ISSN 1726-5479

SENSORS & TRANSDUCERS

vol. 112
1 /10

Sensor Instrumentation, DAQ and Virtual Instruments

International Frequency Sensor Association Publishing

IFSA

Sensors & Transducers

Volume 112, Issue 1
January 2010

www.sensorsportal.com

ISSN 1726-5479

Sensors & Transducers Journal (ISSN 1726-5479) is a peer review international journal published monthly online by International Frequency Sensor Association (IFSA).
Available in electronic and on CD.

Sensors & Transducers Journal

Contents

Volume 112
Issue 1
January 2010

www.sensorsportal.com

ISSN 1726-5479

Research Articles

Authors are encouraged to submit article in MS Word (doc) and Acrobat (pdf) formats by e-mail: editor@sensorsportal.com
Please visit journal's webpage with preparation instructions: http://www.sensorsportal.com/HTML/DIGEST/Submition.htm

Sensors & Transducers Journal, Vol. 112, Issue 1, January 2010, pp. 47-63

Sensors & Transducers

ISSN 1726-5479

http://www.sensorsportal.com

Statistical Feature Extraction and Recognition of Beverages Using Electronic Tongue

P. C. PANCHARIYA and A. H. KIRANMAYEE

Digital Systems Group

Central Electronics Engineering Research Institute (CEERI/CSIR), Pilani-333031, India

Tel.: +91-1596-252267, fax: +91-1596-242294

E-mail: pcp@ceeri.ernet.in, kiran@ceeri.ernet.in

Received: 3 November 2009 /Accepted: 22 January 2010 /Published: 29 January 2010

Abstract: This paper describes an approach for extraction of features from data generated from an electronic tongue based on large amplitude pulse voltammetry. In this approach statistical features of the meaningful selected variables from current response signals are extracted and used for recognition of beverage samples. The proposed feature extraction approach not only reduces the computational complexity but also reduces the computation time and requirement of storage of data for the development of E-tongue for field applications. With the reduced information, a probabilistic neural network (PNN) was trained for qualitative analysis of different beverages. Before the qualitative analysis of the beverages, the methodology has been tested for the basic artificial taste solutions i.e. sweet, sour, salt, bitter, and umami. The proposed procedure was compared with the more conventional and linear feature extraction technique employing principal component analysis combined with PNN. Using the extracted feature vectors, highly correct classification by PNN was achieved for eight types of juices and six types of soft drinks. The results indicated that the electronic tongue based on large amplitude pulse voltammetry with reduced feature was capable of discriminating not only basic artificial taste solutions but also the various sorts of the same type of natural beverages (fruit juices, vegetable juices, soft drinks, etc.). *Copyright © 2010 IFSA.*

Keywords: Electronic tongue, Probabilistic neural network, Principal components analysis, Pattern recognition

1. Introduction

An electronic tongue system has been defined as a multi-sensor system, which, comprising an array of nonspecific, low-selective chemical sensors with high stability and cross-sensitivity to different species in solution, uses an appropriate method of multivariate analysis for data processing and also capable of recognizing the qualitative and/or quantitative composition of multi-species solutions of different natures[1].Among various electronic tongues based on potentiommetry [2-4], voltammetry [5], impedance spectroscopy [6-8] etc., the voltammetric electronic tongue developed by Winquist et. al., has shown good performance due to its sensitivity and simplicity, which makes this technology ideally suited for on-line process monitoring and quality control. It has been successfully tested for numerous applications in agricultural products as well as in industries, beverages, dairy products and food products, etc. [9-15]. Voltammetry is an interfacial electrochemical method of electroanalytical chemistry that is based upon the electrical properties of an analyte when it is made a part of an electrochemical cell, which, in addition to the electrolyte solution comprises of working electrode(s), a reference electrode and an auxiliary (counter) electrode connected to a potentiostat either in three electrode configuration or in two electrode configuration by coupling two functions into one physical unit (reference and auxiliary electrodes). A potentiostat controls the potential of the interface under investigation. The fundamental parameters are the applied potential, the resulting current and the time. Thus, the information about the analyte (the solution under test) is derived from the measured current response as a function of the applied potential.

In the case of the electronic tongue system based on voltammetry, a fixed or continuous potential or a pulse sequence of any shape, pulse, staircase, cyclic, ramp, sinusoidal etc is applied and resulting current response is recorded. In recent literatures are described an electronic tongue based on voltammetry in which a pulse sequence (i.e. large amplitude pulse voltammetry (LAPV), small amplitude pulse voltammetry (SAPV), staircase voltammetry and multifrequency large amplitude pulse voltammetry [13, 16]) with varying amplitude is applied to an array of nonspecific metallic working electrodes in an electrochemical cell and current responses due to the applied potential signal are registered. This generated current signals that are measured have mainly two components: a capacitive component and a faradic component. The capacitive current corresponds to the current required to charge the electric double layer at the interface of the working electrode(s) and the solution. The electric double layer is inherent to interfacial electrochemical phenomena and acts like an electric capacitor. The faradic current corresponds to the current produced by the electrochemical reactions of oxidation-reduction that occur at the working electrode(s). This current is generally governed by the diffusion of electroactive species inside the gradient of concentration caused by the applied potential at the working electrode(s). The magnitude of the faradic current depends not only on the concentration, but also on electro activity (kinetics) and easiness of diffusion of considered species. These current response signals present a distinct response for a specific group of chemical compounds i.e. the corresponding signature. Thus, the system establishes a ‘signature’ of a specific compound in a mixture allowing samples to be grouped on the basis of their current response i.e. voltammogram similarities which is further processed by the pattern recognition methods to perform classification (qualitative as well as quantitative) of samples under investigation. Therefore whole current response curve is very important for interpretation of the desired results.

The pattern recognition refers to techniques in which a priori knowledge is used to develop rules that may be later used for classification of new samples. The classification model is developed on a training set of samples with known categories. The model performance is evaluated by the use of a validation set by comparing the classification predictions with the true categories [17]. There are numerous classical pattern recognition methods [19-23], such as linear discriminant analysis (LDA), soft independent modeling of class analogy (SIMCA), discriminant partial least squares regression (DPLS), locally weighted regression (LWR), K-nearest neighbor (KNN), and many more. According to voltammetric response information, these recognition methods can discriminate and analyze milk, tea, juice, drinking water and mold growth in liquid media [9-16]. These studies demonstrated a high degree of discriminant success of using voltammetric responses and pattern recognition methods.

In E-tongue based on LAPV, the pulse-sequences involve many pulse steps and becomes complex especially when multi-electrode arrangements are used, wherein each pulse-sequence has to be repeated for each electrode. As the response signal contains the information about the electrochemical dynamics of the liquid media, each data point is very important and considered as a dimension. This results in a complex large data matrix which makes enormously cumbersome to any pattern recognition method. Therefore faithful reduction of data dimension without compromising the meaningful information is an essential preprocessing step before attempting for any pattern recognition method. Apart from the data size reduction, data compression is also as essential to extract significant features from the response signal, besides the elimination of irrelevant content, such as noise or redundancies [21, 22]. These preprocessing techniques have manifold advantages such as increased training speed, reduction of memory needs, better generalization ability of the model, enhanced robustness versus noise, and simpler model representations [21].

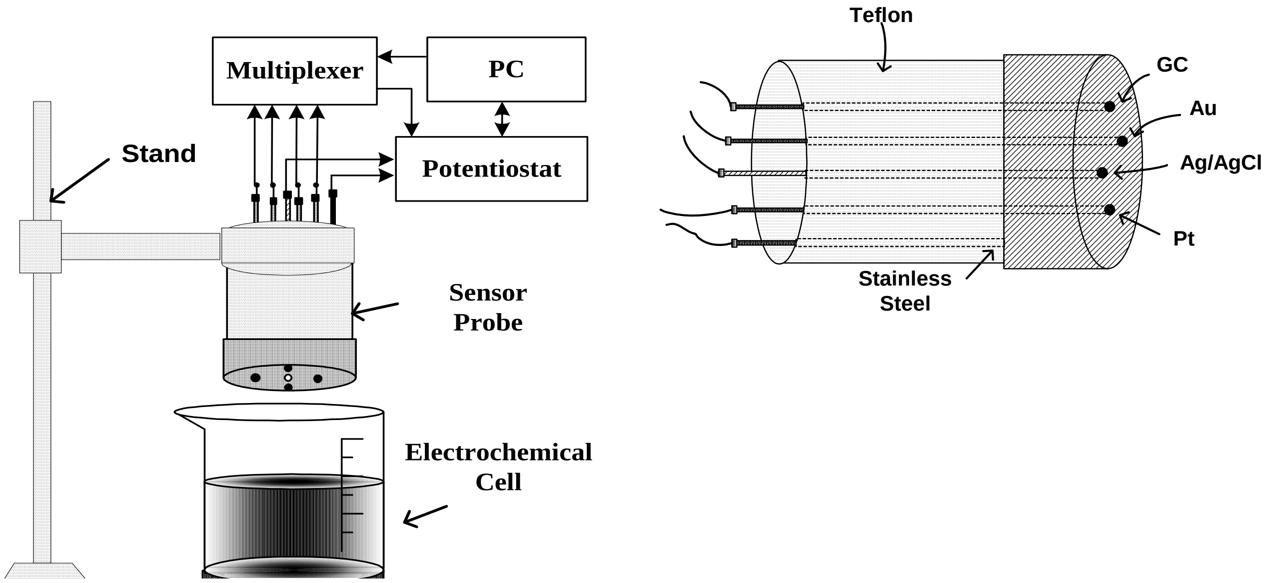
When working with voltammetric electronic tongues, different options have been attempted to reduce the complexity of the acquired information. These techniques include principle component analysis (PCA), hierarchical principal component analysis (HPCA), Fourier transform (FT), discrete wavelet transform (DWT), parametric functions (i.e. based on a sum of exponential decays with some electrochemical phenomena) and various combinations of these methods [23-26]. These data reduction techniques were combined with ANNs for modeling and classification purposes [27-29].

