	0.11	0.11	42.84	16.27	49.08	206.16
59	C	2.53	0.18	0.09	0.18	0.04	0.28	19.38	12.63	21.05	163.50
60	C	0.15	0.04	0.03	0.02	0.10	0.16	13.20	16.25	19.17	74.90
61	C	1.74	0.15	0.04	0.12	0.11	0.35	97.81	36.55	2.05	197.74
62	C	0.76	0.04	0.08	0.08	0.11	0.10	87.50	10.63	43.98	198.05
63	C	3.64	0.06	0.07	0.10	0.03	0.13	18.65	33.44	2.96	200.27
64	C	1.92	0.09	0.09	0.14	0.04	0.36	18.51	10.89	2.75	117.38
65	C	2.39	0.10	0.07	0.03	0.03	0.32	159.14	16.36	6.28	192.84
66	C	2.01	0.10	0.08	0.07	0.03	0.09	28.72	19.30	7.52	179.27
67	C	2.26	0.06	0.07	0.07	0.04	0.10	17.11	24.03	5.72	194.37
68	C	0.15	0.06	0.03	0.09	0.11	0.14	16.62	12.60	6.64	208.11
69	C	2.80	0.12	0.04	0.07	0.07	0.38	16.66	20.99	21.25	162.82
70	C	2.89	0.21	0.04	0.03	0.04	0.20	11.87	12.54	45.23	162.91
71	O	0.04	0.03	0.03	0.04	0.11	0.05	25.52	11.49	5.30	97.88
72	O	0.86	0.04	0.02	0.11	0.11	0.04	27.28	7.18	39.15	95.60
73	O	4.07	0.03	0.02	0.02	0.11	0.04	15.01	7.83	41.17	91.99
74	O	2.60	0.05	0.03	0.05	0.11	0.07	55.21	11.83	5.65	94.58
75	O	2.64	0.04	0.03	0.10	0.04	0.04	43.53	7.37	9.44	98.39

Table 3 (*continued*)

Sample	Code	Fe	Mn	Ni	Cu	Co	Zn	Ca	Mg	Na	K
76	O	0.97	0.08	0.03	0.06	0.10	0.05	62.55	23.65	7.42	120.62
77	O	0.18	0.09	0.03	0.11	0.11	0.04	112.70	17.04	3.71	96.13
78	O	0.19	0.05	0.03	0.11	0.11	0.07	58.05	18.02	7.47	93.82
79	O	3.24	0.06	0.03	0.11	0.11	0.09	15.64	9.77	9.19	105.47
80	O	2.62	0.09	0.08	0.06	0.04	0.11	37.05	16.00	7.44	113.55
81	O	3.06	0.06	0.06	0.06	0.03	0.11	55.75	12.89	12.44	121.94
82	O	3.18	0.07	0.01	0.05	0.11	0.09	58.56	20.44	12.60	120.55
83	O	3.17	0.06	0.06	0.10	0.04	0.16	28.48	9.73	3.24	64.95
84	O	2.52	0.06	0.05	0.08	0.03	0.19	28.24	11.24	3.92	138.26
85	O	0.41	0.09	0.07	0.06	0.04	0.19	41.84	17.98	3.61	136.21
86	O	2.93	0.08	0.03	0.05	0.05	0.08	33.47	18.23	3.32	187.46
87	O	1.21	0.04	0.01	0.13	0.11	0.13	56.10	17.18	5.02	151.11
88	O	2.39	0.06	0.07	0.07	0.04	0.14	33.33	16.24	4.85	129.81
89	O	1.60	0.09	0.08	0.05	0.04	0.08	18.22	16.92	40.95	89.27
90	O	1.90	0.06	0.01	0.07	0.11	0.09	33.52	14.59	41.38	87.35
91	O	2.12	0.10	0.05	0.10	0.11	0.10	22.31	33.76	39.81	64.95
92	O	2.20	0.07	0.02	0.11	0.11	0.09	26.81	6.54	40.02	63.72
93	O	1.76	0.07	0.06	0.11	0.11	0.12	56.95	47.53	5.55	186.90
94	O	2.52	0.05	0.08	0.10	0.04	0.13	13.80	9.27	5.60	61.55
95	O	1.15	0.09	0.06	0.05	0.04	0.14	28.27	13.41	15.86	63.25
96	O	2.17	0.10	0.01	0.08	0.11	0.14	21.74	12.05	12.38	102.75
97	O	3.11	0.05	0.07	0.13	0.11	0.24	25.59	8.49	27.11	86.45
98	O	2.85	0.13	0.09	0.08	0.04	0.15	44.20	19.18	5.24	184.90
99	O	2.37	0.05	0.07	0.07	0.03	0.21	43.86	14.18	3.73	140.89
100	O	2.60	0.06	0.07	0.12	0.03	0.20	46.02	18.02	13.19	130.79
101	O	2.71	0.18	0.02	0.09	0.11	0.19	19.07	14.58	6.47	184.15
102	O	2.53	0.07	0.07	0.12	0.03	0.09	36.29	20.41	33.56	180.52
103	O	3.96	0.05	0.08	0.06	0.04	0.27	74.85	30.13	43.06	189.02
104	O	1.67	0.03	0.01	0.06	0.11	0.08	65.15	19.59	6.38	181.52
105	O	2.56	0.03	0.04	0.18	0.04	0.20	53.75	26.91	9.37	65.58
106	O	2.40	0.06	0.08	0.09	0.03	0.16	74.78	20.48	7.62	51.08
107	O	4.77	0.12	0.07	0.20	0.11	0.21	30.68	12.09	5.46	50.38
108	O	3.06	0.04	0.07	0.09	0.04	0.11	42.08	18.79	9.36	170.86
109	O	4.18	0.05	0.08	0.13	0.06	0.23	65.17	29.43	7.44	172.78
110	O	2.29	0.11	0.06	0.07	0.06	0.11	16.81	11.80	8.73	37.02
111	O	3.06	0.09	0.05	0.08	0.11	0.10	49.70	14.27	12.34	128.54
112	O	2.79	0.05	0.01	0.08	0.11	0.09	48.41	20.74	11.64	101.13
113	O	4.19	0.22	0.09	0.06	0.04	0.15	63.59	26.64	5.61	47.01
114	O	2.85	0.06	0.07	0.04	0.03	0.09	48.89	14.37	4.66	35.83
115	O	1.15	0.12	0.07	0.06	0.11	0.27	49.63	12.57	4.28	51.93
116	O	3.66	0.08	0.07	0.13	0.04	0.20	73.91	19.19	3.18	94.65
117	O	3.86	0.08	0.01	0.09	0.11	0.10	66.31	18.95	4.50	98.64
118	O	1.80	0.07	0.04	0.04	0.11	0.10	52.10	31.57	4.46	110.73
119	O	2.40	0.21	0.04	0.10	0.10	0.20	74.04	12.23	38.46	117.80
120	O	2.76	0.10	0.04	0.06	0.04	0.10	73.65	20.65	42.83	82.28
121	O	3.99	0.07	0.04	0.05	0.04	0.08	60.63	26.70	41.15	87.73
122	O	4.10	0.03	0.07	0.05	0.03	0.05	66.04	33.32	38.88	87.90
123	O	4.57	0.04	0.01	0.06	0.03	0.05	64.13	18.63	15.36	121.25
124	O	5.16	0.04	0.02	0.09	0.04	0.15	19.18	21.03	33.86	185.32
125	O	3.31	0.11	0.09	0.08	0.04	0.15	18.51	14.42	24.56	119.27
126	O	4.31	0.07	0.07	0.08	0.11	0.21	46.50	14.50	25.89	179.84
127	O	5.94	0.05	0.04	0.06	0.11	0.10	48.20	13.93	7.73	192.79
128	O	4.33	0.08	0.04	0.06	0.11	0.09	58.21	20.48	7.69	50.33
129	O	4.35	0.08	0.06	0.04	0.04	0.09	20.63	31.31	6.62	78.46
130	O	3.97	0.04	0.05	0.06	0.04	0.11	21.31	19.79	6.47	165.19

