FEATURE EXTRACTION OF ARTIFICIAL TONGUE DATA USING GRAM-SCHMIDT ORTHONORMALIZATION

Iasen Hristozov[1], Tania Pencheva[1] and Selim Eskiizmirliler[2,3]

[1]Centre of Biomedical Engineering "Prof. Iv. Daskalov"
Bulgarian Academy of Sciences
105 Acad. G. Bonchev Str., 1113 Sofia, Bulgaria
E-mail: *hristozov@gbg.bg*, *tania. pencheva@clbme.bas.bg*

[2]Center for Applied Autonomous Sensor Systems (AASS), Dept. of Technology, University of Orebro, SE-70182, Orebro, Sweden
[3]Université Paris VII - Denis Diderot et INSERM U.742, ANIM, 9, Quai Saint Bernard, 75005, Paris, France
phone: +33 (0)1 44 27 23 79, fax: +33 (0)1 44 27 34 38
E-mail: selim@ccr.jussieu.fr

ABSTRACT

In this paper we present a combined feature extraction approach for an electronic tongue. The use of wavelet decomposition technique for feature extraction, followed by orthonormalization, decreases the number of classifier inputs to the multiplication of number of classes and number of sensors. This approach leads to a higher computational efficiency. Two experiments are presented to demonstrate the procedure.

1. INTRODUCTION

The big interest to the concept of "soft" measurement techniques inspired the development of the so-called electronic tongue - a multi-sensor system for wet-chemical applications. Several different types of electronic tongues are known. For example, Legin et al. [1] have shown an electronic tongue, based on an array of potentiometric cross-sensitive chemical sensors, and pattern recognition and multivariate calibration for the analysis of Italian red wines. Winquist et al. [2] have introduced the voltametric electronic tongue. The paper describes how various voltammetric techniques such as large and small- amplitude pulse voltammetry can generate information when they are combined with a multivariate analysis method. Ivarsson et al. [3] have investigated three different waveforms - large amplitude voltammetry, small amplitude voltammetry and staircase voltammetry, for discrimination of tea by means of voltametric electronic tongue. To evaluate the discrimination of the data, they have used Principal Component Analysis (PCA). An electronic tongue, combined with PCA, has been used by Lindquist et al. [4] to monitor the quality of water in a production plant for drinking water. PCA have been used to examine the possibility to separate the measurement data from water with different quality.

A typical measurement with the electronic tongue is characterized by a large array of numbers (sometimes several thousands) presented in a vector or a matrix. In order to increase the interpretability of the measurements, decrease the computer calculations and reduce the noise, an alternative, more compact representation of the measurements could be made. It would allow the important features of the measurement to be well described but with a much smaller vector. There are a big number of studies that attempt to compress the data from electronic tongue measurement applying different feature extraction methods. Data fusion of electronic nose and electronic tongue data has been presented by Sundic et al. [5]. The authors have used seven basic features per interval that leads to the reduction of the data matrix. For further feature reduction they have used three different approaches - feature selection, based on Fisher's weight, forward and backward selection algorithms. In this way the number of features has been reduced to four per each interval. Holmin et al. [6] have investigated three data compression methods - wavelet transform, hierarchical PCA and parameters of a physical/chemical model to determine their ability to reduce the large data set obtained by a voltametric electronic tongue. In [7], an improvement of the model described in [6] has been made. Five model parameters characterizing the original signal are extracted. In this way the number of parameters has been reduced between 80 and 199 times. Artursson et al. [8] have also used wavelet transform with two different wavelet selection algorithms - variance and discriminance, in two different cases. In both cases the number of variables was significantly reduced.

The aim of this paper is to investigate the possibility of application of the combined approach for feature extraction, developed and demonstrated by the authors in [9] and concerning an electronic nose (e-nose). In comparison with the e-nose, the data sets from e-tongue are larger, which leads to some modifications in the developed method. In the other hand the smaller sensors' drift in electronic tongue allow us to change the algorithm for bases creation. The feasibility of this new approach is illustrated with on data from an e-tongue for two substances - coffee and vinegar.