The selection of data reduction, compression or selection of an algorithm depends on the computational complexity involved, the speed and requirement of memory space especially for the development of instruments for field applications. Therefore, the objective of this research is to investigate the potential of statistical feature extraction algorithms ideally containing only salient information or features of the voltammetric signals for classifying liquid food such as soft drinks and fruit juices with basic five tastes such as sweat, sour, salt, bitter and umami and whether the selected feature vectors chosen are effective in the discrimination of the same category of food with different quality grades.

2. Experimental

2.1. The Measurement Setup

As shown in Fig. 1, the electronic tongue consists of three working electrodes made of platinum, gold and glassy carbon, an Ag/AgCl electrode for reference electrode (saturated KCl, diameter 2 mm), and stainless steel counter electrode for standard three-electrode systems. For better potential stability, the surface area of counter electrode was kept large as compared to that of the working electrode. The metal wires that served as working electrodes had a diameter of 2mm and a purity of 99.9 %. All the electrodes were made by CHI Instruments, USA. The potentiostat used in this measurement setup is from Gamry Instruments, USA. The electrode configuration was mounted in a housing of stainless steel, which was inserted in the liquids under investigation. The switching of electrodes was performed by relay module consisting of relays (built at the lab of Digital System Group, Central Electronic, Engineering Research Institute, Pilani, India) which was controlled by a personal computer (PC). It enables the working electrodes to be connected consecutively one by one in a three-electrode configuration, thereby enabling the potential pulses/steps to be impressed on each of the working electrodes in sequence. The PC was used to set and control the potential pulses, measure and store current responses via potentiostat. A thermostat water bath was used to maintain the cell at a constant temperature.



(a) (b)

Fig. 1. Experimental setup for Electronic tongue system.

2.2. Measurement Principle and Procedure

The developed pulse voltammetry based electronic tongue with three working electrodes made of gold, platinum and glassy carbon is used in the measurements as described in Section 2.1. Current was measured between the working electrode and the counter electrode when a potential pulse was applied over the working electrode and the reference electrode. Initially, the working electrode is held at a base potential and after a fixed waiting period, the potential is stepped to a final potential. A current will then flow to the electrode, initially sharp when a Helmholtz double layer of charged species is formed and electroactive compounds next to the electrode surface are oxidized or reduced. The current will then decay as the double layer capacitance is charged and electroactive compounds are consumed, until only the diffusion limited faradic current remains. When the electrodes potential is stepped back to its initial value, similar but opposite reactions occur. The size and shape of the transient current responses reflect the amount and diffusion coefficients of both redox active and charged compounds in the solution.

The applied potential waveform consists of three cycles i.e. electrochemical cleaning cycle, conditioning cycle and measurement cycle respectively as shown in Fig. 2. In electrochemical cleaning cycle a positive potential of 2 V was applied for 500 ms, thereafter a negative potential of -2 V was applied for the same period. After the electrochemical cycle, the next cycle is conditioning cycle in which the potential is kept at 0 V for 10 s. The final cycle is the measurement cycle which is based on successive voltage pulses of gradually changing amplitude between which the base potential is applied, and the current is continuously measured. The frequency of the pulse was kept at 1 Hz for all these measurements. The potential range for all the measurements was varied from 600 mV to -400 mV in steps of 100 mV.

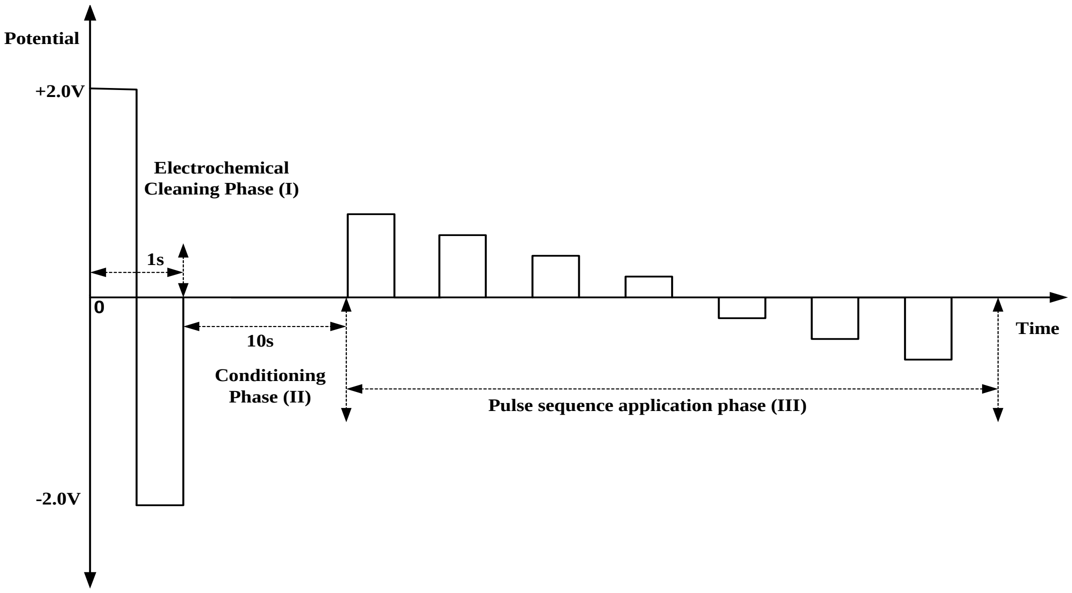


Fig. 2. Experimental pulse sequence.

2.3. Experimental Samples and Measurements

2.3.1. Artificial Taste Solutions

Taste is comprised of five basic taste qualities i.e. sour, sweet, salt, bitter and umami [30, 31]. Sourness can be produced by hydrogen ions of hydrochloric acid, acetic acid, citric acid and so on; saltiness can be from sodium chloride; bitterness can be produced by quinine, caffeine, L-tryptophan and magnesium chloride; sweetness due to sucrose, fructose, glucose, L-alamine and so on; and the umami, which is the Japanese term implying 'deliciousness', can be produced by monosodium glutamate (MSG) contained mainly in seaweeds, disodiuminosinate (IMP) in meat and fish and disodium guanylate (GMP) in mushrooms. Five typical primary taste substances, HCl (sour), NaCl (salty), $MgCl_2$ (bitter), sucrose (sweet) and Glutamic acid (umami) were used in preparing the solutions indicative of these taste qualities. Since the experimental data from the electronic tongue was distributed in the wide range of potentials, they were preprocessed (i.e. by mean normalization) prior to analysis to treat the variances and the average values in a similar scale range. Five samples corresponding to each taste solution were investigated. Each sample solution was analyzed three times successively and the data from three measurements were averaged to one measurement for the further analysis. Each measurement cycle has generated an array which is of the size of 1×4180 points (i.e. acquired current response data points while applying the measurement pulse sequence) for every electrode. The complete experiments for five taste solutions with five samples each generate a data matrix of (5×5)×4180 for a single electrode.

2.3.2. Soft Drinks

Six soft drinks (Coca Cola, Mountain Dew, Fanta, Mirinda, Sprite and Pepsi) bought from local market in Pilani, India were selected as samples for investigation using the developed electronic tongue. All the soft drinks were produced by two different Indian companies in 2008. The task was to discriminate these soft drinks by their brand names. Each soft drink was sampled five times (five samples) so that sampling error can be minimized. Eighty milliliters of each sample of every soft drink was used for analysis by the electronic tongue at temperature (22±1 ^{0}C) in random. Each sample solution was analyzed three times successively and then the data from the three measurements were averaged to one data sample for the analyzed solution. The complete measurement yielded a data matrix of the size (5×6)×4180 for each electrode.

