Sensors and Actuators B 183 (2013) 52–57

Contents lists available at SciVerse ScienceDirect

Sensors and Actuators B: Chemical

journal homepage: www.elsevier.com/locate/snb

# Application of a GA–PLS strategy for variable reduction of electronic tongue signals

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ARTICLE INFO

*Article history:*
Received 30 January 2013
Received in revised form 13 March 2013
Accepted 26 March 2013
Available online 3 April 2013

*Keywords:*
Electronic tongue
Variable reduction
Genetic algorithm (GA)
Partial least square (PLS) regression
Wine ageing

ABSTRACT

A genetic algorithm (GA) combined with partial least squares (PLS) regression was applied in order to reduce the considerable number of variables of electrochemical signals recorded by a voltammetric electronic tongue. The algorithm was specifically designed for improving the analysis of data matrices with high collinearity, providing good solutions in terms of both predictive ability and interpretability and, at the same time, minimising the risk of overfitting.

The variable reduction was carried out within a wine characterisation performed with an electronic tongue based on voltammetric sensors. In more detail, the aim was the evaluation of differences among wines aged by means of two different processes: the traditional ageing process in oak wood barrels and an alternative method based on the use of stainless steel tanks and oak wood chips or staves. The results show that the variables selected are at least as good as the full signals to separate the two different classes, even though the number of parameters has been reduced from 1980 to 280 variables; furthermore, the models obtained are simpler and more easily interpretable. In fact, it is important to point out that the variables selected by the genetic algorithm are related to the electrochemical activity of the polyphenolic fraction of wine.



## 1. Introduction

The so-called electronic tongues are analytical systems usually applied to analysis of liquid samples and formed by sensor arrays which generate multidimensional information [1–4]. As for the electrochemical techniques, voltammetry is one of the most widely applied in such analytical systems, thanks to its high selectivity, sensitivity and signal-to-noise ratio and to the variety of measurement modes available [3,4].

The performance of a voltammetric multisensor system can be improved including in the array chemically modified electrodes, in particular sensing units modified with electroactive materials such as phthalocyanines [5,6]. Voltammograms show peaks of two different origins: peaks associated with the oxidation–reduction of the analytes present in the solution and transient responses associated with the electrode material. In addition, that the interactions that occur between the electrode and the solution can improve extraordinarily the selectivity of the electrodes.

Electrodes modified with transition metal complexes, have the ability to catalyse the oxidation or reduction of solved compounds by lowering the potential required for the catalysed redox systems. Similarly, the nature of the ions present in the wine (that diffuse inside the electrode) or the antioxidant properties of substances such as phenols present in the analysed liquid can modify the electrochemical response of the phthalocyanines. All these redox processes and interactions give rise to rich voltammograms with a high degree of selectivity. Such arrays based on phthalocyanines have been applied for the analysis of wines with different organoleptic characteristics. In addition, good correlations have been found between the signals obtained with the electronic tongue and the chemical parameters. Moreover, the electrochemical signals have been successfully employed to estimate chemical parameters related to the polyphenolic content or the pH such as the tannins content [7–9].

Chemometric processing is generally required for the exploitation and interpretation of these complex data [10]. In fact, the data matrices resulting from the measurements are usually formed by a set of voltammograms, usually composed by hundreds or thousands of variables – the current values recorded at each potential – considerably inter-correlated. The purpose of data analysis differs depending on the application. It can be, for example, the recognition of the presence of structures (clusters, correlation) among the samples and/or the variables studied, the identification

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http://dx.doi.org/10.1016/j.snb.2013.03.114

of chemical species or the determination of their concentration [11,12].

However, independently of the type of problem under study, due to the complexity of the signals arising from artificial tongues, application of suitable signal preprocessing corrections may be advantageous for three main purposes, namely: (i) elimination or reduction of random noise, (ii) elimination or reduction of unwanted systematic variations – often due to instrumental hurdles, as well as to the experimental conditions and/or to physical characteristics of the samples – and (iii) data reduction or compression in order to capture the most relevant information from signals [4,10].