2. ELECTRONIC TONGUE

An electronic tongue is an acronym for a multi-sensor system for wet-chemical applications. The electronic tongue used in this work is made of four different noble metals as working electrodes, an Ag/AgCl reference electrode and an auxiliary electrode of stainless steel working in standard three-electrode configuration based on large pulse voltammetry (LAPV) principle. In voltametric measurements, the current between the working electrode and the reference electrode is measured when a voltage is applied over the working and the reference electrodes. The test signal is a waveform constructed from a sequence of pulses in such way that maximum relevant information can be extracted from the output data. If there are electrochemically active substances in the solution, a current of charged particles in the liquid sample rushes towards the electrode and the electroactive compounds near the electrode surface are oxidized or reduced depending in their potential. The redox reactions cause an exchange of electrons with the electrode.

The amplitude and form of the electric current signals contain information concerning the nature of the sample. The current pattern is rather complex and thus multivariate analysis methods are needed to interpret the data. The dimension of the electronic tongue data increases rapidly when the sampling rate, the number of electrodes or the number of pulses is increased. Consequently, the data sets often become very large. A variable is defined as a single sample in the time sequence of the electrical current, resulting from the voltage pulses. Each variable depends both on the applied voltage and the time instant at which the voltage was applied. Moreover, the response of the e-tongue depends on the type of material used for the electrodes and the chemical contents of the solution.

The electronic tongue used for the experiments in this article is developed in AASS of Orebro University, Sweden and its main application is in water and food quality assessment. This e-tongue has 4 electrodes and a typical measurement data set contains over 5000 readings. More details about its construction and principles of operation can be found in [4].

3. A COMBINED METHOD FOR FEATURE EXTRACTION AND CLASSIFICATION OF ELECTRONIC TONGUE DATA.

In this section we outline the main steps of the proposed method. More theoretical details could be found in [9].

1. The input data consists of M sets of measurements performed with C different substances. The data sets contain the responses from S sensors of the tongue. From each measurement, we take a data matrices $F_m, m \in 1 \div M$ of dimension $S \times N$, where $N = R.2^K$ is the number of readings per sensor.
2. K-level wavelet transform is applied to the signal of each sensor (each row of the data matrices $F_m, m \in 1 \div M$). In this way, for each measurement m we obtain S sets of wavelet coefficients vectors of the form $[a_{K,m,s},\ d_{K,m,s},\ d_{K-1,m,s},\ \ldots,\ d_{1,m,s}], m \in 1 \div M, s \in 1 \div S$.
All operations of convolution and downsampling can be represented as a multiplication of the signal with two matrices W_k and V_k, (see [10]), therefore approximation coefficients a_1 and the detail coefficients d_1 from the first decomposition level can be respectively obtained as
$$\begin{aligned} a_1 &= V_1.f \\ d_1 &= W_1.f \end{aligned} \tag{1}$$
where f is the data vector (a row of matrix F_m). For each of the next decomposition levels k, the approximation coefficients a_k and the detail coefficients d_k are obtained as
$$\begin{aligned} a_k &= V_k.a_{k-1} \\ d_k &= W_k.a_{k-1} \end{aligned} \tag{2}$$
3. A *features' vector* $v_{m,s}$ consists of the approximation coefficients $a_{K,m,s}$ from K-level wavelet decomposition of the signal from s^{th} sensor of the m^{th} measurement. The next steps are performed on these vectors.
4. A basis $q_{c,s}$ is obtained by orthonormalization of mean value $z_{c,s}$ of some features' vectors of the substance c and the sensor s using the Gram-Schmidt procedure [11]:
a) At the first step the vector $q_{c,1}$ is obtained as a division of the vector r_1 and its length:
$$q_{c,1} = \frac{z_{c,1}}{\left\| z_{c,1} \right\|} \tag{3}$$
b) At the step s we subtract from $z_{c,s}$ its components in the directions that are already settled:
$$z'_{c,s} = z_{c,s} - \left(q_{c,1}^T z_{c,s}\right) q_{c,1} - \ldots - \left(q_{c,s-1}^T z_{c,s}\right) q_{c,s-1} \tag{4}$$
c) Then $q_{c,s}$ is a unit vector:
$$q_{c,s} = \frac{z'_{c,s}}{\left\| z'_{c,s} \right\|} \tag{5}$$
Each basis has a length of R. Applying the simplified projection matrix in the following way
$$T_{c,s} = q_{c,s} q_{c,s}^T . \tag{6}$$
on these bases, C projection matrices $T_{c,s}, c \in 1 \div C, s \in 1 \div S$, of dimension $R \times R$, are constructed for each sensor s.
5. The features' vectors $v_{m,s}$ are projected onto the C bases
$$p_{c,m,s} = T_{c,s}.v_{m,s},\ c \in 1 \div C,\ m \in 1 \div M,\ s \in 1 \div S . \tag{7}$$
That is, C projections $p_{1,m,s}\ \ldots\ p_{C,m,s}$ with length R are obtained for features' vector of each sensor.
6. For each projection, the standard deviation is calculated by
$$d_{c,m,s} = \sqrt{\frac{1}{R-1}\sum_{r=1}^{R}\left(p^r_{c,m,s} - \frac{1}{R}\sum_{r=1}^{R} p^r_{c,m,s}\right)}, \quad c \in 1 \div C,\ m \in 1 \div M,\ s \in 1 \div S \tag{8}$$
7. The values of $d_{c,m,s}$ are used as inputs to the linear vector quantization (LVQ) network [12]. Note that the network has $C.S$ inputs and C outputs, where C is also the number of classes.