2.3.3. Juices

The developed electronic tongue was used to analyze different juices i.e. of Mango, Grape, Guava, Litchi, Orange, Pineapple, Mixed fruit juice and Mixed fruit-vegetable. All the eight juices of fruits and vegetables were manufactured by the Indian company (Dabur) in 2008. All samples of juices were stored at −20 ^{0}C before test. Five samples, each of eighty milliliters, of each juice were chosen for the analysis by the electronic tongue. Therefore, a total of 40 samples were chosen for the experimentation. The experiments on the samples were conducted in random at room temperature (25±1 ^{0}C). The experiment for each of the samples is repeated thrice followed by averaging out the resulting data sets to one data set. The result of the experiments carried out for total samples is a data matrix containing 40×4180 data sets resulting in a total of 40 sample points or observations for each electrode.

2.4 Data Processing

In our experiment, a statistical feature extraction (SFE) technique for the voltammetric signals was proposed. Probabilistic neural network (PNN) is used as classifier with the extracted features as inputs to the network. The features were also extracted using the principal component analysis (PCA) techniques and also utilized as inputs to the PNN. The results from the both approaches i.e. SFE-PNN and PCA-PNN have been compared. The data obtained were evaluated using the following two commercial software package: Unscrambler (version 9.5, 2007, CAMO ASA, Trondheim, Norway) and Matlab (version 7.1, Mathworks, USA) for programming the feature extraction and the pattern recognition techniques.

The PCA was carried out on the sensor array data. The PCA is a statistical method that could deduct dimensions and observe a primary evaluation of the between-class similarity. It is also a projection method that allows an easy visualization of all the information contained in a data-set. In addition, it also helps to find out in what respect a sample is different from others and, which variables contribute most to this difference. The PCA method intends to summarize almost all variance contained in the response signal on a fewer number of axes (the PCs) with new coordinates called scores which are mutually orthogonal, obtained after data transformation. Few selected scores (which explain the maximum variance) can be used as inputs to any ANNs for quantitative analysis. However, it can fail to preserve the nonlinearity of a data set, as it is a linear projection technique. If there are some nonlinear characteristics in the response signal, these will be considered as outliers or noise and will not be described by the first PCs as in a linear case. Data were preprocessed before analysis. The preprocessing included a scaling and dividing by the standard deviation.

For classification purposes, a probabilistic neural network (PNN) [32] has been used. The PNN, introduced by Donald F. Specht in 1990 firstly, is relatively new compared to other neural networks like back-propagation artificial neural networks (BP-ANN) and radial basis function networks (RBFN). It takes its basic concept from the Bayesian statistical classifier which is the optimal statistical classifier. It maps the Bayes rule into a feed forward multilayer neural network. PNN associates an unknown pattern to the class to which this pattern is most likely to belong. PNN constitutes a classification methodology that combines the computational power and flexibility of ANNs. The main advantages of PNN over other ANNs include their simplified architecture which overcomes the difficulty of specifying an appropriate ANN model as well as their easy implementation during training and testing.

This type of network is composed of four layers. In the input layer there are three elements that correspond with the first three components of the PCA that carry almost 100% of the old variables. The next layer is the pattern layer. This layer has a number of neurons equal to the training pattern vectors, grouped by classes, where the distance between the test vector and a learning pattern is assessed. The purpose of this layer is to measure and weigh with a radial function, the distance of the input layer vector with each training set element. The third layer, the summation layer, contains one neuron for each class. This layer adds the outputs of the pattern neurons belonging to the same class. Finally, the "output layer" is simply a thresholder that seeks for the maximum value of the summation layer. Then the highest one is selected and takes one as a result. The other outputs are set to 0. In Fig. 3 a schematic diagram of the PNN network is shown [33]. A validation method was applied to the network in order to check the performance of the network. The method consisted of validating N distinct nets (in this case, N is the number of measurements) by using $N-t$ training vectors and t testing vectors which were excluded from the training set for each group.

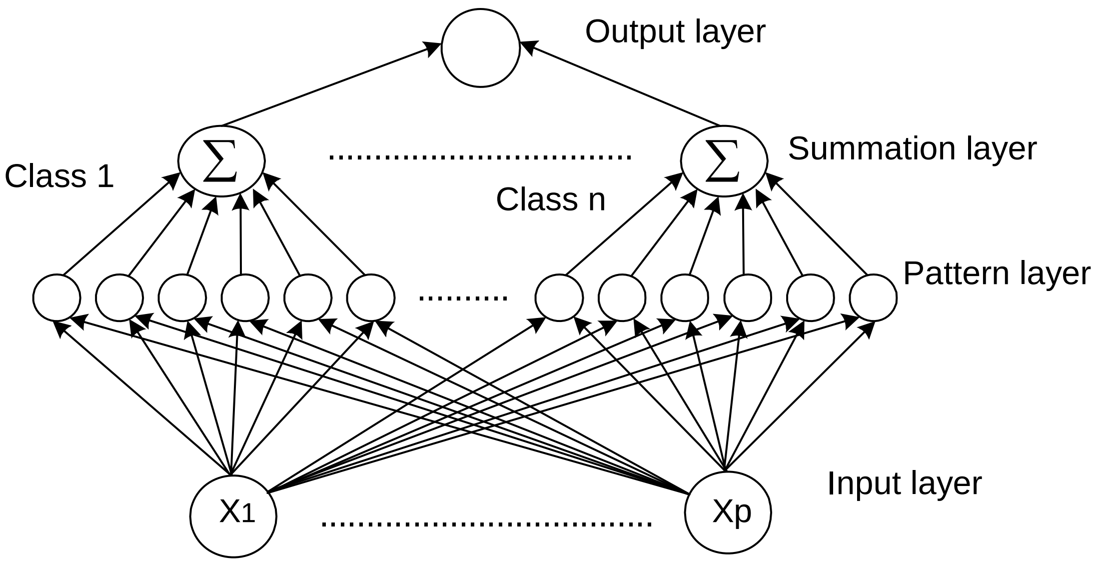


Fig. 3. A typical probabilistic neuronal network (PNN).

3. Results and Discussion

3.1. Large Amplitude Pulse Voltammetry (LAPV) Response to the Samples

The response signals of the electrode array (three working electrodes) for 25 taste samples, 30 soft drinks samples and 40 juices samples were collected using the developed E-tongue system. Each curve represents the variation in current of each electrode with time for a given applied pulse sequence. The initial data points of electrochemical cleaning cycle and conditioning cycle were removed.

3.2. Statistical Feature Extraction and Selection

Data samples can have thousands of values. Descriptive statistics are a way to summarize data into a few numbers that contain most of the relevant information. These descriptive statistics can be categorized in terms of measures of central tendency (location) of data by computation of parameters such as geometry mean, harmonic mean, mean, median, and trimmed mean of the data and also measures of dispersive parameters such as inter quartile range (IQR), MAD, range, standard deviation, variance etc. Some times higher order statistical parameters such as higher order moments, skewness and kurtosis provide important information about the data. In this section, first some of the robust parameters are described and their application for feature extraction procedure applied for feature extraction on voltammetric signals is discussed.

3.2.1. Average Value, the Median Value, the Trimmed Mean Value and the Standard Deviation

The average or mean value (AV) of the response of kth sample is defined as follows:

$$AV_k = \frac{1}{M}\sum_{i=1}^{M} x_i \ , \tag{1}$$

where, M is the no. of measurement points in the final response vector. The median value (MV) of the response vector is the 50th percentile of the response vector. The median is a robust estimate of the center of a sample of data, since outliers have little effect on it. The trimmed mean calculates the mean of a sample x excluding the highest and lowest percent/2 of the observations. The trimmed mean is a robust estimate of the location of a sample. If there are outliers in the data, the trimmed mean is a more representative estimate of the centres of the body of the data. If the data is all from the same probability distribution, then the trimmed mean is less efficient than the sample average as an estimator of the location of the data. The standard deviation (SD) is the standard deviation of the data points in the final response vector $X^{j}_{1\times M}$ is calculated as:

$$SD_k = \left[\frac{1}{M-1}\sum_{i=1}^{M}\left(x_i - AV_k\right)^2\right]^{1/2} , \tag{2}$$

where, $AV_k = \frac{1}{M}\sum_{i=1}^{M} x_i$

3.2.2. Interquartile Range (IQR), Kurtosis and Skewness

The interquartile range is the difference between the 75th and the 25th percentiles of the sample in x. The IQR is a robust estimate of the spread of the data, since changes in the upper and lower 25% of the data do not affect it. If there are outliers in the data, then IQR is more representative than the standard deviation as an estimate of the spread of the body of the data. The IQR is less efficient than the standard deviation as an estimate of the spread, when the data is all from the normal distribution. The kurtosis is a measure of how outlier-prone a distribution is. The kurtosis of the normal distribution is 3. Distributions that are more outlier-prone than the normal distribution have kurtosis greater than 3 and the distributions that are less outlier-prone have kurtosis less than 3. The kurtosis of a distribution is defined as:

$$k = \frac{E\left(x-\mu\right)^4}{\sigma^4} \ , \tag{3}$$

where $E(x)$ is the expected value of x. The skewness is a measure of the symmetry of the data around the sample mean. If the skewness is negative, the data are spread out more to the left of the mean than to the right. If skewness is positive, the data are spread out more to the right. The skewness of any perfect symmetric distribution is zero. The skewness of a distribution is defined as:

$$y = \frac{E\left(x-\mu\right)^3}{\sigma^3} , \tag{4}$$

where $E(x)$ is the expected value of x.

