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Characterization of Catalan red wines by pattern recognition methods

by

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Caractérisation des vins rouges catalans aux moyens de méthodes de reconnaissance de modèles (pattern recognition)

Résumé: On a distingué et différencié selon leur origine géographique 52 vins rouges catalans produits au département de Tarragone (Catalogne, Espagne) du cru de 1983. Les vins appartiennent à 4 contrées différentes: Priorat, Terra Alta, Camp de Tarragone et Falset. La caractérisation a été réalisée sur la base de 17 paramètres mesurés pour chaque échantillon de vin et 3 méthodes de reconnaissance de modèles: SQDA, KNN et LLM. Les variables les plus remarquables dans cette étude ont été les ions métalliques manganèse, magnésium, fer et sodium, en plus les paramètres oenologiques teneur en alcool éthylique, alcalinité des cendres et acidité totale.

Le manque de différences variétales associé aux conditions climatiques et culturelles assez semblables dues à la proximité géographique des zones étudiées mène à une capacité de prédiction maximale de 87 % en utilisant la méthode LLM.

Key words: red wine, differentiation, analysis, manganese, magnesium, iron, sodium, ethanol, acidity, statistics, Spain.

Introduction

Organoleptic examination has constituted, until the present, the major procedure for determining the quality of wines. A well trained expert could distinguish good wines from poor quality ones as well as wines from different geographic origin. However, this requires at least several years of training. Therefore, it seems convenient to establish a faster and more objective method to recognize unknown wines. Pattern recognition techniques have proved a valuable tool in this field. Several recent studies have been made on this very promising area with different aims as correlating chemical constituents with sensory characteristics (1, 4, 10, 13, 18, 19), differentiating wines according to their geographic or varietal origin (9, 11, 15, 16, 22) or distinguishing wines according to the vinification process (5, 17).

In this study, the differentiation and classification of 52 red wines, originating from four distinct Catalan areas, vintage 1983, have been attempted on the basis of 17 measurements of different sample constituents and by using three supervised methods of analysis, i. e. a parametric technique (7), Statistical Quadratic Discriminant Analysis (SQDA), and two non-parametric techniques (8, 23), K-Nearest Neighbour (KNN) and Linear Learning Machine (LLM). Results obtained from the various pattern recognition methods have been compared.

Material and methods

Samples

52 red wines, all from 1983 vintage, were collected in the production areas: 13 samples from Priorat, 10 samples from Camp de Tarragona, 17 samples from Falset and 12 samples from Terra Alta. All wines were guaranteed by the Spanish D.O. (Denominación de Origen: Certified Brand of Origin).

Chemical analyses

7 enological parameters were determined including measurements of density (Den, $g \cdot l^{-1}$), ethanol content (EtOH, % v/v), ash content (A, $g \cdot l^{-1}$), alkalinity of ashes (AA, $g \cdot l^{-1}$ expressed as Na_2CO_3), titratable acidity (TA, $g \cdot l^{-1}$ of tartaric acid), pH and electrical conductivity (COND, $mS \cdot cm^{-1}$), all of them determined according to the OIV standard methods (14), jointly with 10 metal ion concentrations: sodium (Na, $mg \cdot l^{-1}$), potassium (K, $mg \cdot l^{-1}$) and lithium (Li, $mg \cdot l^{-1}$) determined by flame emission spectroscopy and calcium (Ca, $mg \cdot l^{-1}$), magnesium (Mg, $mg \cdot l^{-1}$), strontium (Sr, $mg \cdot l^{-1}$), iron (Fe, $mg \cdot l^{-1}$), copper (Cu, $mg \cdot l^{-1}$), zinc (Zn, $mg \cdot l^{-1}$) and manganese (Mn, $mg \cdot l^{-1}$) determined by atomic absorption spectroscopy. Enological parameters were determined at the Viticulture Enological and Fruticulture Station of Reus (INCAVI) and metal ion concentrations were measured by using an Instrumentation Laboratory AA/AE 551 spectrophotometer.

Pattern recognition methods

Discriminant analysis

In Statistical Discriminant Analysis, several discriminant functions, which can be associated to axes situated in the n-dimensional space, are computed. The class-separating functions result from weighting and linearly combining the discriminating variables (analytical parameters in this case) in such a way that the projection of the data points of the classes (the 4 sets of different wines) on these axes exhibit the maximum separation.