4. EXPERIMENTAL RESULTS AND DISCUSSION

The method was tested on the measurement data sets of two substances - coffee and vinegar. For each substance, 20 measurement data sets were available. Ten of them were used for network training and another ten - for network testing. Each measurement data set captures the signals from four sensors. The typical e-tongue response for a substance (coffee) is shown in Fig. 1.

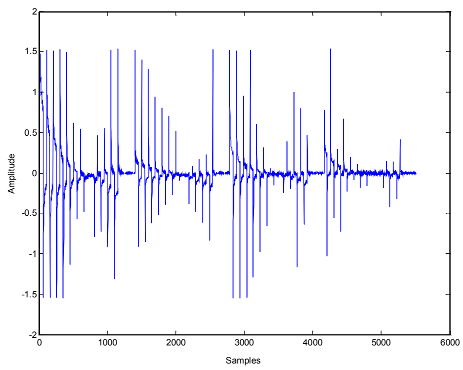

Fig. 1. Typical e-tongue output for coffee

In this paper, a wavelet function, called Daubichies-2, is used. Daubichies-2 LPF and HPF are represented by four coefficients (Table 1):

Table 1 Daubichies 2 coefficients

c_1	c_2	c_3	c_4
$\frac{1+\sqrt{3}}{4\sqrt{2}}$	$\frac{3+\sqrt{3}}{4\sqrt{2}}$	$\frac{3-\sqrt{3}}{4\sqrt{2}}$	$\frac{1-\sqrt{3}}{4\sqrt{2}}$

The two matrices W_k and V_k, mentioned in Eqs. (1 - 2), in the case of Daubechies-2 have the following forms:

$$V_k = \begin{bmatrix} c_1 & c_2 & c_3 & c_4 & 0 & & & & & \cdots & 0 \\ 0 & 0 & c_1 & c_2 & c_3 & c_4 & 0 & & & \cdots & 0 \\ 0 & \cdots & & 0 & c_1 & c_2 & c_3 & c_4 & 0 & \cdots & 0 \\ \vdots & & & & & & & & & & \vdots \\ c_3 & c_4 & 0 & & & \cdots & & & 0 & c_1 & c_2 \end{bmatrix}_{(N_k/2 \times N_k)} \tag{9}$$

$$W_k = \begin{bmatrix} c_4 & -c_3 & c_2 & -c_1 & 0 & & & & & \cdots & 0 \\ 0 & 0 & c_4 & -c_3 & c_2 & -c_1 & 0 & & & \cdots & 0 \\ 0 & \cdots & & 0 & c_4 & -c_3 & c_2 & -c_1 & 0 & \cdots & 0 \\ \vdots & & & & & & & & & & \vdots \\ c_2 & -c_1 & 0 & & & \cdots & & & 0 & c_4 & -c_3 \end{bmatrix}_{(N_k/2 \times N_k)} \tag{10}$$

where k is the number of current decomposition level, $N_k = N/2^{k-1}$ and N is data length.

