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THEORETICAL ADVANCES

Chilean wine varietal classification using quadratic Fisher transformation

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Abstract This paper deals with the Chilean red wine varietal classification problem. The problem is solved here by using one of the simplest statistical classification methods based on quadratic discriminant analysis (QDA) together with a new recently introduced nonlinear feature extraction technique called quadratic Fisher transformation. Classification is based on liquid chromatograms of polyphenolic compounds present in wine samples, obtained from a high performance liquid chromatograph with diode alignment detector. For comparison purposes three other feature extraction methods are studied: linear Fisher transformation, Fourier transform and wavelet transform, maintaining QDA as classification scheme. From experimental results it is possible to conclude that when using quadratic discriminant analysis as classification method, the percentage of correct classification was improved from 91% (obtained for the case of wavelet extraction) to 99% when employing quadratic Fisher transformation as feature extraction method.

Keywords Feature extraction · Nonlinear feature extraction · Quadratic feature extraction · Fisher transformation · Linear Fisher transformation · Nonlinear Fisher transformation · Quadratic Fisher transformation · Wavelet transform · Fourier transform · Quadratic discriminant analysis · Fisher discriminant analysis

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1 Originality and contribution

The main contribution of this research is in the application of a new feature extraction technique [quadratic Fisher transformation (QFT)] recently developed by the authors [17], to the problem of Chilean wine classification according to variety. This is the first time that QFT is applied to this type of problems. There are not known results on this subject where a nonlinear feature extraction technique (nonlinear feature transformation) is used to classify wines.

The main idea was to investigate if QFT can be successfully used in this particular classification problem and compare its performance with those obtained from three other feature extraction techniques commonly used [linear Fisher transformation (LFT), Fourier transform (FT) and wavelet transform (WT)].

The emphasis of the study is not on the pattern recognition method but in the influence of the feature extraction used in the stage previous to the classification procedure. That is why only one classifier is employed in the study. The selected classifier was QDA since it is one of the most commonly used in practice and it is a rather simple classifier.

Nevertheless, extensive simulations performed in our Lab with more advanced pattern recognition methods [support vector machines (SVM), radial basis function neural networks (RBFNN) and probabilistic neural networks (PNN)], not shown in this study because they go beyond the scope of the paper, reveal that the same kind of conclusions can be drawn as far as the advantages of the QFT technique over other feature extraction techniques studied is concerned (Wavelet transform, Fourier transform and linear Fisher transformation). Then we can confidently state that the advantages exhibited by QFT over other feature extraction methods are independent of the classifier used in the pattern recognition process.

2 Introduction

During the last few years world wine industry has experienced a large growth. In particular, Chilean wine industry is nowadays one of the most dynamical and important sectors of country's economy. Adding technology to this industry is a key issue for successfully competing in international markets.

Developing objective methods for determining varietal and geographical wine origin has become an important problem in order to guarantee wine quality. Most of the previous works on wine variety classification are based on the concentration of specific compounds present in the wine which are obtained from liquid or gas chromatography (see for example [1–4]). In a chromatogram the concentration of a compound corresponds to the area under the peak, and compounds are determined by comparison with pattern solutions containing the pure compound. While more than 600 compounds have been identified in the wine, which of them characterize the wine variety still remains as an open problem. Origin of wines based on their chemical content and mineral and trace elements has also been investigated. Capron et al. in [23] used the multivariate classification techniques partial least squares-discriminant analysis and kernel support vector machines to identify wines from four different countries. Provenance and authenticity of wines were recognized on the basis of typical mineral and trace element patterns by means of chemometric methods [24]. Alvarez et al. [25] analyzed 50 wines from three origin denominations of Valencia using 35 components grouped according to the conventional parameters, alcohols and polyols, and esters. A correct classification of 98% was reached.

A different approach has been followed in the last few years in which all the information contained in the chromatogram rather than certain peaks is used for classification purposes [5–7]. This approach has two main advantages since it is not necessary to specifically identify each compound and its concentration, and the whole information contained in the signal is used. The main drawback is that the dimension of the characteristic vector (features) increases dramatically making difficult the direct use of pattern recognition techniques. Nevertheless, preprocessing techniques and feature extraction methods applied previous to the classification stage can be used to face this problem.