3.2.3. Proposed Feature Extraction Method for Voltammetric Signal

Let us assume that the voltammetric system consists of d number of working electrodes. These electrodes are excited by a potential pulse sequence, $\{v_l \,|l = 1...t\}$, of t no. of decreasing potential pulses in sequence. Due to the excitation of different working electrodes it generates a current response vector, $\left\{\left(x_j\right)^{\mathrm{k}} \;|j = 1,2,....,p \;\&|\mathrm{k}=1,2,....\mathrm{K}\right\}$ of a sample for a single selected working electrode, where, K is no. of electrodes; p is the no. of data points generated by each electrode.

The final response vector, $X^i_{1\times M}$, for i^{th} sample from all working electrodes is a vector obtained by appending the response vectors generated from each working electrode as:

$$X^i_{1\times M} = x^k_{1\times pK} = [x^1_{ip}, x^2_{ip}, ...x^K_{ip}], \tag{5}$$

where $M = pK$. Let us assume that there are N samples under investigation then the complete data set matrix is considered as a $N \times M$ matrix and is denoted as $\mathbf{z}$ matrix where, each data point $z_i,[i = 1,....,N]$, is a vector of M dimension.

$$Z = [X^1, X^2,.....X^N]^T \tag{6}$$

or

$$Z = \begin{bmatrix} z_{11}z_{12}...z_{1M} \\ z_{21}z_{22}...z_{2M} \\ . \\ . \\ z_{N1}z_{N2}...z_{NM} \end{bmatrix} \tag{7}$$

It is obvious that each and every data point recorded during experiments may not contain the meaningful information. The collected data may contain redundant information as well as noise too therefore careful selection of data points is necessary. An example of the recoded data using the e-tongue system for taste samples are illustrated in the Fig.4. It can be observed from the fig. 4 that there are redundant data points. The change of response signal due to variation in samples properties can be easily visualized from the response curves. It is propose to segment the final current response vector $Z_{i\times M}$ corresponding to the each pulse excitation signals $\{v_l \,|l = 1...t\}$ into t segments say $\mathbf{Z}^l = [\mathbf{Z^1}_{N\times n}, \mathbf{Z}^2{}_{N\times n},.....\mathbf{Z}^t{}_{N\times n}]$ segments where, n, the no. of data points falling in a particular pulse step signal. These $\mathbf{Z}$ segments are further labeled as S, significant segments of continuous data variables i.e. meaningful segments where response signal variation is high for different samples and

$\Re$, non significant segments where response signal variation is low. The $\Re$ segments are discarded and S segments are retained for further computation. The statistical features of these S segments are extracted for forming final feature vector and used as inputs to the classifier.

The procedure for feature selection and extraction can be summarized as follows:

(1) Select a response vector Z^i from total response data matrix.

(2) Segment the response vector into $\mathbf{Z}^l = [\mathbf{Z}^1{}_{N\times n}, \mathbf{Z}^2{}_{N\times n}, ...\mathbf{Z}^t{}_{N\times n}]$ segments corresponding to each pulse excitation signals.

(3) Now, label each segment as significant segments, $\mathrm{S}^u = [\mathrm{S}^1_{N\times n}, \mathrm{S}^1_{N\times n}, ..., \mathrm{S}^r_{N\times n}]$ & non significant segments, $\Re^m = [\Re^1_{N\times n}, \Re^1_{N\times n}, ...\Re^q_{N\times n}]$ where, $t = r + q$, based on their response variation due to change in sample properties.

(4) Extract the statistical features of each S prominent segment individually and discard $\Re$ segments.

(5) Form a feature matrix, F as inputs for further processing

(6) Go to (1) until $i = N$ or all response vectors are considered.

The final feature vector of a response signal can be written as:

$$\begin{aligned}\mathrm{F} = \{&[f_1(\mathrm{S}^1), f_2(\mathrm{S}^1), ...f_w(\mathrm{S}^1)], [f_1(\mathrm{S}^2), f_2(\mathrm{S}^2), ...f_w(\mathrm{S}^2)],\\ &............, [f_1(\mathrm{S}^r), f_2(\mathrm{S}^r), ...f_w(\mathrm{S}^r)]\}\end{aligned} \tag{8}$$

where, w the no. of statistical parameters selected for computation for all significant segments, S. The final feature vector, $\mathrm{F} = [\mathrm{F}^1, \mathrm{F}^2, ...\mathrm{F}^N]^T$ is a vector of wr dimension i.e. the total size of the final feature matrix, F is $N \times wr$. This will be used as an input matrix for further computation i.e. the classifier etc. The proposed statistical feature extraction technique has been applied to basic taste solutions as shown in Fig. (4) and thereafter on different beverages such juices, soft drinks etc.

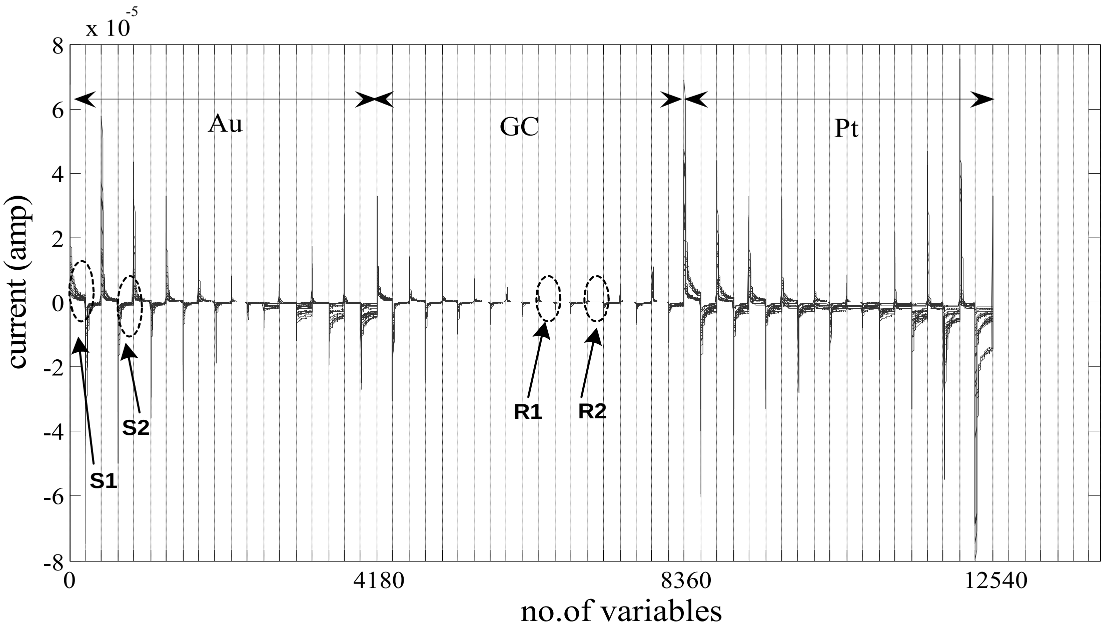
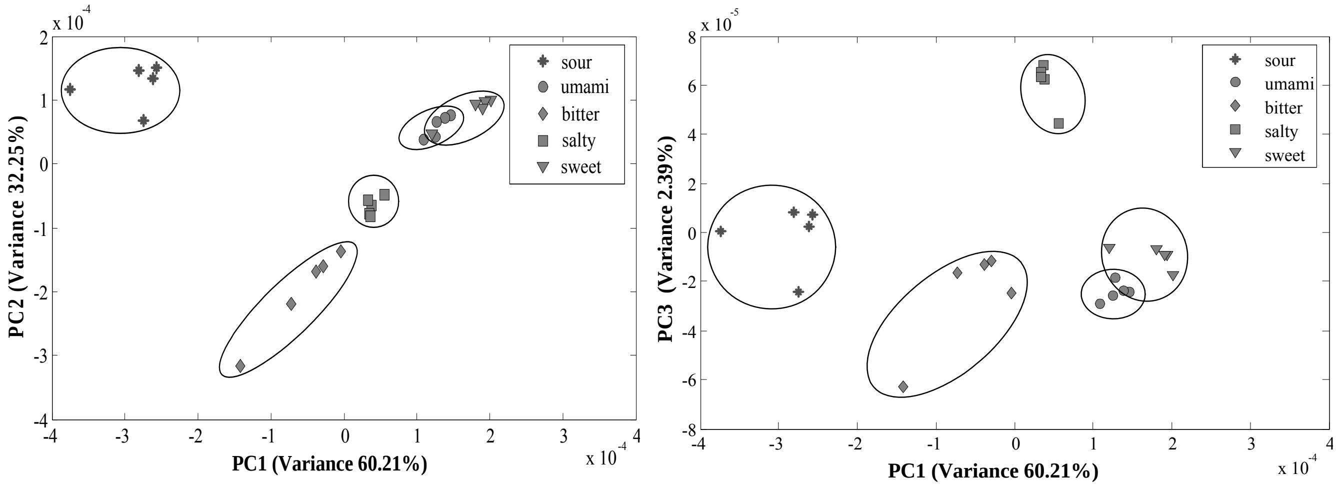


Fig. 4. E-tongue data for taste solutions.

