Intelligent Systems with Applications 16 (2022) 200143

Contents lists available at ScienceDirect

Intelligent Systems with Applications

journal homepage: www.journals.elsevier.com/intelligent-systems-with-applications

Yogurt classification using an electronic tongue system and machine learning techniques

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ARTICLE INFO

Keywords:
Yogurt classification
Multistep amperometry
Electronic tongue
Dimensionality reduction
t –SNE
k –NN

ABSTRACT

Electronic tongue sensor arrays allow the analysis of liquid substances and provide information for classification tasks to artificially emulate a taste recognition system. These kinds of devices are needed for the alimentary industry because they ensure their products' quality; however, they are still in the development phase because of the components required for their robustness. This paper presents an electronic tongue system for yogurt classification to contribute to developing automatic systems for this industry. The developed system uses a sensor array with Screen-Printed Electrode sensors, a potentiostat, and a multiplexer to handle eight different sensors. A pattern recognition methodology for the processing of multi-step amperometry signals is defined. It comprises the following stages: First, a data unfolding process to build a two-dimensional matrix with the information from the sensors is applied. Next, raw data is normalized using the mean-centered group scaling method. Then, a dimensionality reduction stage is applied. Two methods are evaluated, the t-distributed stochastic neighbor embedding (t-SNE) and Principal Component Analysis (PCA). Subsequently, a supervised machine learning classification algorithm is used. Five methods were evaluated to determine the best classifier: LDA, classification trees(C4.5), naive Bayes, k-NN, and SVM. A dataset of 151 samples of 8 different yogurts is used for the methodology validation. This validation is executed through a Leave One Out Cross Validation (LOOCV) method. Final classification accuracy of 100% was obtained When PCA and LDA or t-SNE and k-NN were used; however, from the computational point of view, a shorter execution time was evidenced for PCA and LDA, showing the convenience in its use in the methodology.

1. Introduction

Discrimination of different liquid food drinks is an essential task in the food industry Christinelli et al. (2021), since it allows identifying adulteration in food trying to achieve high quality or preserving the flavor in the production process Wei et al. (2018). This process is usually performed by a panel of expert tasters Lanza and Amoruso (2020) or by costly and time-consuming tests performed in the laboratory using high-performance liquid chromatography (HPLC) Cheah and Fang (2020).

In this context, electronic tongues emerge as a portable and inexpensive alternative to performing analysis of liquid substances. According to the IUPAC technical report Vlasov et al. (2005), an electronic tongue is an analytical instrument including an array of non-selective chemical sensors with partial specificity to different solution components and an appropriate pattern recognition instrument, capable of recognizing quantitative and qualitative compositions of simple and complex solutions. Different transductive methods exist to perform the analysis of liquids, and electrochemical sensors have predominated in electronic tongues. Some electrochemical techniques have been used to perform the experiments in the electronic tongue type sensor arrays Ozer and Henry (2021), such as square wave voltammetry Ye et al. (2020), cyclic voltammetry Cetó and Pérez (2020) Głowacz et al. (2021), pulse voltammetry Yang et al. (2021), multifrequency large amplitude pulse voltammetry (MLAPV) Liu et al. (2020), among others.

Some works have used electronic tongues to discriminate against yogurts. For example, a study Li et al. (2019) discriminates against five classes of yogurt using an electronic tongue. The authors employed Linear Discriminant Analysis (LDA) and Principal Component Analysis (PCA) as pattern recognition tools to perform the recognition task. In

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https://doi.org/10.1016/j.iswa.2022.200143
Received 27 June 2022; Received in revised form 12 October 2022; Accepted 17 October 2022
Available online 26 October 2022

both cases, LDA and PCA reached 95.1% of the discrimination index (DI). PCA and the discriminant function analysis (DFA) were used to process electronic tongue signals for the classification of six categories of yogurts Wei et al. (2013). The best yogurt classification results were obtained using PCA and the multifrequency staircase pulse voltammetry (MSPV) waveform. In 2017, PCA and DFA based on the fusion data of multifrequency rectangular pulse voltammetry (MRPV) and MSPV-area data Wei et al. (2017) was used to classify a set of yogurts in the stages of fermentation, post-ripeness, and storage. It was found that data fusion worked better than the sole usage of either the MSPV- or MRPV area data.