The main objective of the paper is to verify if the new nonlinear feature extraction recently introduced in [17] is suited to face wine classification problems. To this extent a comparative study is presented for Chilean red wine varietal classification into classes Cabernet Sauvignon, Merlot and Carménère. Discrimination is based on the information of polyphenolic compounds contained in a liquid chromatography provided by a high performance liquid chromatograph with diode alignment detector (HPLC-DAD) [8]. Four feature extraction techniques are analyzed and compared using a single classifier based on quadratic discriminant analysis (QDA). The extraction techniques compared are linear Fisher transformation (LFT) [16], Fourier transform (FT) [13], wavelet transform (WT) [12] and quadratic Fisher transformation (QFT) [17].

The paper is organized as follows. In Sect. 3 the main theoretical aspects of the QFT method are presented. In Sect. 4 the experimental information used in this study is described. Next, in Sect. 5, a brief description of the methodology employed is presented. Section 6 contains the experimental results together with some comments on each method. Some conclusions are drawn in Sect. 7.

3 Description of the quadratic Fisher transformation

The new nonlinear feature extraction method used in this study is based on developments contained in [17] and is called quadratic Fisher transformation (QFT). The method is a generalization of the nonlinear Fisher discriminant analysis (FDA) for the multi-class problem, maximizing the Fisher criterion. It considers any smooth nonlinear transformation that can be expressed using linear and quadratic basis functions. The method does not make use of numerical algorithms and it has an analytical (closed-form) solution. Moreover, no assumptions on the class probability distribution functions are needed. A brief description of QFT is given in what follows.

Let C^2 be the space of functions defined on $\Re^n \to \Re^m$, having continuous partial derivatives of order 1 and 2. Our objective is to find a function $Y = Z(X) \in C^2$ (with $Y \in \Re^m$ and $X \in \Re^n$), such that the Fisher index evaluated in the space generated by $Z(X)$ is maximized. Then we have to considerer the problem of optimizing the Fisher index defined as

$$J = Tr\left\{\tilde{S}_w^{-1}\tilde{S}_b\right\} \tag{1}$$

where $\tilde{S}_w \in \Re^{m\times m}$ is the within-class scatter matrix in the transformed space and $\tilde{S}_b \in \Re^{m\times m}$ is the between-class scatter matrix in the transformed space. We choose a transformation containing linear and quadratic terms of the form

$$Z(X) = \begin{bmatrix} A_1X + X^TB_1X \\ A_2X + X^TB_2X \\ \vdots \\ A_mX + X^TB_mX \end{bmatrix}, \quad Z \in \Re^m, \quad \text{and} \quad X \in \Re^n \tag{2}$$

which can be written in a compact form as

$$Z(X) = \Omega^T \Phi(X) \quad (3)$$

where

$$\Phi(X) = \begin{bmatrix} x_1^2 \\ x_1x_2 \\ \vdots \\ x_1x_n \\ x_2^2 \\ x_2x_1 \\ \vdots \\ x_2x_n \\ \vdots \\ x_nx_1 \\ x_nx_2 \\ \vdots \\ x_n^2 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \Re^{n^2+2n} \quad (4)$$

$\Phi(X)$ is a vector of dimension $n^2 + 2n$ and $\Omega \in \Re^{m\times(n^2+2n)}$ is a constant matrix. The dimension of $\Phi(X)$ can be reduced by considering the cross-terms only once, if extra conditions on matrices A_i, are imposed, i.e., $A_i = A_i^{\mathrm{T}}$.

It is proven in [17] that the extreme condition is given by

$$(S_w^{-1}S_b)\Omega = \Omega(\tilde{S}_w^{-1}\tilde{S}_b) \quad (5)$$

Since the Fisher index is invariant under nonsingular transformation, we can use the simultaneous matrix diagonalization lemma [16, 18] in the transformed space to transform equation (5) into an eigenvalue–eigenvector equation without altering the solution [17].

Since the dimension of $\Phi(X)$ is high, we can use the method stated in [17, 18] to solve the Fisher optimization problem. To this extent we will use the method stated by Fukunaga [16], Kirby and Sirovich [21] and Turk and Pentland [22], to efficiently compute the eigenvalues and eigenvectors of matrix $S_w^{-1}S_b$.