Regarding the reduction of the number of variables, these tools can lead to improvements in multivariate data processing for a number of reasons. First of all, because the presence of features that contain irrelevant information may cause problems. Additionally, collinearity present within variables may affect the prediction results [13]. Finally, when a model is built from data characterised by a considerable number of variables, a larger number of training samples would be required to provide reliable predictions on new samples. In particular, the number of samples required grows considerably with the number of input variables, and this often makes a dimension reduction necessary to obtain a reliable model. This is usually referred to as the "curse of dimensionality" [14].

One feasible solution is to use the wavelet transformation (WT) [15]. Another successful approach has been the use of the kernel method [6]. It has already been shown that tools such as genetic algorithms (GA) applied to PLS regression can be successfully used as a feature selection technique [16]. Leardi and Lupiáñez Gonzalez proved that GA, after suitable modifications, produce more interpretable results in the case of continuous signals, since the variables selected are less dispersed than with other selection methods [17].

In this paper the benefits of the application of PLS–GA to process the voltammetric signals recorded by an electronic tongue dedicated to the analysis of red wines are described and discussed. The algorithm applied in this study is an evolution of the original algorithm, particularly targeted to the analysis of continuous signals.

The electronic tongue employed consists of an array of voltammetric sensors chemically modified with electroactive substances (phthalocyanines and ferrocene). These materials are sensitive to several components present in wines, including species affecting the pH and species with a redox reactivity [5,18]. The same device has already been successfully employed in the discrimination of wines of different grape variety or aged in different types of oak barrels [6,7]. In addition, in a previous study, the possibility of using this device to discriminate between bottled wines previously aged in barrels or treated with oak chips was shown [7,8,18].

The present study was carried out with two sets of red wines both aged in traditional oak wood barrels of different origins (French or American) and aged in stainless steel tanks, in which pieces of wood of different sizes and origin were added. In the case of stainless steel tanks, artificial micro-oxygenation was carried out in tanks, in order to simulate as much as possible the diffusion of oxygen that naturally occurs through the barrel pores. The differences between the two wines are related to the denomination of origin where the wines were produced – Toro and Ribera del Duero, respectively.

## 2. Experimental

### 2.1. Electronic tongue

Electrochemical measurements were carried out using a three-electrode cell. The reference electrode was an Ag|AgCl/$KCl_{sat}$ and the counter electrode was a Pt wire. Chemically modified carbon paste electrode (CPE) sensors were used as the working electrodes. The electrodes were selected according to the previous experience of our group [18]. Three phthalocyanines (Lu and Gd bisphthalocyanines, and Co phthalocyanine) and electroactive compounds such as ferrocene (Fc) were used as chemical modifiers for the CPEs. In addition, one unmodified carbon paste electrode and one Pt electrode were included in the array.

Graphite powder (high purity Ultracarbon®, Ultra F purity, Bay City, USA) and high purity mineral oil (Nujol®, Fluka) were used in the preparation of the carbon paste. The carbon paste electrodes were prepared by mixing the carbonaceous material with the corresponding electroactive modifier (15%, w/w) and binder (Nujol) and the blend was mixed until a homogenous paste with the appropriate consistence was obtained. Once prepared, 0.1 g of the mixture were introduced in a PVC syringe (1 mL), and compressed. Appropriate packing was achieved by pressing the electrode surface against a filter paper. A copper wire was used as a contact. The CPEs were finally smoothed manually by a clean filter paper.

The electrochemical experiments were carried out following a previously published method [7,8]. For the electronic tongue measurements, Square Wave Voltammetry (SWV) was performed at a potential scan ranging from −1.0 to +1.3 V, using $f$ = 15 Hz; Esw = 90 mV; $\Delta$Es = 7 mV (except in the case of CoPc, $\Delta$Es = 5 mV). All the electrochemical experiments were performed at a controlled temperature (25 ± 1 °C).