SVM classification that is able to model non linear frontiers between classes.

3.2.2. SVM

Support vector machines (SVM) are revolutionary methods for pattern recognition based on statistical learning theory and kernel latent variables [13–15]. The purpose of SVM is separate the classes in a vectorial space independently on the probabilistic distribution of pattern vectors in the data set [29]. This separation is performed with the particular hyperplane which maximizes a quantity called margin. The margin is the distance from a hyperplane separating the classes to the nearest point in the data set. The training pattern vectors closest to the separation boundary are called support vectors. When dealing with a non linear boundary, the kernel method is applied. The key idea of kernel method is a transformation of the original vectorial space (input space) to a high dimensional Hilbert space (feature space), in which the classes can be separated linearly. The application of SVM classification to our data set leads to a prediction ability of 93.1%. This confirms the fact of SVM is the tool of choice for classification with non-linear boundaries between classes. In previous studies, when comparing wines from different denomination of origin (DO) in Spain, we also observed differences in the effectiveness of the classification methods employed. Thus, Artificial Neural Networks (ANN), was more adequate classification procedure than LDA [8,30]. This affirmation is in agreement with Balabin et al., [16,17,23–25] who classified different multivariate methods into three groups: the most effective ones (SVM, PNN), methods of medium effectiveness (KNN, MLP) and the least effective ones (RDA, SIMCA, PLS).

Table 4
Mineral contents in conventional ($n=70$ samples) and organic ($n=60$) mangoes samples.

Element	Conventional			Organic		
	Mean ± SD (mg/100 g)	Median	Range of quantified values (mg/100 g)	Mean ± SD (mg/100 g)	Median	Range of quantified values (mg/100 g)
Ca	47.30 ± 45.75	28.10	4.20–241.72	44.50 ± 20.57	44.20	13.80–112.70
Co	0.07 ± 0.04	0.05	0.03–0.17	0.07 ± 0.04	0.06	0.03–0.11
Cu	0.07 ± 0.06	0.04	0.00–0.33	0.08 ± 0.03	0.08	0.02–0.20
Fe	1.97 ± 1.44	1.87	0.00–6.41	2.76 ± 1.26	2.68	0.04–5.94
K	146.60 ± 93.97	135.00	24.21–500.74	112.03 ± 45.57	101.00	35.83–192.79
Mg	18.08 ± 10.99	15.80	2.59–68.79	17.96 ± 7.82	17.40	6.54–47.53
Mn	0.09 ± 0.07	0.07	0.02–0.30	0.07 ± 0.04	0.07	0.03–0.22
Na	11.44 ± 11.68	7.16	0.62–51.01	15.26 ± 14.01	7.69	3.18–43.06
Ni	0.07 ± 0.03	0.07	0.01–0.12	0.05 ± 0.03	0.05	0.00–0.09
Zn	0.20 ± 0.18	0.15	0.00–1.31	0.13 ± 0.06	0.11	0.04–0.27

4. Conclusion

The two different mangoes crops have been suitably discriminated when using the metal content profile and applying SVM classification method. Accordingly, our results are in good agreement with the prior working hypothesis of differentiation between mangoes coming from locations where different cultivation methods were employed (conventional and organic). Samples of class C was well separated from class O. This fact supports the importance of the cultivating techniques, correlated to the metal content, in the mangoes differentiation.

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