Notice that in QFT the dimension of Φ (X) increases as n^2, $(n = \dim(X))$, and therefore a high computational effort may be needed.

Same as in the LFT method, the dimension of the original feature vectors is reduced to *C-1*, where *C* is the number of classes.

4 Experimental information

The information used in this study for wine classification corresponds to polyphenolic compounds of low molecular weight contained in liquid chromatograms obtained from an HPLC-DAD [8]. The equipment used in the experiments corresponds to a Merck-Hitachi, model L-4200 UV-Vis detector with pump and column holder Thermostat. The column is a Novapack C18, length 300 mm and inner diameter 3.9 mm. For separation of the different phenolic compounds the following solvents were used:

(A) 98% H_2O and 2% acetic acid,
(B) 78% H_2O, 20% acetonitrile and 2% acetic acid,
(C) 100% acetonitrile.

The gradient used in the separation has the following characteristics:

- 0–55 min, 100% of A (flux = 1 ml/min),
- 55–57 min, 20% of A and 80% of B (flux = 1 ml/min),
- 57–90 min, 10% of A and 90% of B (flux = 1.2 ml/min).

Each chromatogram is a 90-min signal sampled every 800 ms, containing 6,751 points. Each of the peaks on the chromatogram has been identified by researchers in the area of chemistry and agronomy [9, 10]. As example, Fig. 1 shows a typical normalized profile corresponding to a Merlot wine supplied by the HPLC-DAD.

Since the size of the maxima in the chromatograms depends upon the wine volume injected to HPLC, and volumes ranging from 20 to 100 ml of prepared wine sample were injected into the HPLC, a normalization procedure for the amplitudes was used. The normalization procedure was done using the following transformation:

$$\tilde{z}_i = \frac{z_i - z_{im}}{z_{iM} - z_{im}} \quad (6)$$

where $\tilde{z}_i$ corresponds to the scaled (normalized) signal amplitude at point i within the interval [0,1], z_i is the real amplitude, z_{im} is the minimum amplitude and z_{iM} is the maximum amplitude.

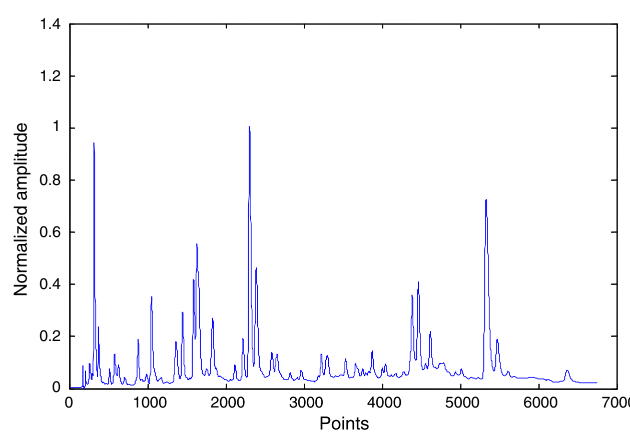

Fig. 1 Typical phenolic normalized liquid chromatogram of a Merlot sample

In this study, 172 Chilean wine chromatograms were employed. They were obtained from reliable wine samples distributed as 80 Cabernet Sauvignon, 35 Merlot and 57 Carménère, coming from different valleys of the central part of Chile (Maipo, Rapel, Curicó, Maule and Itata) and from 2000 and 2001 vintages [5].

5 Methodology

5.1 Information pre-processing

In order to decrease data dimensionality some signal analysis tools were used previous to classification process. Frequency content (power spectrum) of each signal was examined to determine the Nyquist frequency. This Nyquist frequency was determined for each chromatogram by computing the power spectrum of each signal and determining the frequency over which there is little information content in the signal. The criterion used in this study to determine Nyquist frequency was 90% of information content measured in terms of the signal power. Since profiles are different amongst them even those corresponding to the same variety (class), Nyquist frequencies are also different. In order to use the "Sampling Theorem" [11] and to apply it correctly, the highest Nyquist frequency was determined. Then the chromatograms will be re-sampled with a sampling period based on this Nyquist frequency maintaining the original information contained in the chromatograms. In this case it was determined that the maximum Nyquist frequency was $f_n = 0.125$ Hz. The illustration of the Nyquist Frequency for one chromatogram is shown in Fig. 2, where there is a vertical line indicating the Nyquist frequency for that particular chromatogram.