If classes have identical variance-covariance matrices, the separating surface between groups is linear and the method is known as Statistical Linear Discriminant Analysis (SLDA). If there is a certain degree of dissimilarity among the variance-covariance matrices of the different groups, the separating surface is curved and the method is referred to as Statistical Quadratic Discriminant Analysis (SQDA) (22).

Calculations were performed by using a special option of the DISCRIMINANT subprogram of the statistical package SPSS (12). All runs were done on a UNIVAC 1100/80 at the MEC (Madrid) which was accessed through a DCT 2000 terminal at the CCUPC (Barcelona).

K-Nearest Neighbour

In this method, the distance matrix, which contains all interpoint distances in the n-dimensional space, is computed. The unknown object is then assigned to the class to which the majority of its K-closest neighbours belong (3).

Calculations with K = 1, 3, 4, 5, 7 and 9 were performed by applying the routine KNN of the general pattern recognition package ARTHUR (6).

Linear Learning Machine

The method classifies unknown objects by locating decision surfaces in the n-dimensional space, so that the objects for different classes in the training set fall on distinct sides of the hyperplane (20). The separating surfaces are built by an empirical method without using statistical properties of the training group.

Calculations were performed by using the ARTHUR routine PLANE which finds a hyperplane for each pair of groups. All calculations were carried out on a IBM 3083 at the Informatic Centre of the University of Barcelona. The original VAX version was modified by one of us (A.S.) to be adapted to a IBM computer with a VM/CMS operating system.

Results and discussion

Chemical results

The results of the chemical analyses, and of the one-way analysis of variance test for equality of group means on a single variable, are given in Table 1. As it can be deduced from these values, the chemical characterization of each zone, i. e. the definition of a set of parameters whose characteristic values determine the assignation of each wine to its region of origin, is not straightforward. Apart from the ethanol content, which is the most relevant parameter in order to discriminate between the regions according to the F ratios, the individual separation power of the variables is limited. The fact might be due to the scarce differences occurring among the distinct regions of origin. All of them belong to the Tarragona province which implies certain homogeneity in the climatic, edaphologic, varietal and cultural conditions. Nevertheless, some differences have to be emphasized, the inner more mountainous zones of Falset, Priorat and Terra Alta have more extreme climatic conditions than the coastal Camp de Tarragona region. A large percentage in the ethanol differences could be associated with this fact which would imply a lesser sugar content in the musts and, therefore, a lesser alcohol content in the Camp de Tarragona wines compared to those of all other regions.

The varietal differences between the considered zones are kept to a minimum, being the varieties Carignane and Grenache employed in similar percentages.

The most remarkable differences in the edaphologic conditions arise from the Priorat zone whose soils are conformed by the characteristic shales 'licorella', which define this region. Therefore, the metal ion concentration of the wines is expected to contribute to the geographic differentiation due to the relationship between soil and wine composition recently pointed out (21).

Only certain interdependence has been found between pairs of variables. The maximum Pearson correlation coefficient encountered corresponds to the pair conductivity/ash content ($r = 0.68$, significance = 0.000). Positive correlations over the entire data set above $r = 0.5$ are observed in the correlation matrix (not reported) for the following measurement combinations: titratable acidity/density ($r = 0.59$, significance = 0.000), pH/ash content ($r = 0.56$, significance = 0.000), pH/alkalinity of the ashes ($r = 0.56$, significance = 0.000) and conductivity/alkalinity of the ashes ($r = 0.59$, significance = 0.000). These values indicate the lack of independence between the variables, but they are not high enough to consider the parameters redundant. Therefore, reduction of the initial data set of variables has not been considered appropriate at this step.

Feature selection

The F ratios previously computed yield an estimate of the importance of each individual variable to differentiate the studied groups; however, they do not take into account the correlation between features previously selected and, therefore, this crite-

Table 1

Chemical results and univariate F ratios, 1983 vintage of Catalan red wines

Résultats d'analyses des vins rouges Catalans, récolte de 1983, et analyse de la variance pour chaque variable