Hence, three-level Daubichie-2 wavelet decomposition was applied on each sequence. In order to apply wavelet transform, the number of samples per sensor must be proportional to a number, which is a power of two. For this aim each measurement set (which is consisted of 5461 readings) is reduced to 5376 samples ($1344=168.2^3$ for each of the four sensors) without loss of information. Fig. 2 shows some typical coefficients obtained from the wavelet decomposition. Fig. 3 shows comparison between the original and the reconstructed signals, accomplished only on the base of approximation coefficients

The features' vector of each measurement is constructed from the 168 approximation coefficients of the four sensors. These coefficients account for 81% from signal's energy. The mean values of features' vectors from first ten measurements are used to construct a basis and a projection matrix for each of the two substances, applying Gram-Schmidt orthonormalization.

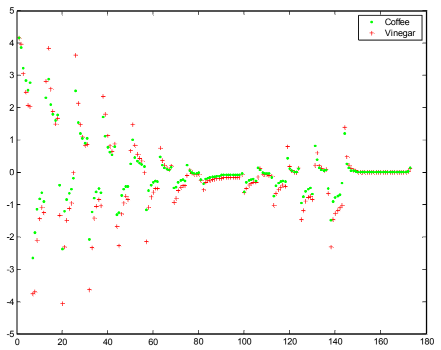

Fig. 2. Approximation coefficients from three-level wavelet decomposition of the first sensor signal

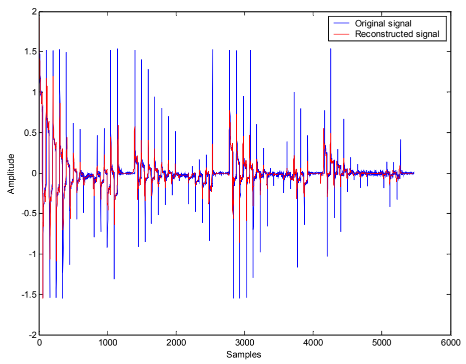

Fig. 3. Original and reconstructed signal for coffee

Each features' vector of the training data sets is projected onto these bases (see Fig. 4).

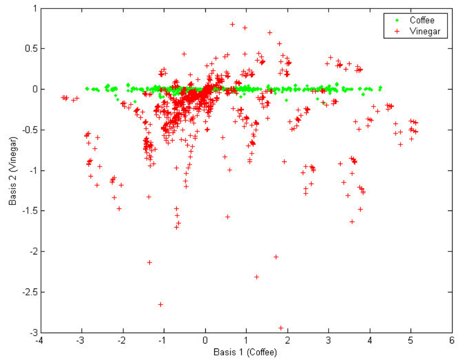

Fig. 4. Projections onto the bases for the first sensor

Fig. 5 presents the standard deviations of the two projections for each measurement.

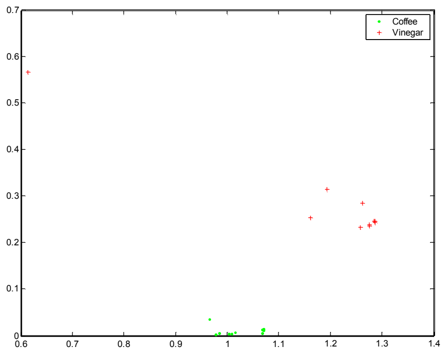

Fig. 5. Standard deviations of the projections for the first sensor

These values for 20 measurements are used as inputs in training of a LVQ neural network. A perfect learning (0% error) is achieved after two steps. In the test phase, performed with 20 unseen examples (10 measurements for each of the 2 substances), 0% classification error was registered.

The second experiment was inspired from the work of Artursson et al. [8] and it was performed on the mirrored and flipped signals from each sensor (see Fig. 6).