3.3. Discrimination Capability of the Electronic Tongue

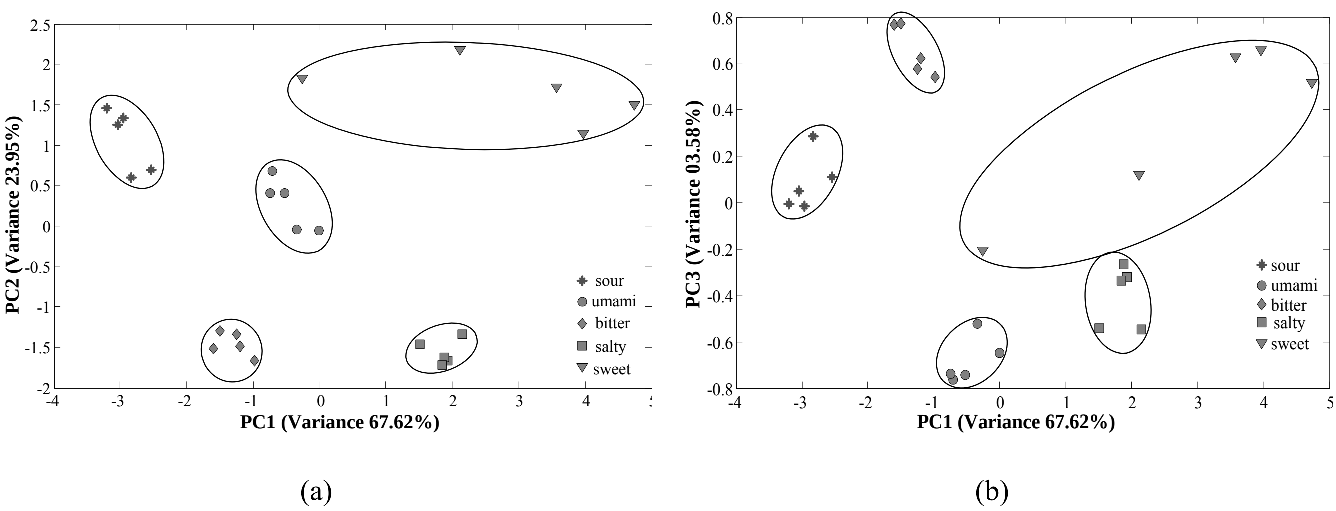
3.3.1. Principal Component Analysis (PCA)

The data obtained from the E-tongue for eight classes of juices, six classes of soft drinks and five classes of basic taste solutions are analyzed using PCA. The PCA method can indicate the data trend in visualizing dimension spaces based on the score plot of the two components. The two-dimensional scatter plots of PCA of the complete data set for the five basic taste solutions are shown in Fig. 5. Fig. 6 and & Fig. 7 shows the PCA plots of the reduced segments data set and extracted statistical features data set respectively. All the five classes are well separated. The explained variance plot is shown in Fig. 8 (a) for raw data set and in Fig. 8(b) for statistical feature as data set. Only first two principal components of statistical features explain the total variance of 96.02 % (PC1 (77.86 %) and PC2 (18.16 %)) whereas the PCA of raw data sets only explained total variance of 92.46 % (PC1 (60.21 %) and PC2 (32.25 %)). The total explained variances of only two principal components show the power of the discrimination capability of the proposed feature extraction techniques.



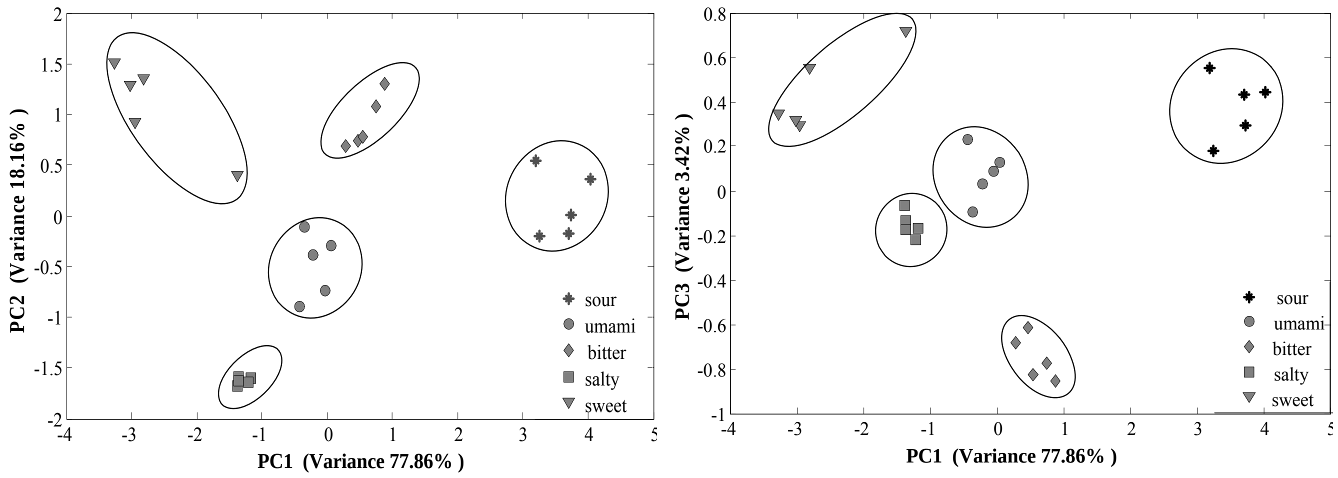
(a) (b)

Fig. 5. Principal component plots for complete data set of taste solutions.



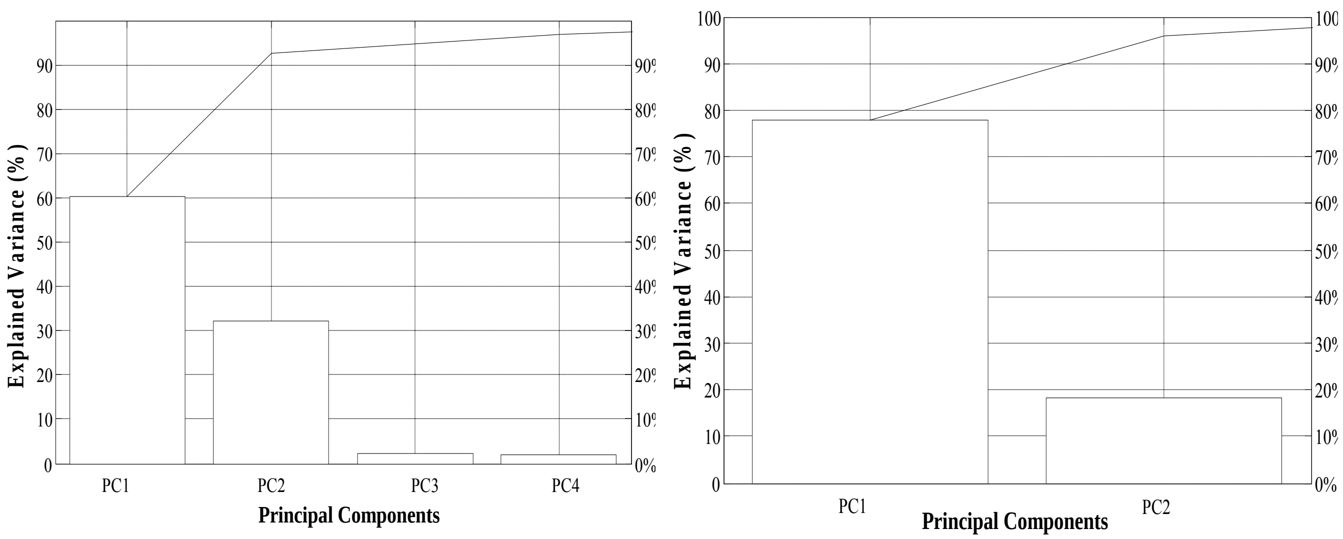
(a) (b)

Fig. 6. Principal component plots for reduced segment data set of taste solutions.