## 3. Wine samples

Two different sets of wine samples were prepared and submitted to analysis (Table 1). In particular, grapes of the variety *Tempranillo*, coming from two different Spanish areas (Geographic Denominations or DO) the D.O. Ribera del Duero and the D.O. Toro, were considered. After fermentation, the wine obtained was submitted to ageing processes following two different methodologies.

In the first method, wines were aged in barrels (225 L capacity) using American and French oak wood (traditional wine ageing). In the second method, wines were matured in 100 L stainless steel tanks, in which pieces of oak wood were added (alternative method for wine ageing). These samples were obtained by adding wood pieces of different sizes (chips or staves), different origins (American and French) and toasting levels (light, medium, heavy). In order to assure a comparable surface of wood to be in contact with wine (both in barrels and tanks), the amount of wood added was calculated considering the surface/volume ratio of the barrel. Thus, 600 g of chips were added to each tank to reproduce the wood surface/volume ratio of barrels. Similar calculations were carried out for staves. D.O. Toro wines were analysed after 30 days (T1) and after 90 days (T2) of ageing.

## 4. Data analysis

All the samples were measured seven times with each sensor. The data analysis involved an initial pre-processing of the electrochemical signals using the standard normal variate (SNV) transform. Data were also autoscaled column-wise in order to give the variables the same importance a priori [10]. Data processing was performed using in-house routines under Matlab environment (The Mathworks Inc., Natick, USA). The GA algorithm routines are described in [19,20].

It is worth considering that – as it was shown in previous studies – the performance of the GA decreases when >200 input variables are used [7,19,20]. This is due to the fact that a higher variables/objects ratio increases the risk of overfitting and that the size of the search domain becomes too great. The signals used in

**Table 1**
Wines samples prepared and analysed in this study.

| D.O. Toro | | | | D.O. Ribera del Duero | | | |
|---|---|---|---|---|---|---|---|
| Traditional ageing | | Alternative ageing | | Traditional ageing | | Alternative ageing | |
| Number of samples | Type of barrel | Number of samples | Characteristics of the pieces of wood | Number of samples | Type of barrel | Number of samples | Characteristics of the pieces of wood |
| 1 | -French oak<br>-Light toast | 3 | -Chips<br>-French oak<br>-Light toast | 2 | -French oak<br>-Medium toast | 2 | Chips<br>French oak<br>Medium toast |
| 1 | -French oak<br>-Medium toast | 3 | -Chips<br>-French oak<br>-Medium toast | 2 | -American oak<br>-Medium toast | 2 | Staves<br>French oak<br>Medium toast |
| 1 | -French oak<br>-Heavy toast | 3 | Chips<br>-French oak<br>-Heavy toast | | | 2 | Chips<br>American oak<br>Medium toast |

this study originally contained 1980 variables. To reduce this number, the average of 10 consecutive points was taken (198 resulting variables). Such a large averaging window size might determine a loss of fine features characterising the voltammograms, potentially important for the calibration model. On this data set, an iterative approach was applied, which allowed the window to be progressively reduced to a size which preserved the electrochemical features of interest. Several independent GA runs were performed, starting from the complete set of variables. The consecutive analyses were examined visually and the portions of the signals that were never chosen by the GA were removed. The entire cycle was then repeated on the selected portions of the voltammograms, thus allowing the window size to be reduced. This was repeated until no more regions to be deleted were found.

All the models were evaluated by cross-validation with a leave-one-out scheme. Cross-validation was also used during the GA procedure. In this case, the data were split into five deletion groups.

## 5. Results

Fig. 1 illustrates the typical response of the array of sensors immersed in a red wine. The voltammograms showed that wines have considerable complex electroactivity within the potential window between 0.3 V and 1.0 V (vs Ag/AgCl), in which it is possible to identify oxidation processes associated with different types of phenolic compounds at ca. 0.5–0.7 V [21] and oxidation processes associated to the electrode material (at −0.4 and 0.6 V for LnPc2; at 1.2 V for CoPc and 0.6 V for ferrocene; the Pt electrode shows the decomposition of the hydroalcoholic solution at −0.7 V). In addition, the interactions between the electrode and the wine (i.e. influence of antioxidants in the response of the sensor or the electrocatalytic effect of the electrode on the redox behaviour of the wine) also contribute to the complexity of the signals. For these reasons each electrode showed a particular response towards red wine samples and the electrochemical signals can be used as a fingerprint to discriminate among wines with different characteristics. This cross-selectivity is evident by the different current vs potential profiles represented in Fig. 1.