According to the sampling theorem [11], data can be sampled with a period $T_n = 1/2f_n$ without information losses, i.e., every 4 s in our case. As a consequence of this preprocessing, it was possible to reduce data dimension from the 6,751 points to only 1,351 points.

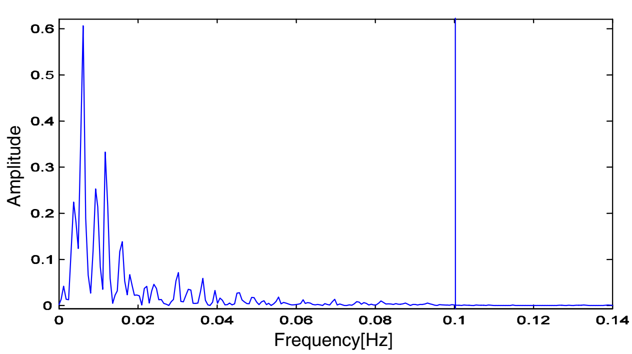

Fig. 2 Power spectrum and Nyquist frequency of a typical chromatogram

Another preprocessing of the information was done previous to the classification stage; the normalization process of the amplitude signals so that amplitudes lie into the interval [0,1]. This normalization process was explained in detail in Sect. 4.

5.2 Feature extraction methods

Although the nonlinear (quadratic) feature extraction method [17] is the main interest of this paper, three other feature extraction methods were selected for comparison purposes. After the re-sampling and normalization processes a feature extraction stage was applied to data. Four techniques were applied in total including linear Fisher transformation (LFT), wavelet transformation (WT), Fourier transform (FT) and quadratic Fisher transformation (QFT).

To see if the feature extraction methods produce statically significant differences in the classification process McNemar test [13] was employed.

5.2.1 *Fourier transform*

The discrete Fourier transform (DFT) *F(k)* of a discrete-time signal *f(nT)* is given by [12]

$$F(k) = \sum_{n=0}^{N-1} f(nT) e^{-\frac{j2\pi nk}{N}} \quad (7)$$

To determine the number of coefficients to be considered Parseval Theorem [12] is usually employed. In this study the criteria was to maintain the 90% of the energy signal. In our case this means that data dimension is reduced from 1,351 to 271, which is the number of DFT coefficients.

5.2.2 *Wavelet transform*

Wavelet transform of an L^2-function $f(t)$ can be represented as [12]

$$f(t) = \sum_{k=-\infty}^{\infty} c_k \Phi_k(t) + \sum_{j=0}^{\infty} \sum_{k=-\infty}^{\infty} d_{j,k} \psi_{j,k}(t), \qquad j, k \in Z \quad (8)$$

where $\psi_{j,k}(t)$ and $\Phi_k(t)$ are sets of orthonormal functions (basis functions) satisfying certain properties. Coefficients c_k and $d_{j,k}$ (approximation and detail coefficients, respectively) correspond to the wavelet coefficients of the function and they are computed as the inner product (projection) of the function with respect to the basis functions. Sub-index j is known as decomposition level and sub-index k is the time delay. In this study the mother wavelets Haar will be used mainly for its simplicity. Several decomposition levels were analyzed to determine the best one. It was found for this study that the best decomposition level is 8, which means the use of 40 wavelet coefficients.

5.2.3 Linear Fisher transformation

The goal of the Fisher transformation [14–16] is to get a data representation in a lower dimensional space maintaining the discrimination power of the original data. Thus, classes are separated as much as possible (maximize the inter-class mean) and dispersion around the class mean is reduced (minimize the intra-class mean), which corresponds to the well-known Fisher criteria or Fisher index. The solution to this problem is obtained by solving an eigenvalue–eigenvector problem [16]. Using this technique the dimension of the original feature vectors is reduced to *C-1*, where *C* is the number of classes.

5.2.4 Quadratic Fisher transformation

This new nonlinear feature extraction method [17] has been already described in Sect. 3. The main advantage over the standard LFT is that it allows a larger separation of patterns belonging to a same class when projected onto the space generated by the Fisher transformation (see Fig. 6 and compare with Fig. 5). Once the QFT is applied the dimension of the original feature vectors is reduced to *C-1*.