Parameter	Mean values ± 95 % confidence interval					
	Priorat[1]	C. Tarragona[2]	Falset[3]	Terra Alta[4]	F ratio[5]	Signi-ficance
Density (Den, $g \cdot l^{-1}$)	993.1 ± 0.5	994.9 ± 0.6	993.8 ± 1.0	993.0 ± 1.0	2.74	0.0545
Ethanol (EtOH, % v/v)	15.43 ± 0.43	12.83 ± 0.54	14.51 ± 0.41	14.81 ± 0.46	12.43	0.0000
Ash content (A, $g \cdot l^{-1}$)	2.52 ± 0.17	2.38 ± 0.19	2.22 ± 0.11	2.36 ± 0.13	2.48	0.0731
Alkalinity of ashes (AA, $g \cdot l^{-1}$ of Na_2CO_3)	1.64 ± 0.09	1.84 ± 0.10	1.57 ± 0.07	1.74 ± 0.11	4.59	0.0070
Titratable acidity (TA, $g \cdot l^{-1}$ of tartaric acid)	5.89 ± 0.20	6.20 ± 0.35	7.00 ± 0.73	5.55 ± 0.31	4.19	0.0108
pH	3.37 ± 0.06	3.36 ± 0.08	3.25 ± 0.06	3.36 ± 0.08	2.04	0.1218
Electrical conductivity (COND, $mS \cdot cm^{-1}$)	1.97 ± 0.07	2.24 ± 0.12	1.94 ± 0.06	2.07 ± 0.06	7.22	0.0005
Sodium (Na, $mg \cdot l^{-1}$)	31 ± 4	28 ± 3	22 ± 1	19 ± 3	8.10	0.0002
Postassium (K, $mg \cdot l^{-1}$)	1060 ± 58	1001 ± 76	1003 ± 57	894 ± 73	3.29	0.0291
Calcium (Ca, $mg \cdot l^{-1}$)	57 ± 6	71 ± 7	76 ± 12	86 ± 5	5.08	0.0042
Magnesium (Mg, $mg \cdot l^{-1}$)	167 ± 15	215 ± 31	150 ± 22	217 ± 19	4.97	0.0046
Strontium (Sr, $mg \cdot l^{-1}$)	1.58 ± 0.22	2.30 ± 0.96	1.69 ± 0.47	2.76 ± 0.49	4.06	0.0124
Lithium (Li, $mg \cdot l^{-1}$)	0.04 ± 0.01	0.06 ± 0.02	0.15 ± 0.01	0.06 ± 0.01	1.85	0.1512
Iron (Fe, $mg \cdot l^{-1}$)	9.9 ± 1.8	13.8 ± 2.5	9.4 ± 0.96	12.7 ± 1.6	4.05	0.0125
Copper (Cu, $mg \cdot l^{-1}$)	0.24 ± 0.09	0.59 ± 0.34	0.23 ± 0.24	0.18 ± 0.09	1.72	0.1759
Zinc (Zn, $mg \cdot l^{-1}$)	0.75 ± 0.12	1.24 ± 0.38	0.77 ± 0.16	0.73 ± 0.09	2.45	0.0949
Manganese (Mn, $mg \cdot l^{-1}$)	1.71 ± 0.35	1.11 ± 0.22	0.95 ± 0.06	0.99 ± 0.08	8.17	0.0002

[1]) 13 Samples. [2]) 10 Samples. [3]) 17 Samples. [4]) 12 Samples.
[5]) One-way analysis of variance test for equality of group means on a simple discriminant variable (with 3 and 44 degrees of freedom).

Table 2

Comparison of the selection methods · Order of variable selection

Comparaison des divers critères de sélection des variables · Ordre de sélection des variables

Selection method	Order of variable inclusion	Classification ability (%)
WILKS	EtOH COND Na Sr TA A Fe Mn Mg AA Cu K pH Ca Zn Den Li	98.08
	EtOH COND Na TA A Fe Mn Mg AA Cu K Sr pH Ca	94.23
	COND Na TA A Fe Mn EtOH Mg AA Cu	96.15
	EtOH COND Na Sr TA	88.46
MAHAL	AA Na Sr Ca EtOH A TA Mg Mn Cu K Fe COND pH Den Li Zn	98.08
	AA Na Sr Ca EtOH A TA Mg Cu K Fe pH COND Mn	94.23
	Na Sr Ca EtOH A TA Mg Cu Fe K pH	94.23
	AA Na Sr Ca EtOH TA Mg Cu K Fe	96.15
MAXMINF	Ca A COND Na TA Fe Sr Mg EtOH Cu AA Mn K Den Li pH Zn	98.08
	Ca A COND Na TA Fe Sr Mg EtOH Cu AA Mn K pH	94.23
	A COND Na TA Fe Mn EtOH Mg AA Cu	96.15
	AA Mn Mg Fe TA Na EtOH	96.15
MINRESID	EtOH COND Na Sr A Fe Mn pH K Mg Cu TA AA Ca Zn Den Li	98.08
	EtOH COND Na Sr A Fe Mn pH K Mg Cu TA AA Ca	94.23
	EtOH COND Na A Fe Mn TA Mg AA Cu	96.15
	EtOH COND Na Sr TA	88.46
RAO	EtOH Na Sr K pH Fe Mg Mn Cu TA Ca A AA COND Zn Den Li	98.08
	EtOH Na Sr K pH Fe Mg Cu TA Ca A AA Zn	96.15
	EtOH Na Sr K pH Fe Mg Mn Cu TA Ca	94.23
	EtOH Na Sr K pH Fe Mg Mn	88.46