In the present study, the capability of the electronic tongue to distinguish between wines aged by different methods was evaluated using principal component analysis (PCA). Seven measurement replicates of each sample were carried out and the average signal was computed for the subsequent data processing. Figs. 2 and 3 show the score plots of the first two PCs for wine samples from D.O. Toro and D.O. Ribera del Duero, respectively. This analysis was carried out with the total variable set (1980 variables, i.e. 330 variables for each of the six sensors).

The 24 wine samples shown in Fig. 2 refer to the sampling times T1 and T2.

From the visual inspection of the score plot it was not possible to adequately differentiate the ageing processes based on the first two PCs, which explain 46% of the total data variability (PC1 = 26% and PC2 = 20%). In particular, wine samples aged in barrels (represented by stars and crosses) appear to overlap samples aged in stainless steel tanks with oak wood insertion (represented by triangles and squares).

The score plot of wines from Ribera del Duero is presented in Fig. 3. In contrast with the results previously reported, some differences between the two types of ageing are noticeable. As in the previous case, samples aged in oak barrels are represented by stars, while wines matured in stainless steel tanks are marked with triangles, which appear to be well separated according to PC2 (accounting for 26% of total variability).

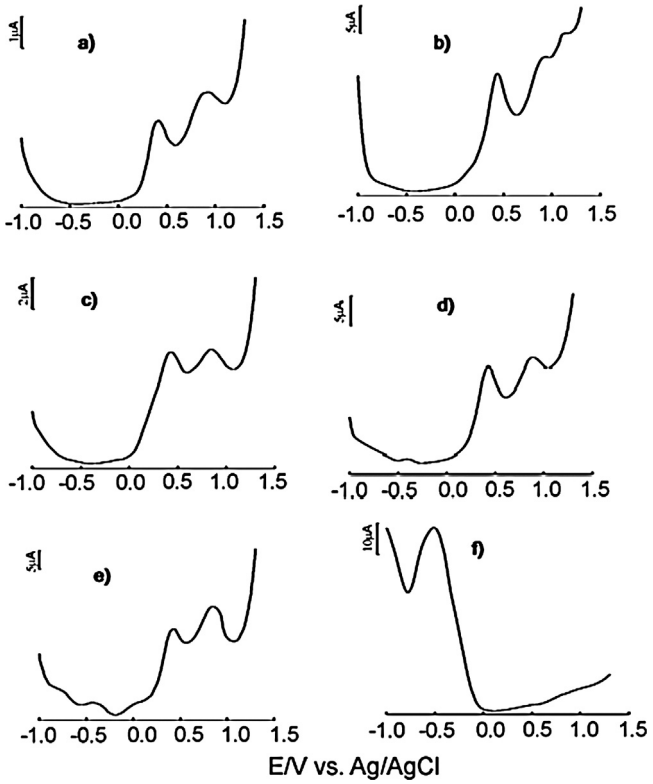


**Fig. 1.** Voltammograms of the carbon paste electrodes towards a D.O. Ribera del Duero wine aged in stainless steel tank where staves of French oak were added: (a) unmodified Carbon paste electrode; (b) cobalt phthalocyanine modified; (c) ferrocene modified; (d) gadolinium bisphthalocyanine modified; (e) lutetium bisphthalocyanine modified and (f) platinum electrode.