6 Classification results for Chilean red wines

Since the aim is to study the performance of the new feature extraction method QFT when used in a classification problem, the quadratic discriminant analysis will be used as pattern recognition technique. This QDA was chosen as classifier because it is a statistical rather simple pattern recognition method commonly used in a wide range of practical applications. The emphasis therefore is not in the pattern recognition method. However, extensive simulations performed in our Lab with more advanced pattern recognition methods such as support vector machines (SVM), radial basis function neural networks (RBFNN) and probabilistic neural networks (PNN), not shown in this work because they go beyond the scope of the paper, indicate that the same conclusions can be drawn as far as the advantages of the QFT technique over other feature extraction techniques.

Next, classification results obtained for Chilean red wines are presented using the database described in Sect. 4. Table 1 shows the average and standard deviation of the classification rates using each one of the four feature extraction methods studied employing QDA as classification method.

Since the number of patterns is rather low (172 samples), tenfold cross validation technique was used to assess the classifier accuracy. Data was randomly divided into ten subsets using nine of them for training-validation and one for testing purposes. This procedure was repeated 100 times.

From Table 1 we can state the following ranking for the analyzed methods in this application ordered from best to worse:

Rank	Feature extraction method	Classification method
1	QFT	QDA
2	WT	QDA
3	FT	QDA
4	LFT	QDA

Table 2 contains the values of the McNemar test of hypothesis [13] applied to the results of each feature extraction method. Recall that if the test *P*-value is greater than 3.84, the difference between the methods is statistically significant.

From Table 2 it is seen that differences among methods are indeed statistically significant.

In what follows, comments and remarks for each particular method are made. Since the problem has three classes and Fisher transformation maps data into a *C-1* space (where *C* is the number of classes) we can use Fisher transformation to plot the point distribution in the characteristic space along with the boundary decision. We will plot the pattern scattering using the Fisher transformation to project those points onto a two-dimensional space in order to visualize them.

6.1 Extraction using Fourier transform

It is important to point out that in contrast to LFT, when using Fourier transform we do not use information regarding the classes, and therefore Fourier method is considered a nonsupervised feature extraction method.

Table 1 Classification rates of Chilean red wines

Feature extraction method	Average (%)	Standard deviation (%)
Fourier transform	82.10	0.34
Wavelet transform	91.30	0.22
Linear Fisher transformation	71.80	0.30
Quadratic Fisher transformation	99.73	0.01

Table 2 *P*-values of the McNemar test of hypothesis

	Fourier transform	Wavelet transform	Linear Fisher transformation	Quadratic Fisher transformation
Fourier transform		5.23	4.82	6.78
Wavelet transform	5.23		7.08	4.85
Linear Fisher transformation	4.82	7.08		8.87
Quadratic Fisher transformation	6.78	4.85	8.87	