An E-tongue system obtained a success rate of 98.7% on data classification of pasteurized milk Carrillo-Gómez et al. (2021). Pulse voltammetric electronic tongues have been used in different food applications, for example, monitoring adulterations in honey Sobrino-Gregorio et al. (2018). Machine learning methods, such as support vector machines (SVM), have been employed to classify electronic nose signals with high accuracy Zhang et al. (2020). In 2021, a computational intelligence approach for black tea discrimination reached average classification accuracy of 91.34% Acharya et al. (2021).

Recently, some machine learning methodologies have been developed to process (MLAPV) signals in classification tasks of liquid substances. In 2020, a machine learning-based method to classify seven different aqueous matrices reached a 96.83% of classification accuracy Leon-Medina et al. (2020). Similarly, another methodology was described in Leon-Medina et al. (2019) for classifying a dataset of 13 different liquid substances, obtaining a 94% of accuracy.

Although there are multiple solutions to tackle the liquid classification problem, it remains open due to the need to improve the results. For this reason, as a contribution, this paper shows the development of an electronic tongue system composed of a sensor array, a data acquisition system, and a pattern recognition unit. First, its parts are described for the electronic tongue developed, and its characteristics and operation are exposed. Subsequently, multi-step amperometry is used as an electrochemical technique in the developed experiments, and its configuration parameters are detailed. Finally, an electronic tongue signal data processing methodology based on machine learning techniques is described. This signal processing methodology compromises several stages, including a dimensionality reduction stage. Two different algorithms were compared for performing the dimensionality reduction: PCA and t-distributed stochastic neighbor embedding (t-SNE). Following a k-nearest neighbors (KNN) algorithm is used as a supervised machine learning classifier. Finally, a leave-one-out cross-validation (LOOCV) is used to find a resulting confusion matrix, and the classification accuracy is calculated as a performance measure.

This paper is organized in the following structure. Section 2 describes the material and methods and provides information about the electronic tongue system with each of its parts. Besides Section 2 describes the methodology for yogurt classification, introducing the signal processing of the acquired signals through a pattern recognition approach. Subsequently, the results and discussion are shown in section 3, including the details of data scaling, data unfolding, data reduction, classification, and leave one out cross-validation(LOOCV). Section 4 presents a discussion of the results and finally, Section 5 outlines the principal conclusions of this work.

2. Materials and methods

2.1. Hardware setup of the electronic tongue system

The electronic tongue system described in this work is composed of an array of Screen Printed Electrode (SPE) Sensors from the BVT Technologies Company. The selected potentiostat is the Palmsens4 offered by the Palmsens company; however, due to the number of sensors and the number of input channels in the potentiostat, it was necessary the use of a MUX8R2 multiplexer equipment also from the Palmsens company. This multiplexer allows handling up to 8 sensors. The data acquisition hardware requires the use of a laptop to apply the pattern recognition stage. Specifically, in this work, this task is performed on an HP ProBook 440 G5 computer with an Intel Core i5 8250U processor and 8GB of RAM. The schematic diagram of the system is presented in Fig. 1 where the components of the electronic tongue system are illustrated.

2.2. Integration of the electronic tongue system with all its components.

The integration of the entire electronic tongue system is described below. Among its parts are: the sensors, couplings, cables, multiplexer, potentiostat, and computer software. First, the sensors are connected to each of their couplings, as shown in Fig. 2. Second, the container for the liquid to be evaluated is defined, and the sensors are arranged in such a way that all of them are simultaneously submerged in the liquid. The influence of the fact that the sensors must remain fixed in the tests is also evaluated, since their movement may alter the measurements. Connection cables and adapters were used for the 8 sensors. Due to the nature of the multiplexer cables, where there are two cables and each cable commands 4 sensors, it was decided a rectangular arrangement of sensors, where 4 and 4 sensors will face each other, as illustrated in Fig. 2.