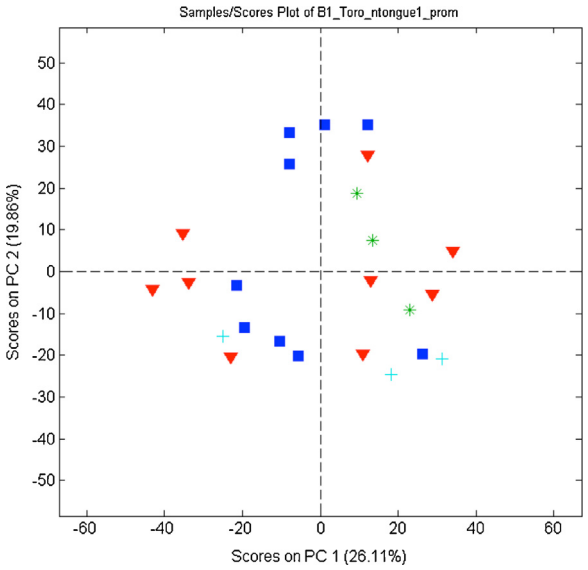


**Fig. 2.** Wine samples of D.O. Toro. PC1 vs PC2 score plot from the whole dataset (1980 variables). Green stars: barrel at T1; cyano crosses: barrel at T2; red triangles: stainless steel at T1; blue squares: stainless steel at T2. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

Assuming that a supervised selection of the most informative sensors and/or of the appropriate regions of signal can improve the recognition of these differences, GA–PLS was applied as a strategy for variable selection, as described in Section 4. Since the number of variables was considerably larger than 200, it was necessary to reduce them, as previously described.

Fig. 4 represents each stage of the GA runs. The black line indicates the voltammetric profiles recorded at each sensor of the array. Broken lines at the bottom indicate the regions selected by the GA through the three stages carried out in this study. These regions of the voltammograms provided a better differentiation between samples according to the ageing procedure.

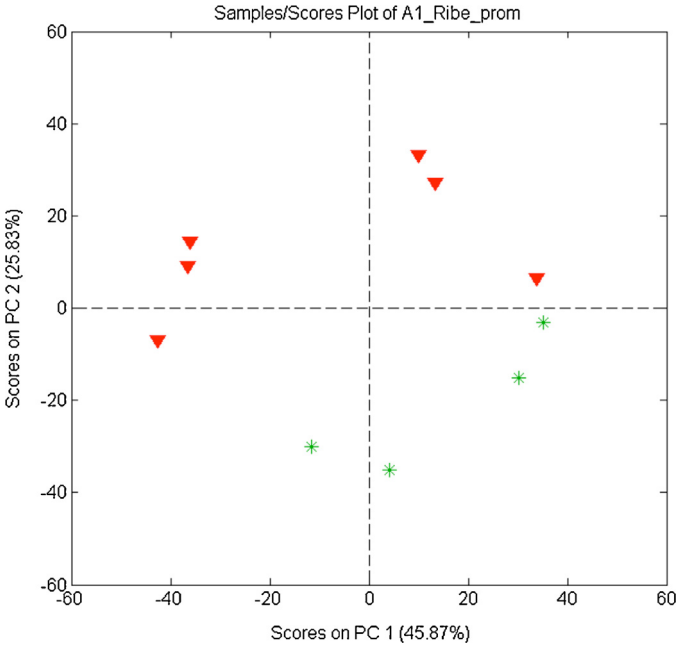


**Fig. 3.** Wine samples of D.O. Ribera del Duero. PC1 vs PC2 score plot. Green stars: oak barrels; red triangles: stainless steel. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