(a) (b)

Fig. 7. Principal component plots for features as input variables of taste solutions.

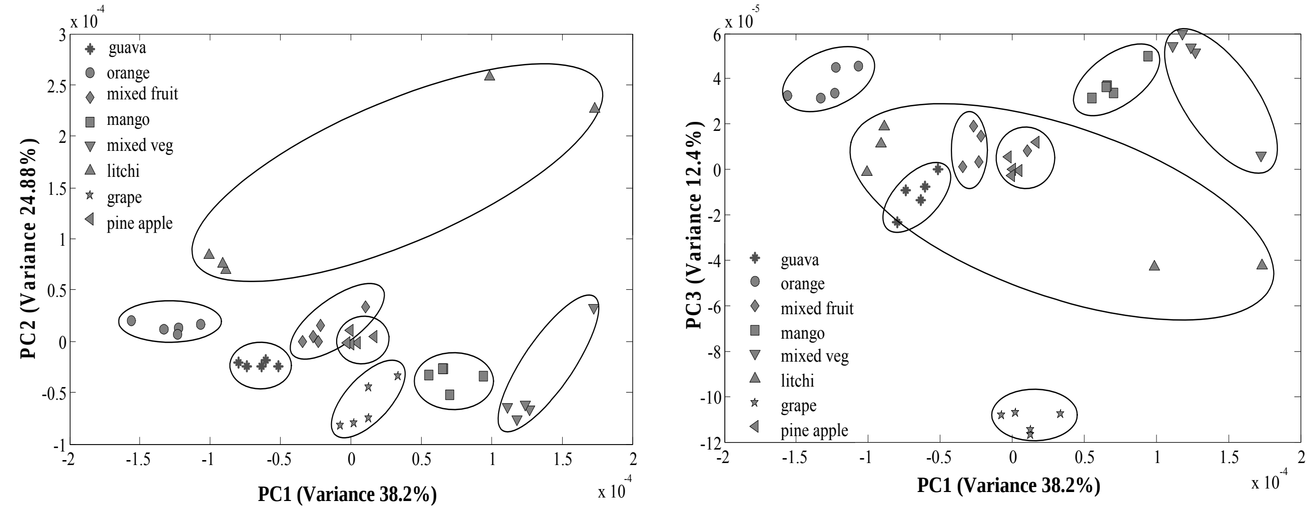


(a) (b)

Fig. 8. Explained variance plot of (a) raw data (b) statistical features of taste solutions.

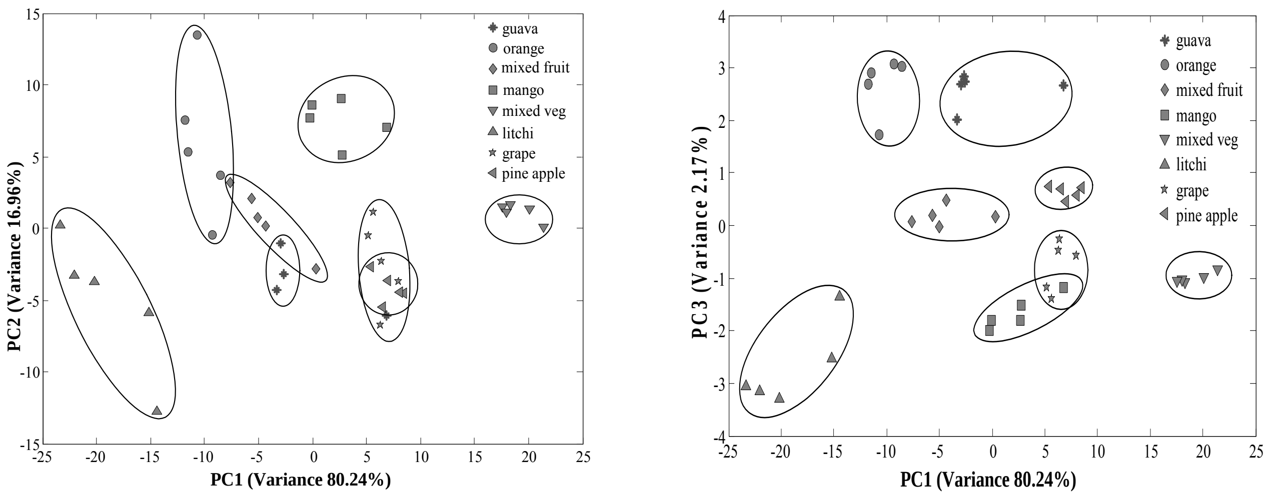
A similar principle component analysis was done for different types of juices and soft drinks. The PCA plots of raw data sets and extracted statistical feature data sets for eight juices classes are shown in Fig. 9 and Fig. 10 respectively. The explained variance plots for these data sets are shown in Fig. 11. Similarly, Fig. 12 and Fig. 13 shows the PCA plots of raw data sets and extracted statistical feature data sets for six classes of soft drinks respectively.

In Fig. 14, the explained variance plots of raw data sets and feature data sets are illustrated. In case of juices and soft drinks samples, the only first two principal components of the proposed feature extraction techniques explain the total variance of 97.10 % and 85.02 % (for juices PC1(80.24 %) and PC2 (16.96 %) and for soft drinks PC1(50.19 %) and PC2 (34.83 %).



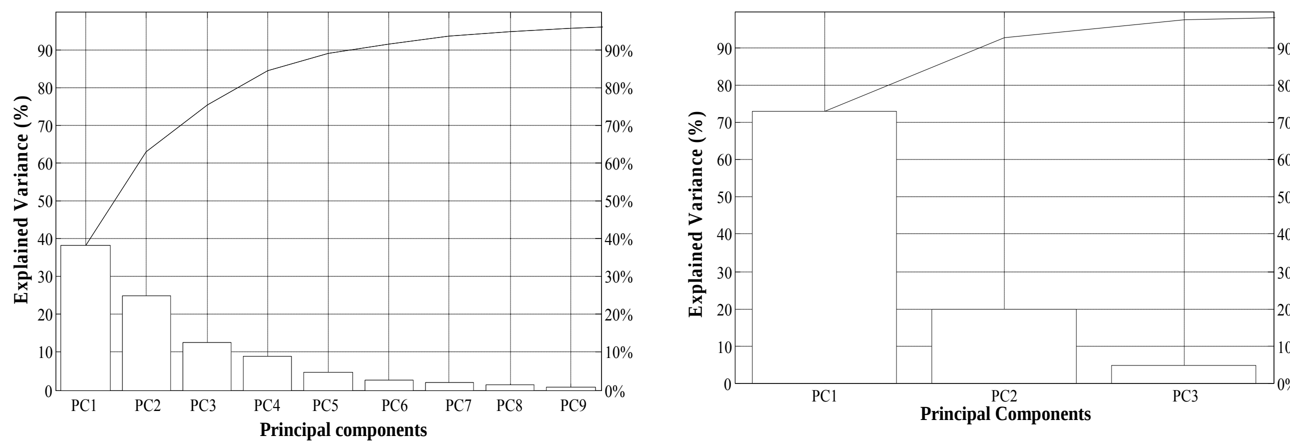
(a) (b)

Fig. 9. Principal component plots for complete data set of juices.



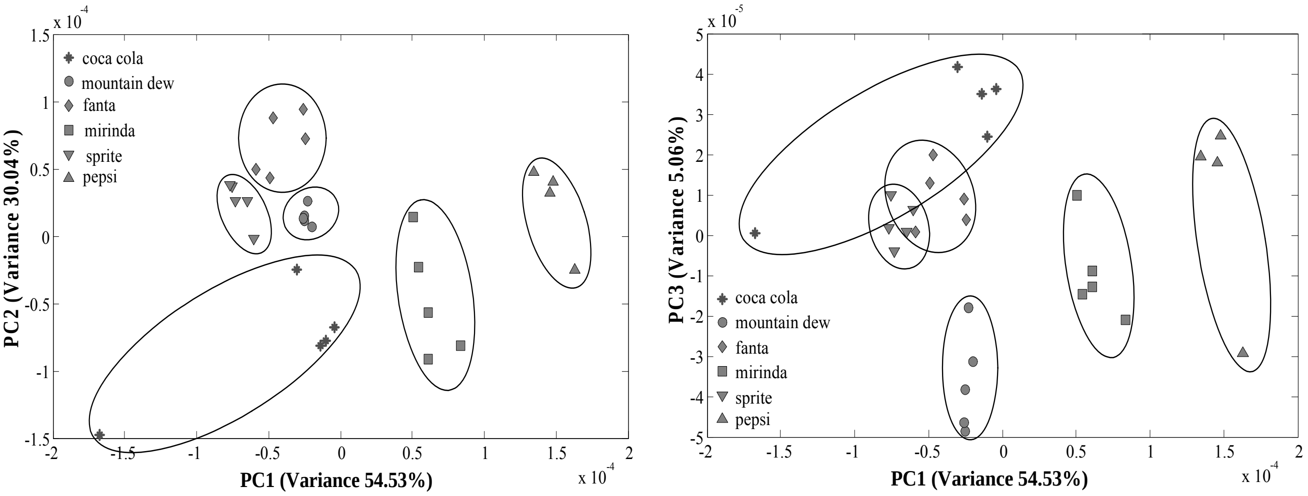
(a) (b)

Fig. 10. Principal component plots for extracted feature data set of juices.