Each cable must handle four sensors when connecting the MUX8R2 multiplexer cables to the sensor couplings. Due to the space that each cable covers and the assembly of the sensors in the container of the liquid to be evaluated, it was decided to use a rectangular arrangement so that the sensors remain rigid in their position inside the red rectangular container as shown in Fig. 2. The next step in the assembly of the system contemplates the connection between the multiplexer and the potentiostat. Finally, the last connection is made between the potentiostat and the computer by using a USB type C cable. The software that commands the process is the PSTrace 5 from the Palmsens company.

2.3. Screen printed electrode sensors

As explained earlier, sensors of the screen printed electrode (SPE) type from BVT technologies were selected. Each sensor is formed on a corundum ceramic base. The working, reference and auxiliary electrodes are applied to this surface. The working and auxiliary electrodes are made of a variety of materials. At the end of the sensor, a contact field is connected to the active part by silver conductive paths covered by a dielectric protection layer. A biochemically active substance can be immobilized on the working electrode of the sensor to create a biosensor. Since the MUX8R2 multiplexer has the ability to command up to 8 different channels and there are 5 working electrode materials, the remaining 3 channels were completed by repeating some materials. Therefore, the channels were occupied as follows: 3 sensors with the platinum working electrode, 2 sensors with a silver working electrode, and 1 single gold, graphite, and gold-platinum alloy working electrode. The sensor identifier number, with its reference and working electrode material, are described in Table 1.

For working electrodes, W1 = Gold, W2 = Platinum, W3 = Silver, W4 = Graphite and WS = gold-platinum alloy. For the reference electrodes, R1 = silver / silver chloride and R2 = silver covered by AgCl. Fig. 3 shows an example of the SPE sensors, whose terminals are named as follows: the upper terminal corresponds to the reference electrode, the middle terminal for the working electrode and the lower terminal for the auxiliary electrode.

2.4. Experimental setup for collecting a data set of 8 classes of yogurts

Experiments to capture data for the classification of yogurt data were applied by conducting experiments on 8 different yogurts from a local company. These are produced in the municipality of Firabitova, in the department of Boyacá, Colombia. The selection of the company was because the variety of the flavor of yogurts, however, same steps can be applied to different yogurt references from different producers. These

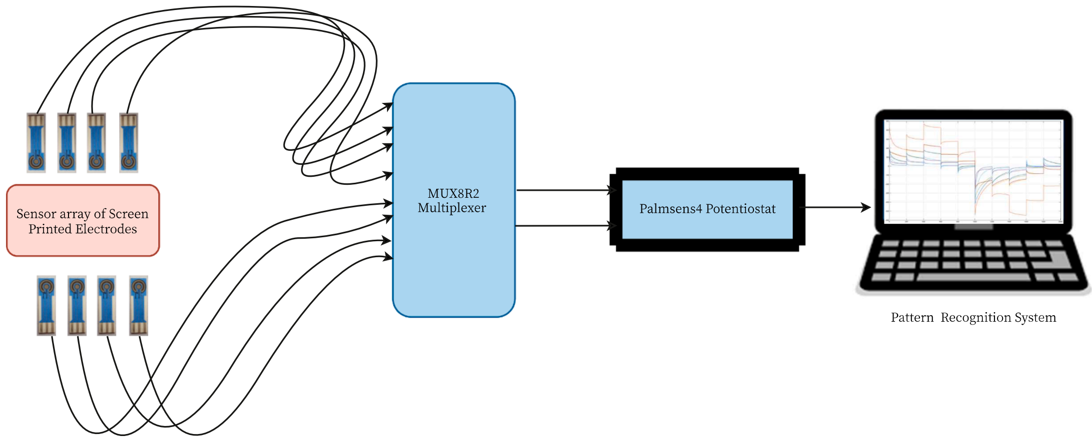

Fig. 1. Schematic diagram of the electronic tongue type system with the SPE sensors, the MUX8R2 multiplexer, the Palmsens4 potentiostat and the computer.