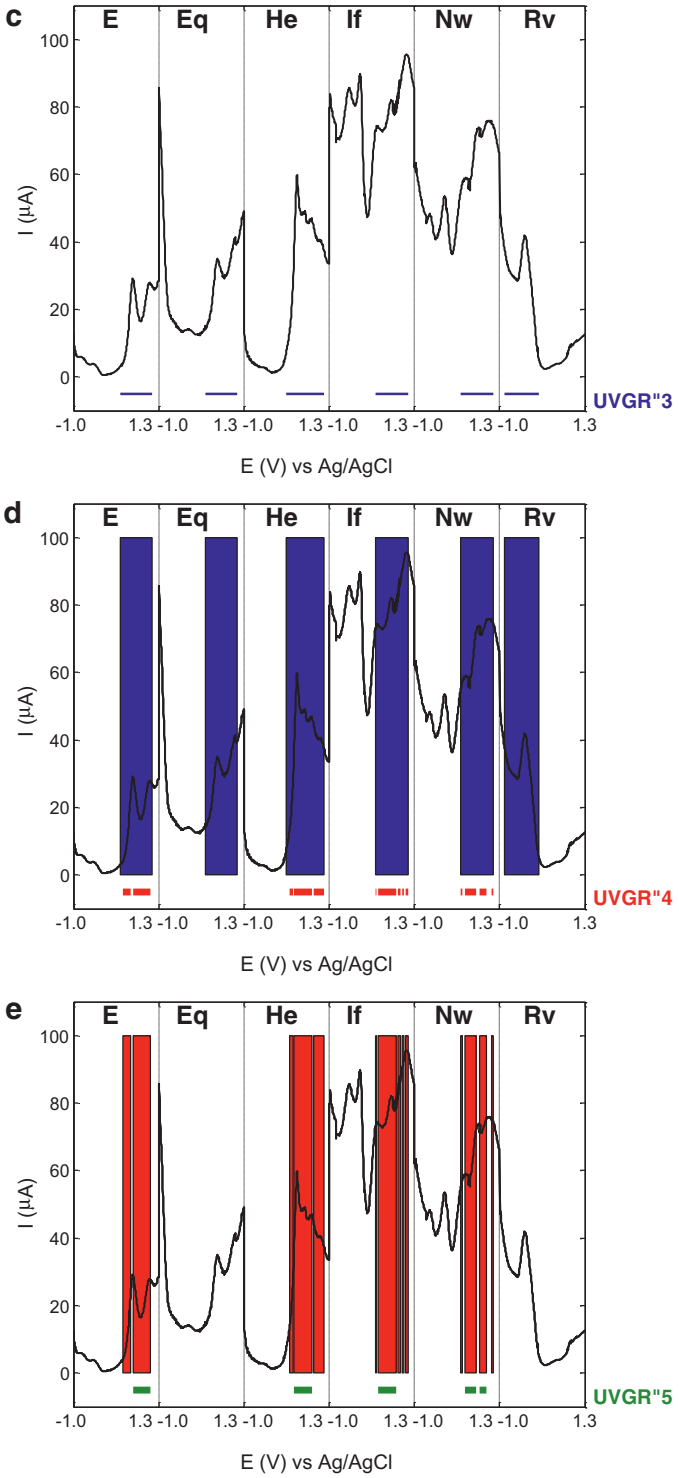


**Fig. 4.** Voltammetric profiles recorded at the six different working electrodes and variable intervals selected by the GA at each step, indicated by broken coloured lines. In the second and third steps, variables retained in the previous selection are highlighted by shadowed rectangles. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

Step 1. The first series of runs is applied on the complete dataset (1980 variables) (Fig. 4a). The number of variables of the data matrix was previously reduced to 198 using the averaging window. The response variable for PLS regression was a vector of zeros and ones, corresponding to the two types of wine ageing processes, respectively. In this way, the GA looks for the portions