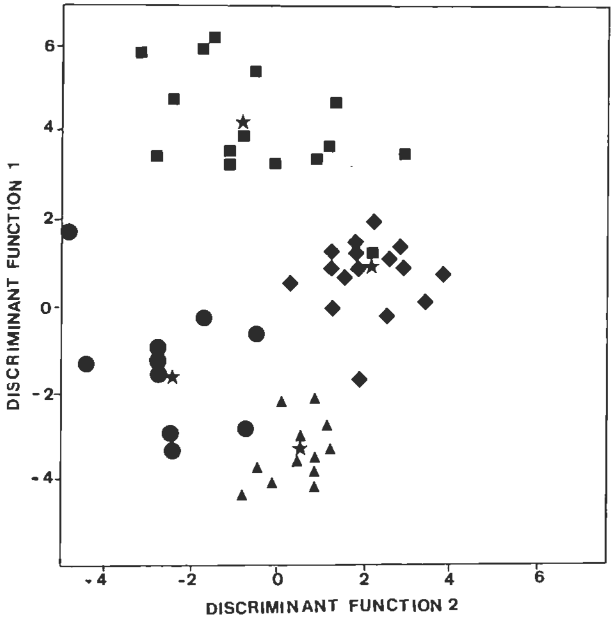

Fig. 1: Representation of 4 groups of Catalan red wines, 1983 vintage, in the best bidimensional discriminant space. — ■ = Priorat, ● = C. de Tarragona, ◆ = Falset, ▲ = Terra Alta. ★ = Group centroids.

Représentation des vins considérés dans le meilleur espace discriminant bidimensionel, récolte de 1983. — ■ = Priorat, ● = C. de Tarragona, ◆ = Falset, ▲ = Terra Alta. ★ = Centre de gravité du groupe étudié.

Table 3

Canonical discriminant functions

Paramètres des fonctions discriminantes derivées

Function	Eigenvalue	% of variance	Canonical correlation
1	8.54	62.68	0.946
2	3.04	22.35	0.867
3	2.04	14.98	0.819

After function	Wilks' Lambda	X^2	Degrees of freedom	Significance
0	0.008	166.85	60	0.000
1	0.081	87.87	38	0.000
2	0.328	38.94	18	0.003

rion is not the best to select the optimum group of variables. For this reason, the stepwise forward selection procedures available in DISCRIMINANT of SPSS has been applied. Previously, the effect of each variable has been equalized by autoscaling (7), that is, the values for each variable have been transformed in such a way that the new values have a mean of 0 and standard deviation of 1.

The order of inclusion of parameters in the stepwise discriminant analysis is given in Table 2. It can be observed that the best classification score (98.08 %) is achieved