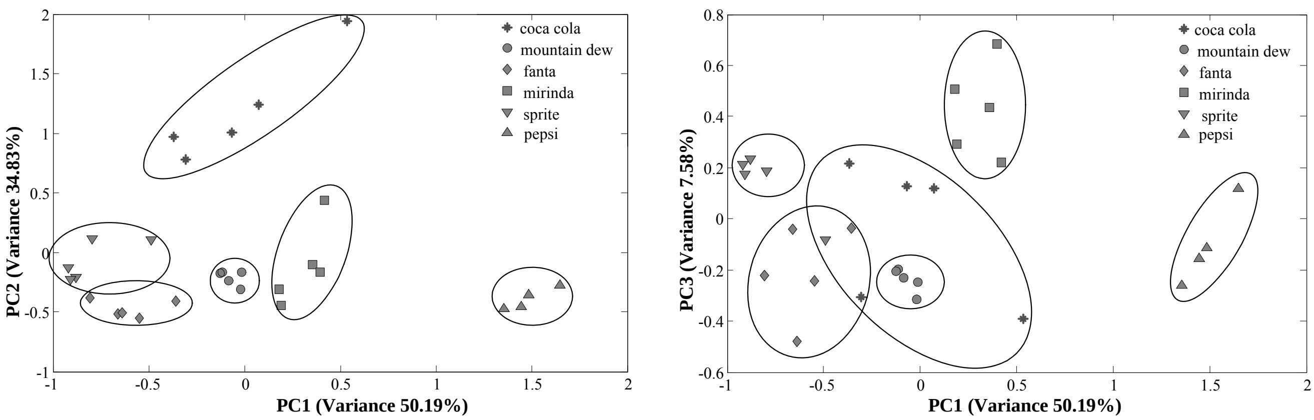
(a) (b)

Fig. 11. Explained variance plot of (a) raw data (b) statistical features of juices.



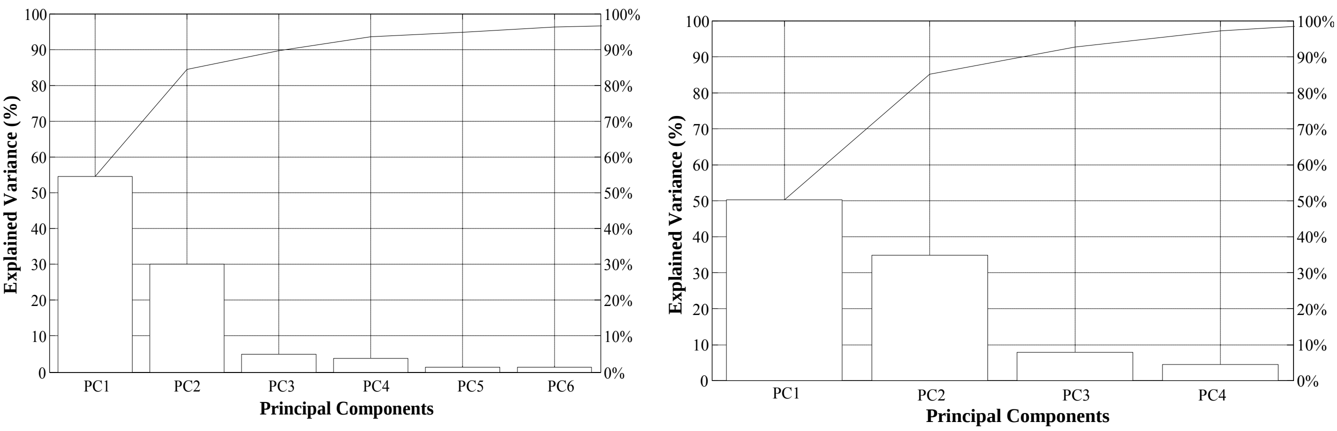
(a) (b)

Fig. 12. Principal component plots for complete data set of soft drinks



(a) (b)

Fig. 13. Principal component plots for extracted feature data set of soft drinks.



(a) (b)

Fig. 14. Explained variance plot of (a) raw data (b) statistical features of soft drinks.

3.4. Classification of Samples

In this study, the classification of different juices, soft drinks and basic taste solutions were realized by using PCA-PNNs and statistical features with PNNs.

3.4.1. Classification of Samples by PCA-PNNs

In this study, the PNNs classification model was applied using the principal component vectors extracted by PCA. PNN classifier is a three-layer, feed-forward, one-pass, learning network that uses sums of Gaussian distributions to estimate the class probability density functions as learned from training vector sets. These functions, in the recall mode, are used to estimate the likelihood of an input feature vector being part of a learned category, or class. The learned patterns can also be combined, or weighted, with a priori probability, also called the relative frequency, of each category to determine the most likely class for a given input vector. Before the input vectors enter the network they are normalized. In this paper, the PNN network contains an input layer which has as many neurons as the dimensions of the extracted features vectors by PCA. It has a pattern layer, which organizes the training set such that each input vector is represented by an individual processing neuron. And finally, the output layer has as many processing neurons as there are classes to be recognized. In order to optimize the PNN model, PCA-PNN architectures with different numbers of inputs (PCs) were examined (1PC to 10 PCs). Finally 3PCs for all types of samples were selected as the inputs to the PNN model. PNN analysis shows an overall 100 % classification success for the training sets for all the samples and 100 % success for the testing sets of juices, soft drinks and 100 % success for basic taste solutions as shown in Table 1.

3.4.2. Classification of Samples by Statistical Features-PNNs

In this study, the PNNs classification model was applied using the extracted statistical features. In order to optimize the PNN model, statistical features-PNN architectures with different numbers of inputs (features) were examined (3 features to 7 features). Finally 7 features for taste and soft drinks samples and 5 features for juice samples were selected as the inputs to the PNN model. PNN analysis shows an overall 100 % classification success for the training sets and testing sets for all the samples as shown in Table 2.

Table 1. Results of PCA-PNN model.

Sample	No. of Classes	No. of training samples	Training accuracy (%)	No. of Test samples	Testing accuracy (%)
Juices	8	24	95.83	40	92.50
Soft drinks	6	17	76.47	30	73.33
Basic taste	5	15	93.33	25	96.00

Table 2. Results of Statistical features-PNN model.

Sample	No. of Classes	No. of training samples	Training accuracy (%)	No. of Test samples	Testing accuracy (%)
Juices	8	24	100	40	100
Soft drinks	6	17	100	30	100
Basic taste	5	15	100	25	100

4. Summary

An 'electronic tongue' based on voltammetry was developed and successfully applied for the recognition of different taste liquids. The possibility of identifying soft drinks and classification of individual fruits and vegetable juice types was achieved by the 'electronic tongue'. The PCA analysis on the data was performed. PCA is used for a linear explorative technique and the dimensionality of the datasets is reduced largely. The results of the PCA clearly show differentiation of the juices and soft drinks samples with different quality grade. However, there are some incorrect classifications among the taste samples of different concentrations. The method needs improvement for similar ones.

An alternative approach, the extraction of statistical features from the voltammetric signal is proposed and used as the input to the PNN which has shown excellent classification results for all the samples under investigation. The use of statistical feature extraction with PNN has reduced data complexity to a greater extent. For comparison, PNN has also been applied to the vectors extracted using the PCA. For PCA-PNN, the classification success is 100% for the training set and 88 % for the testing set. For statistical features-PNN, the classification success is 100% for both the training set and the testing set. The results show that better classification is obtained by statistical features-PNN than by PCA-PNN. The results of statistical features with PNN are encouraging, and it was demonstrated that the E-tongue could be used in the quality classification of beverages, only when the optimum features are extracted. Further results have revealed that E-tongue based on voltammetry has excellent sensitivity to the broad range of beverages with different quality grade. This study demonstrates the feasibility of using E-tongue as an analytical tool for the classification of beverages using statistical features with PNN.

Acknowledgements

The project was supported by Council of scientific and Industrial Research (CSIR), New Delhi through supra institutional project grant on development of smart systems. The authors gratefully acknowledge Dr. Yagnaraman (SECRI, Karaikudi, India) for the useful advice in the electrochemical experiments.