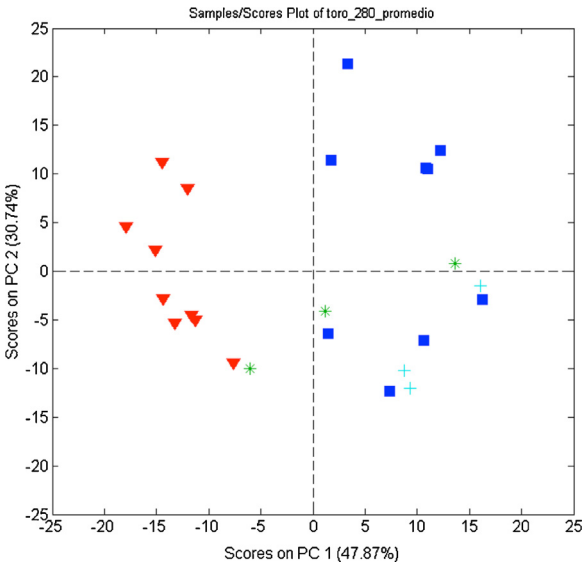


**Fig. 5.** Wine samples of D.O. Toro. PC1 vs PC2 score plot from the reduced dataset (280 variables selected by the GA). Green stars: barrel at T1; cyan crosses: barrel at T2; red triangles: stainless steel at T1; blue squares: stainless steel at T2. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

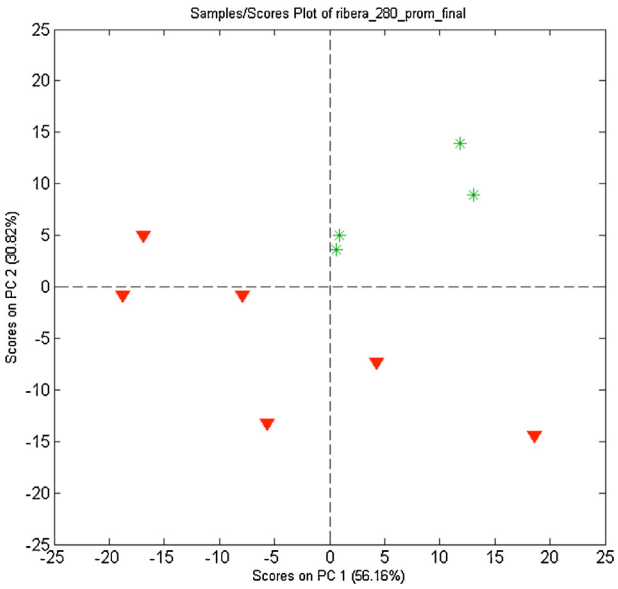


**Fig. 6.** Wine samples of D.O. Ribera del Duero. PC1 vs PC2 score plot from the reduced dataset (280 variables selected by the GA). Green stars: oak barrels; red triangles: stainless steel. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of the article.)

of the voltammograms most important to identify the differences related to the type of wine ageing process. The regions selected are indicated by the blue broken line in Fig. 1a. Intervals between 0.25 V and 1.12 V were chosen for carbon (C), $CoPc_2$ (Co), $GdPc_2$ (Gd) and $LuPc_2$ (Lu) modified electrodes, while for the ferrocene based sensor (Fc), the interval between 0.15 V and 1.02 V was selected, and potentials ranging from −0.87 V to 0.06 V were retained for the platinum based sensor (Pt).

Step 2. The regions selected in the previous step were submitted to a second GA run. In more detail the second selection run was carried out on a subset of 750 original variables, on which an averaging window of 5 datapoints was applied. The outcomes of this second selection, represented by the red broken lines in Fig. 4b, suggested that a more parsimonious model could be obtained by further reducing the set of variables, without using the information provided by the CoPc and Pt sensors.

Step 3. In the third stage, a subset of 400 original variables (100 for each sensor) was used as input for a further GA–PLS selection run, after application of an averaging window of two datapoints. The segments selected, indicated by the green broken line in Fig. 4c, highlight the peaks of the voltammogram associated with the electrochemical activity of polyphenols in wine. In more detail, the portions selected were: 0.60–1.07 V for the C-based sensor, 0.36–0.83 V for the Fc-based sensor, 0.32–0.80 V for the Gd-based sensor and 0.36–0.67 V and 0.75–0.95 V for the Lu-based sensor.

As it can be seen in Fig. 4c, the final run chose almost all the variables that were selected in the previous cycle. A final model was thus developed with a subset of 280 original variables, which correspond to the above mentioned potential intervals. This set was used to compare the ability of discrimination with the original set of 1980 variables.