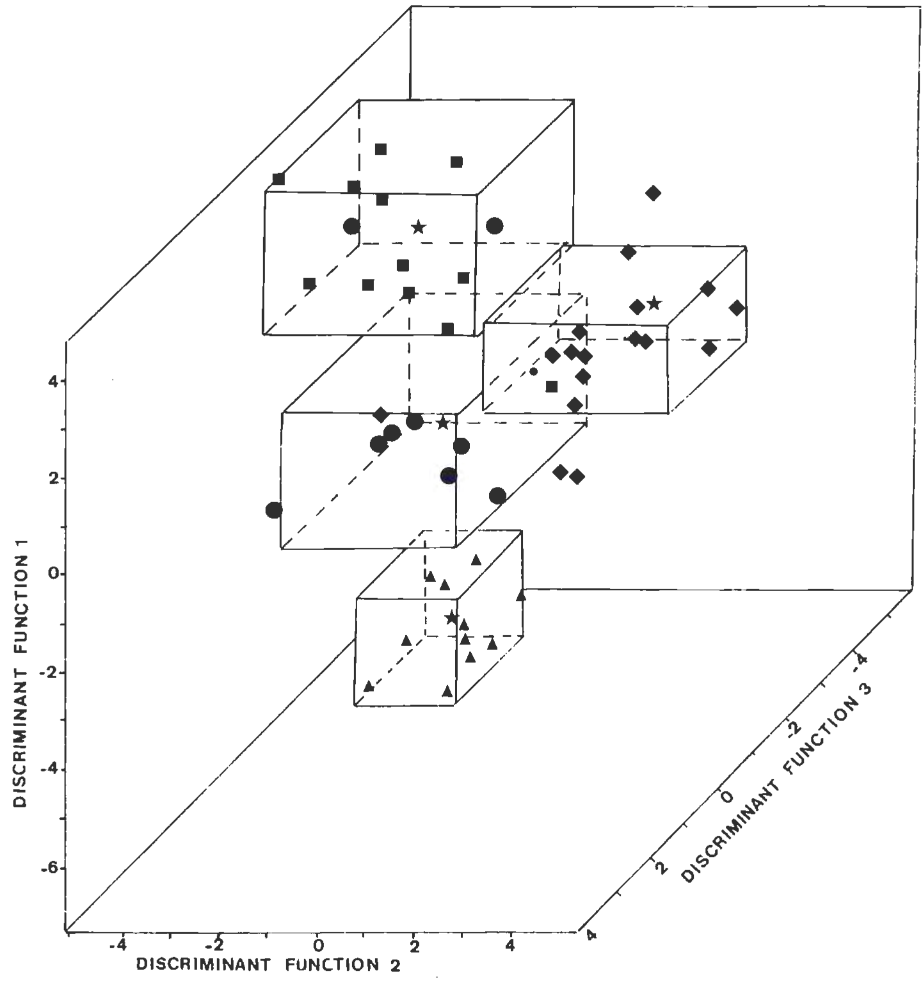

Fig. 2: Representation of the Catalan wines in the three-dimensional discriminant space. Class limits defined as the standard deviation of the groups on each discriminant function. — ■ = Priorat, ● = C. de Tarragona, ◆ = Falset, ▲ = Terra Alta. ★ = Group centroids.

Représentation des vins catalans dans l'espace de trois fonctions de l'analyse discriminante. Limites des classes definies à partir des déviations standard des groupes dans chaque fonction discriminante. — ■ = Priorat, ● = C. de Tarragona, ◆ = Falset, ▲ = Terra Alta. ★ = Centre de gravité de groupe étudié.

Table 4

Classification ability according to discriminant analysis

Capacité de classement suivant l'analyse discriminante

Actual group	No. of samples	Predicted group membership				% Classification ability
		Priorato	Tarra-gona	Falset	Terra Alta	
Priorat	13	13	0	0	0	100.0
Tarragona	10	0	9	1	0	90.0
Falset	17	0	1	16	0	94.1
Terra Alta	12	0	0	0	12	100.0
		Total classification ability 98.1 %				

when all variables are considered in the analysis. However, the number of wines/number of variables ratio must be higher than 3 in any binary classification (23) to attain nonsense classifications and consequently this figure does not constitute a reliable score. Only a reduced loss of classification ability is obtained when decreasing the number of variables (96.15 %, method MAXMINF) down to 7; accordingly, the following variables have been selected to compute the discriminant functions: alkalinity of the ashes (AA), manganese (Mn), magnesium (Mg), iron (Fe), titratable acidity (TA), sodium (Na) and ethanol content (EtOH). A further decrease in the classification score (84.46 %) is obtained if the number of variables is reduced to 5 (method WILKS and

Table 5

Prediction ability as derived from the leave-one-out procedure applied to KNN and discriminant analysis

Evaluation de l'aptitude à la prédiction des résultats dans le cadre de l'utilisation de la méthode des K les plus proches et la méthode d'analyse discriminante linéaire suivant le procédé d'en laisser un échantillon dehors

Group	No. of samples	Correct prediction percentage						
		K-nearest neighbour						Discriminant analysis
		1-NN	3-NN	4-NN	5-NN	7-NN	9-NN	
Priorat	13	92.3	100.0	100.0	100.0	92.3	100.0	76.9
Tarragona	10	60.0	60.0	70.0	70.0	60.0	60.0	70.0
Falset	17	58.8	58.8	70.6	76.5	82.4	64.7	70.6
Terra Alta	12	66.7	66.7	75.0	83.3	83.3	83.3	75.0
Total correct classification		69.4	71.4	78.9	82.5	79.5	77.0	73.1
		76.4						

MINRESID), but this further loss of information can be avoided since a suitable ratio of wines to variables has previously been taken for the analysis. The fact that ethanol is the 7th variable to be selected in the chosen procedure, in spite of having the highest F ratio score, evidences that, because of correlation, the information encompassed by this measurement can be obtained from a combination of different variables.