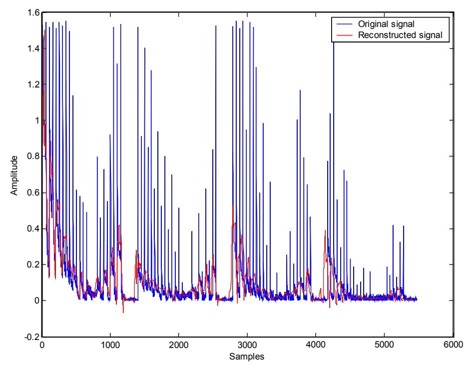

Fig. 6. Original and reconstructed mirrored signal for coffee

We observed that similarly to the previous case, conservation of energy could be achieved with higher-level wavelet transform. The problem was that the difference between the original signal and the one, reconstructed from approximation coefficients became too large. This was the reason for us to look for a compromise between good compression and loss of information. With five-level Daubichies-2 wavelet decomposition we achieved 75% signal energy accounted in fourty-two approximation coefficients for each sensor (Fig. 7).

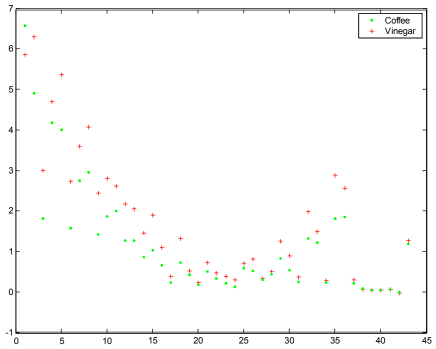

Fig. 7. Approximation coefficients from five-level wavelet decomposition for the first sensor signal

These coefficients were used to construct the features' vector for the measurements. The same steps as in the previous experiment were performed. Fig. 8 presents the projections of measurements features' vectors on the bases, and Fig. 9 - their standard deviations.

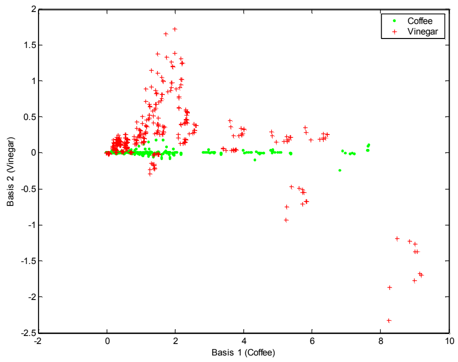

Fig. 8. Projections onto the bases for the first sensor

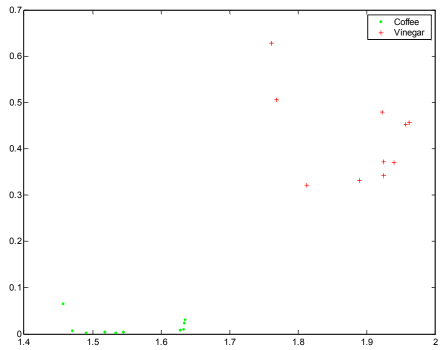

Fig. 9. Standard deviations of the projections for the first sensor

Twenty measurement features' vectors for two different substances were used for network training and another twenty - for network testing. The classification error is again 0%.

5. CONCLUSIONS

The aim of this article was to investigate the applicability of the feature extraction combined approach, based on wavelet transform and Gram-Schmidt orthonormalization, for the electronic tongue data. We concentrated our attention to demonstrate the ability of the method to handle very large data sets. In the future work we plan to investigate its robustness and test the method with greater number of substances. The computational difficulties associated with very large data sets leaded us to idea to modify the original method developed for electronic noses. Namely, in this article we examined data from different sensors separately and formed the bases for each sensor.

The method was evaluated in two experiments - with the original and with mirrored signals. After successful training of the classifier, perfect separation of the substances was achieved. In both cases we reduced the classifier' input variables from above 5000 to only 8. The obtained results demonstrate the possibility of the successful application of the modified combined approach for classification tasks dealing with the large-scale data sets.

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