In order to perform such an evaluation, PCA was applied on the chosen subset of 280 variables. Fig. 5 shows the score plot for wines from D.O. Toro, on the first two PCs that account for 79% of the total variance (PCA after GA variable selection). As it can be observed in the figure, wines aged with a similar method appeared in the same region of the plot. This represents a clear improvement in the possibility to differentiate samples: samples marked with triangles (wines macerated with oak wood chips) appeared well separated from the other samples on the left side of the plot. This outcome indicates that the final subset of variables retained by PLS–GA presents an increased capability to separate classes of red wines according to the type of ageing, though a complete discrimination has not been obtained.

Fig. 6 shows the score plot, after GA variable selection, on the first two PCs for Ribera del Duero wines. The removal of the non relevant variables allowed to further improve the separation between wines aged in barrels and wines aged with alternative systems already shown with the whole data set. It is important to point out that, working with this reduced variable set, it was also possible to distinguish between wines aged in American oak wood barrel and wines aged in French oak wood barrel.

As observed in Figs. 5 and 6, the PLS–GA can be successfully applied to wines of different regions, because the results appear to be related with the effect induced on the electrochemical properties of modified electrodes by a complex mixture like wine. In particular, the oxidation peaks detected as highly informative by the algorithm may be attributed to polyphenolic compounds, characterised by the presence of many hydroxyl groups (high antioxidant activity). Further investigations will be performed on larger sample sets including wines of different geographic origins, varieties of grapes, etc.

## 6. Conclusions

The present study showed Genetic Algorithms to be an efficient and helpful strategy for feature selection on electrochemical data sets. The results were assessed by the visual inspection of PCA score plots and evaluated in terms of capability to characterise two wine samples according to the ageing practice. Variable selection by PLS–GA seemed to improve the efficiency of the electronic tongue. In particular, it allowed to simplify the data treatment, maintaining or improving the capability of the system to distinguish among the different wine samples. Furthermore, the identification of the most relevant regions is helpful for the interpretation of the results from the electrochemical point of view.

## Acknowledgments

Financial supports from the Spanish Ministry of Science (Grant AGL2009-12660/ALI) and from the Italian Ministry of University and Research (PRIN 2008, CUP:D31J0000020001) are gratefully acknowledged. N. Prieto wishes to thanks for grant FPI from University of Valladolid.

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## Biographies

**Natalia Prieto** was born in 1985. She graduated in Physics Engineering and got her doctorate in Physics in 2012 at the University of Valladolid. Her research is mainly focused on the development of chemical and physical sensors for building multisensor systems (electronic nose), as well in the analysis of multivariate data (chemometrics). Recently, she joined the department of physics and mathematics at Autonomous University of Manizales, Colombia.

**Paolo Oliveri** was born in 1982. He obtained MSc degree in Pharmaceutical Chemistry and Technology in 2006, and PhD in Sciences and Technologies of Chemistry and Materials in 2010. He currently works as a post-doctoral fellow at the University of Genova (Italy). His research is mainly focused on Chemometrics and its application in Analytical Chemistry. In particular, his interests are devoted to signal and image processing and pattern recognition techniques. In 2010, he got the Young Researcher Award of the Division of Analytical Chemistry of the Italian Society of Chemistry.

**Riccardo Leardi** was born in 1959. His interests are mainly devoted to problems of classification and regression (applied especially to food, environmental and clinical data), experimental design, process optimisation, multivariate process monitoring and multivariate quality control. His original research focused mainly on genetic algorithms, especially in their application to the problem of variable selection, and three-way methods. He is author of more than 110 papers and more than 100 communications in national and international meetings. He is Editor of Journal of Chemometrics, Editorial Adviser of Analytica Chimica Acta, member of the Editorial Board of the Journal of the Iranian Chemical Research and a regular reviewer for several Journals.

**Monica Gay-Martín** was born in Valladolid (Spain). She received the PhD in Chemistry in 2012 from the University of Valladolid (Spain). She is co-author of 10 papers. She is presently a posdoc fellow at the R&D department of Abengoa (Spain).

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