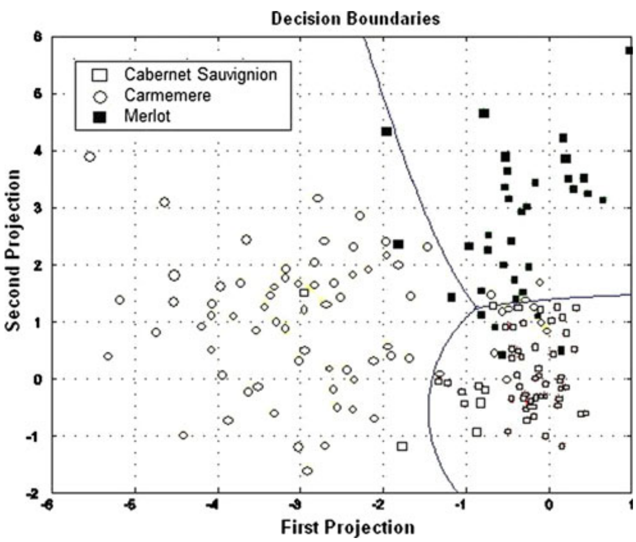

Fig. 3 Decision boundaries and pattern scattering when using FT as extraction

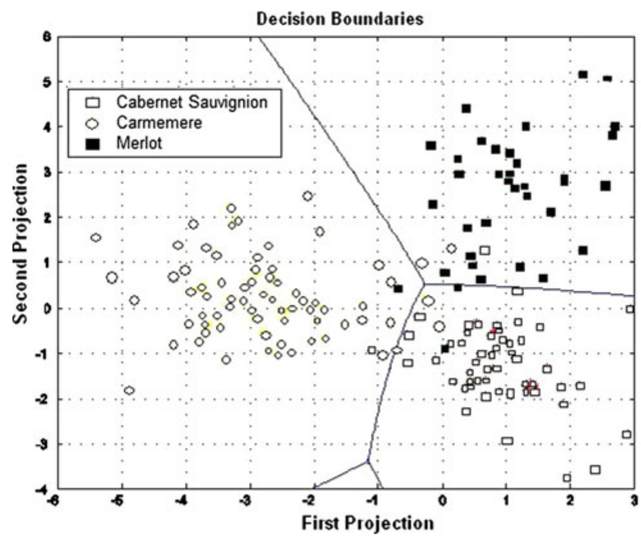

Fig. 4 Decision boundaries and pattern scattering using WT as extraction

The first 271 coefficients of the Fourier series were considered as input vector to the classifier. These 271 points contain 90.7% of the original signal energy.

Figure 3 shows the pattern scattering when using Fourier transform as extraction, plotted using the Fisher transformation as projection, for one run. A nice class separation can be observed from Fig. 3, indicating that classification could be properly performed. Some misclassified samples are also shown.

6.2 Extraction using wavelet transform

Since we are using the approximation coefficients of the WT as input vector to the classifier the decomposition level plays an important role in determining the number of characteristics to be considered. To determine the decomposition level a subset of the patterns was used in the validation procedure using cross-validation leaving-one-out (LOO) resulting that level 8 is the most appropriate for this case with 40 wavelet coefficients.

The results for the case of wavelet extraction, projected using Fisher transformation, are shown in Fig. 4 for one run. It can be observed that classes are quite separated although some misclassification is observed.

The rather modest behavior exhibited by FT can be explained because of the form of the liquid chromatograms signals. They are quite sharp and wavy, and FT is not a good tool to represent this kind of signals with a small number of coefficients, whereas WT represents it in a much better way, improving classification in about 9%.

6.3 Extraction using linear Fisher transformation

When using LFT as extraction method matrix S_w results singular (since original data dimension is 1,351 and only 172 patterns are available). To solve this difficulty inverse simultaneous diagonalization (ISD) method was used, technique proposed by Yu and Yan [18].

Figure 5 graphically shows the scatter of the wine samples when linear Fisher transformation is used as feature extraction method, projected using Fisher transformation for one run. Some important misclassification can be observed.