References

[1]. Y. Vlasov, A. Legin, A. Rudnitskya, C. Di Natale and A. D'Amico, Nonspecific sensor arrays (Electronic tongue) for chemical analysis of liquids (IUPAC technical report), *Pure Appl. Chem.*, Vol. 77, No. 11, 2005, pp. 1965-1983.

[2]. S. Iiyama, S. Ezaki, K. Toko, T. Matsuno, K. Yamafuji, Study of astringency and pungency with multichannel taste sensor made of lipid membranes, *Sensors and Actuators, B, Chem*., 24, 1995, pp. 75–79.

[3]. Legin, Y. G. Vlasov, A. M. Rudnitskaya, E. A. Bychkov, Cross-sensitivity of chalcogenide glass sensors in solutions of heavy metal ions, *Sensors and Actuators, B, Chem*., 34, 1996, pp. 456–461.

[4]. Di Natale, C., Davide, F., Brunink, J. A. J. et al., Multicomponent analysis of heavy metal cations and inorganic anions in liquids by a non-selective chalcogenide glass sensor array, *Sensors and Actuators, B, Chem.*, 34, 1996, pp. 539– 542.

[5]. F. Winquist, P. Wide, et al, An electronic tongue based on voltammetry, *Anal. Chim. Acta*, 357, 1997, pp. 21–31.

[6]. A. Riul Jr., R. R. Malmegrim, F. J. Fonseca, L. H. C. Mattoso, An artificial taste sensor based on conducting polymers, *Biosens. Bioelectron.,* 18, 2003, pp. 1365–1369.

[7]. Montserrat Cortina-Puig, et. al., EIS multianalyte sensing with an automated SIA system—An electronic tongue employing the impedimetric signal, *Talanta*, 72, 2007, pp. 2 774-779.

[8]. Pioggia G., et al., A composite sensor array impedentiometric electronic tongue: Part I. Characterization, *Biosensors and Bioelectronics*, Vol. 22, 11, 2007, pp. 2618-2623.

[9]. Winquist, F., et al., Monitoring of freshness of milk by an electronic tongue on the basis of voltammetry. *Measurement Science and Technology*, 9, 1998, pp. 1937–1946.
[10].F. Winquist, I. Lundström, P. Wide, The combination of an electronic tongue and an electronic nose, *Sensors and Actuators B, Chem*., 58, 1999, pp. 512–517.
[11].F. Winquist, S. Holmin, C. Krantz-Rülcker, P. Wide and I. Lundström, A hybrid electronic tongue, *Anal. Chim. Acta,* 406, 2000, pp. 147–157.
[12].Krantz-Ru¨lcker, C., Stenberg, M., et al, Electronic tongues for environmental monitoring based on sensor arrays and pattern recognition: a review, *Anal. Chim. Acta*., 426, 2001, pp. 217–226.
[13].P. Ivarsson, S. Holmin, et al, Discrimination of tea by means of a voltammetric electronic tongue and different applied waveforms, *Sensors and Actuators, B, Chem*. 76, 2001, pp. 449–454.
[14].C. Söderström, F. Winquist and C. Krantz-Rülcker, Recognition of six microbial species with an electronic tongue, *Sensors and Actuators, B, Chem*. 89, 2003, pp. 248–255.
[15].F. Winquist, R. Bjorklund, et al, An electronic tongue in the dairy industry, *Sensors and Actuators, B, Chem*., 111/112, 2005, pp. 299–304.
[16]Tian Shi-Yi, Deng Shao-Ping and Chen Zhong-Xiu, Multifrequency large amplitude pulse voltammetry: a novel electrochemical method for electronic tongue, *Sensors and Actuators, B, Chem.*, 123, 2006, pp. 1049-1056.
[17].E. P. Derks, M. L. Beckers, W. J. Melssen and L. M. Buydens, Parallel processing of chemical information in a local area network, Part II, A parallel cross-validation procedure for artificial neural networks, *Comput. Chem.,* 20, 1995, pp. 439–448.
[18].R. O. Duda, P. E. Hart and D. G. Stork, Pattern Classification, *Wiley–Interscience*, 2001.
[19].C. M. Bishop, Neural Networks for Pattern Recognition, *Oxford University Press*, Oxford, 1999.
[20].B. G. M. Vandeginste, D. L. Massart, L. M. C. Buydens, S. de Jong, P. J. Lewi and J. Smeyers-Verbeke, Handbook of Chemometrics and Qualimetrics: Part B, *Elsevier*, 1998, pp. 238-239.
[21].Despagne, F. and Massart, D. L., Neural networks in multivariate calibration, *Analyst*, 123, 1998, pp. 157R–178R.
[22].Simons, J., Bos, M., and Van der Linden, W. E., Data processing for amperometric signals, *Analyst*., 120, 1995, pp. 1009–1012.
[23].Borggaard, C. and Thodberg, H. H., Optimal minimal neural interpretation of spectra, *Anal. Chem*., 64, 1992, pp. 545–551.
[24].Holmin, S., Spangeus, et al, Compression of electronic tongue data based on voltammetry—a comparative study, *Sensors and Actuators, B, Chem*., 76, 2001, pp. 455–464.
[25].Artursson, T. and Holmberg, M., Wavelet transform of electronic tongue data, *Sensors and Actuators, B, Chem*., 87, 2002, pp. 379–391.
[26].Artursson, T., Spangeus, P., and Holmberg, M., Variable reduction on electronic tongue data, *Anal. Chim. Acta,* 452, 2002, pp. 255–264.
[27].Moreno-Barón, L., et al, Application of the wavelet transform coupled with artificial neural networks in a voltammetric electronic tongue, *Sensors and Actuators, B, Chem.,* 113, 2006, pp. 487-499.
[28].Ensafi, A. A., Khayamian, T., and Atabati, M., Simultaneous voltammetric determination of molybdenum and copper by adsorption cathodic differential pulse stripping method using a principal component artificial neural network, *Talanta*, 57, 2002, pp. 785–793.
[29].Gutes, A., Cespedes, F., Alegret, S., and del Valle, M, Determination of phenolic compounds by a polyphenol oxidase amperometric biosensor and artificial neural network analysis, *Biosens. Bioelectron*., 20, 2005, pp. 1668–1673.
[30].K. Toko, Taste sensor, *Sensors and Actuators, B, Chem*., 64, 2000, pp. 205–215.
[31].Pioggia G., et al., A composite sensor array impedentiometric electronic tongue: Part II. Discrimination of basic tastes, *Biosensors and Bioelectronics*, 22, 11, 2007, pp. 2624-2628.
[32].D. F. Specht**,** Probabilistic Neural Networks, Neural Networks, 3, 1990, pp. 109-118.
[33].Lozano J., et al., Comparative study of sampling systems combined with gas sensors for wine discrimination, *Sensors and Actuators, B, Chem*., 126, 2007, pp. 616–623.

Guide for Contributors

Aims and Scope

Sensors & Transducers Journal (ISSN 1726-5479) provides an advanced forum for the science and technology of physical, chemical sensors and biosensors. It publishes state-of-the-art reviews, regular research and application specific papers, short notes, letters to Editor and sensors related books reviews as well as academic, practical and commercial information of interest to its readership. Because it is an open access, peer review international journal, papers rapidly published in *Sensors & Transducers Journal* will receive a very high publicity. The journal is published monthly as twelve issues per annual by International Frequency Association (IFSA). In additional, some special sponsored and conference issues published annually. *Sensors & Transducers Journal* is indexed and abstracted very quickly by Chemical Abstracts, IndexCopernicus Journals Master List, Open J-Gate, Google Scholar, etc.

Topics Covered

Contributions are invited on all aspects of research, development and application of the science and technology of sensors, transducers and sensor instrumentations. Topics include, but are not restricted to:

- Physical, chemical and biosensors;
- Digital, frequency, period, duty-cycle, time interval, PWM, pulse number output sensors and transducers;
- Theory, principles, effects, design, standardization and modeling;
- Smart sensors and systems;
- Sensor instrumentation;
- Virtual instruments;
- Sensors interfaces, buses and networks;
- Signal processing;
- Frequency (period, duty-cycle)-to-digital converters, ADC;
- Technologies and materials;
- Nanosensors;
- Microsystems;
- Applications.

Submission of papers

Articles should be written in English. Authors are invited to submit by e-mail editor@sensorsportal.com 8-14 pages article (including abstract, illustrations (color or grayscale), photos and references) in both: MS Word (doc) and Acrobat (pdf) formats. Detailed preparation instructions, paper example and template of manuscript are available from the journal's webpage: http://www.sensorsportal.com/HTML/DIGEST/Submition.htm Authors must follow the instructions strictly when submitting their manuscripts.

Advertising Information