Discriminant analysis

The information to estimate the necessary number of discriminant functions is given in Table 3, the eigenvalues and their associated canonical correlations denote the relative ability of each function to separate the groups. According to these values, the first 2 functions are able to discriminate quite adequately the 4 groups studied, Fig. 1, but the introduction of the 3rd function, accounting for 15 % of total variance, considerably improves the results as seen in Fig. 2. Consequently, further computations are based on all 3 discriminant functions.

The classification ability, resulting from the classification functions, which were computed from the covariance matrix and the group centroids for the discriminating variables, is given in Table 4. It is well known that these results give an optimistic evaluation of the actual classification power of the derived functions (8). As a consequence, the prediction ability has been determined by applying the leave-one-procedure (23). Results are given in Table 5.

Table 6

Classification according to the Linear Learning Machine method · Routine PLANE[1])

Classification des vins à partir de la méthode de la Machine d'Apprentissage Linéaire

Priorat/Tarragona	84.37 %	Tarragona/Falset	65.62 %
Priorat/Falset	78.13 %	Tarragona/Terra Alta	90.62 %
Priorat/Terra Alta	87.50 %	Falset/Terra Alta	87.50 %
	Total prediction ability 87.2 %		

[1]) Average values obtained from 8 different training/test sets (sample ratio 5:1).

K-Nearest Neighbour rule

Results of the KNN classification rule, together with the prediction ability of the discriminant analysis, are given in Table 5 for comparison purposes. It can be observed that, although a higher percentage than in discriminant analysis is obtained when considering 4 or more nearest neighbours, the overall classification percentage is in reasonable agreement in both methods, (76.4 % for KNN and 73.1 % for SQDA). It can be noticed that, in all cases, Priorat samples achieve the best separation from all other groups which is in accordance with the particular soil characteristics mentioned above and the fact that 4 metal ion concentrations intervene in the analysis. The general trend of obtaining smaller classification percentage, as smaller number of nearest neighbours are computed, might be related to the group size differences (2). Poorer results are obtained in all cases when feature reduction has been performed using either variance weight or Fisher weight and applying subroutine SELECT from ARTHUR.

Linear Learning Machine

Table 6 summarises the mean values obtained when computing 8 different training/test sets maintaining in all cases a sample ratio of approximately 5 : 1. The averaged classification ability over all pairs of groups, 87.2 %, is higher than the results obtained with the previous methods, although the discrimination between certain pairs of groups, (e. g. Tarragona/Falset) is difficult to achieve by using this decision surface classification method.

Conclusion

Metal ions along with several enological parameters, among which ethanol content, alkalinity of ashes and titratable acidity are the most relevant ones, constitute the basis for the characterization and differentiation of 4 distinct wine producing zones in the Tarragona province (Spain). In spite of being contiguous geographic zones, which implies a great similarity in soil — except for the Priorat region —, climate and cultural conditions, an appreciable classification score is obtained. However, in order to account for the variability introduced by several vintages, further observations taken over several years are needed to provide more reliable differentiation between wines of different geographic origin.

The search for better discriminating variables, though requiring more sophisticate instrumentation, is recommended and efforts are being made in this direction. The variables related to the soil characteristics of each zone must have a considerable discriminating power in the cases where no appreciable differences are encountered in the varietal composition of each region as in the present study.

Summary

52 red wines produced in the Tarragona province (Catalonia, Spain), 1983 vintage, belonging to 4 different regions, namely Priorat, Terra Alta, Camp de Tarragona and Falset, have been characterized and differentiated according to their geographic origin on the basis of 17 parameters measured for each sample and 3 pattern recognition methods: Statistical Quadratic Discriminant Analysis, K-Nearest Neighbour and Linear Learning Machine. The metal ions manganese, magnesium, iron and sodium, along with the enological parameters ethanol content, alkalinity of ashes and titratable acidity have been found as the most relevant ones in this study. The lack of varietal differences together with quite similar climatic and cultural conditions due to the geographic contiguity of the studied zones leads to a maximum prediction ability of 87 % with the Linear Learning Machine method.

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