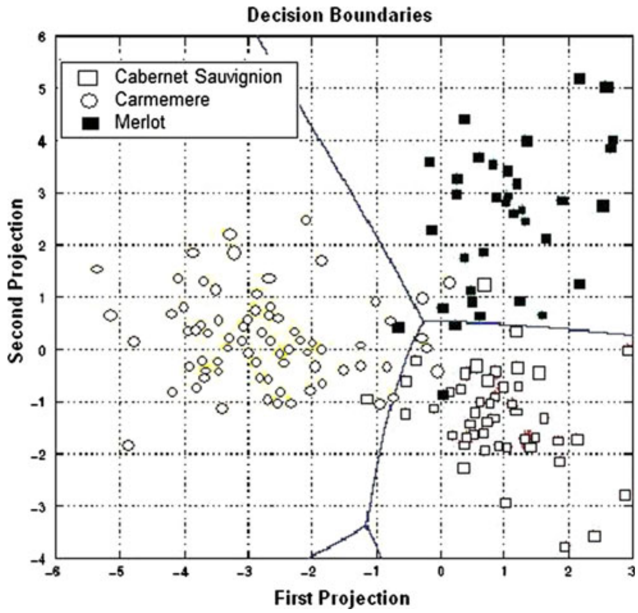

Fig. 5 Decision boundaries and pattern scattering using LFT as extraction method

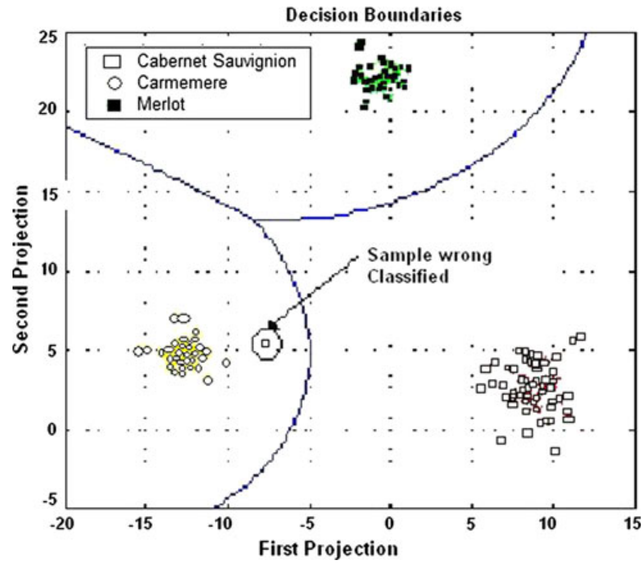

Fig. 6 Decision boundaries and pattern scattering using QFT as extraction

6.4 Extraction using quadratic Fisher transformation

Figure 6 presents the pattern scattering (projected using Fisher transformation for one run) when QFT is used as feature extraction technique. It can be seen that classes are almost completely separated except for sample number 43 that corresponds to a Cabernet Sauvignon wine that was erroneously classified as Carménère.

In the case of the LFT the use of only linear terms in the transformation is not good enough to represent properly the original signals in a reduced dimension space. The inclusion of quadratic terms in the basis functions, as done by QFT, enables a much better representation of the original signals in the reduced space. The introduction of these quadratics terms improves classification in almost 28%.

7 Conclusions and future work

In this paper results for Chilean red wine classification using four different feature extraction methods and one classification method were presented. The wine samples were characterized by the content of polyphenolic compounds measured through an HPLC.

Due to the high dimensionality of the liquid chromatograms and certain nonuniformities in the volume injection, re-sampling and normalization procedures were used previous to the feature extraction stage.

From the experimental results we can conclude that using quadratic Fisher transformation as feature extraction, previous to the classification using QDA, improved the percentage of correct classification from 91.30% (obtained using wavelet extraction) to 99.73%. LFT and FT extractions did not exhibit a good performance by the reasons discussed in Sects. 6.2 and 6.4.

As future research it is proposed to use these techniques in classifying Chilean red wines, but using information supplied by an electronic nose (*z*-nose). Some work is currently underway on this direction and promissory partial results have already been achieved [19, 20].

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Author Biographies

Manuel A. Duarte-Mermoud received the degree of Civil Electrical Engineer from the University of Chile in 1977 and the M.Sc., M.Phil. and the Ph.D. degrees, all in electrical engineering, from Yale University in 1985, 1986 and 1988, respectively.From 1977 to 1979, he worked as Field Engineer at Santiago Subway. In 1979 he joined the Electrical Engineering Department of University of Chile, where he is currently Professor.His main research interests are in robust adaptive control (linear and nonlinear systems), system identification, signal processing and pattern recognition. He is focused on applications to mining and wine industry, sensory systems and electrical machines and drives.Dr. Duarte-Mermoud is member of the IEEE and IFAC. He is past Treasurer and past President of ACCA, the Chilean National Member Organization of IFAC, and past Vice-President of the IEEE-Chile.

Nicolás H. Beltrán studied Electrical Engineering at the University of Chile where he graduated in 1974. He got his Master of Electrical Engineering in 1981 and his Doctoral degree in Applied Sciences in 1985, both from the Katholieke Universiteit Leuven (KUL), Belgium. He was with the Venezuelan Institute for Scientific Research (IVIC) from 1975 to 1979. Since 1985 he is with the Electrical Engineering Department of the University of Chile where he has conducted research in his areas of interest, ceramic sensors and intelligent instrumentation. Dr. Beltran is senior member of IEEE.

Matías A. Bustos was born in Santiago, Chile in 1977. He received his B.Sc. and M.Sc in Electrical Engineering from the Universidad de Chile in 2004. Currently he is working as senior research engineer in the Services and Technology division of the Mining and Metallurgical Research Center of Chile. He is involved in the development of computer vision and image processing algorithms used in soft sensor applications for mining processes.