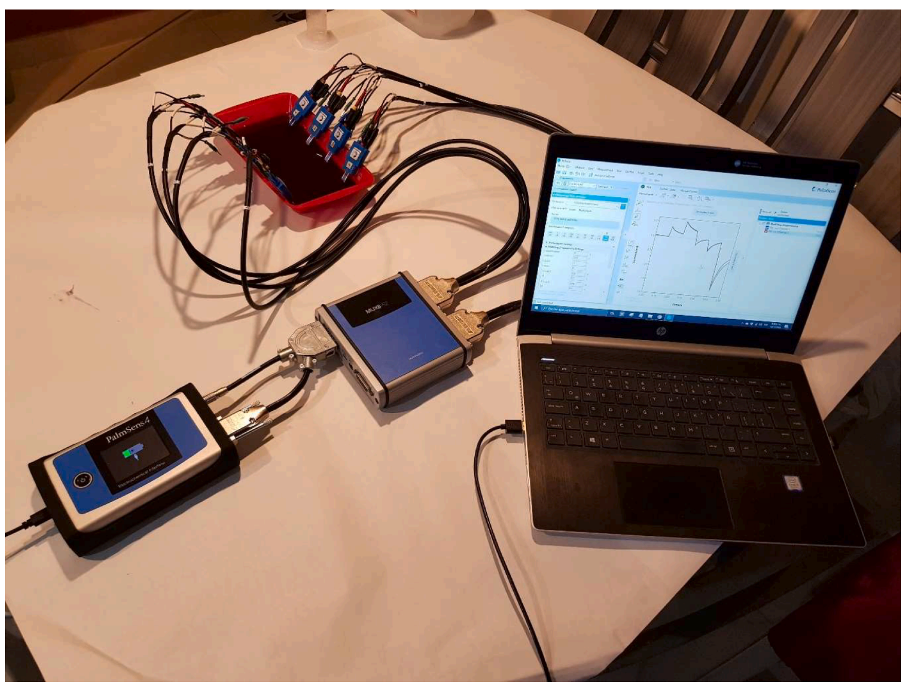

Fig. 2. Detail of the electronic tongue system implemented with all its parts. The computer shows the PSTrace 5 software.

Table 1
Description of the sensors used in the electronic tongue type sensor array for obtaining the yogurt data set.

ID	Referencia	Material of Working Electrode
Sensor1	AC1.W1.R1 DW=2	Gold
Sensor2	AC1.W2.R2 DW=2	Platinum
Sensor3	AC1.W3.R2 DW=2	Silver
Sensor4	AC1.W4.R2 DW=2	Graphite
Sensor5	AC1.W2.R2 DW=2	Platinum
Sensor6	AC1.WS.R2 DW=2	Gold-platinum alloy
Sensor7	AC1.W3.R2 DW=2	Silver
Sensor8	AC1.W2.R2 DW=2	Platinum

are shown in Fig. 4.

For each yogurt, 20 tests were taken except for the strawberry bebigurt yogurt, for which 11 experiments were taken as can be seen in Table 2. Yogurt is a viscous product, so they were diluted in distilled deionized water to create a homogeneous solution.

Fig. 5 a) shows the addition of 40ml of feijoa yogurt in 120ml of distilled deionized water before mixing. It is observed that the eight sensors are submerged in the liquid. Fig. 5b) shows the solution when stirring between yogurt and distilled water.

To carry out the experiments on the 8 different yogurts, a mixture of 50 ml of yogurt with 100 ml of de-ionized distilled water was obtained. The PSTrace 5 software was then configured to perform the multi-step amperometry experiments. For this purpose, the multiplexer configuration shown in Fig. 6a) was used, where the signals from each sensor are acquired consecutively. In addition, the sense connector was connected to the working electrode (Connect Sense to WE) as also illustrated in Fig. 6a). When using the MUX8R2 multiplexer together with the Palmsens 4 potentiostat, the configuration allowed to obtain the signal from a sensor and then the next one until completing the 8 sensors, as shown in the video available online https://youtu.be/KP6l8NmK4KQ.

A signal of 10 different levels was configured as illustrated in Fig. 6b). At each step, a duration interval of 0.1 seconds was set constant, which means a total signal duration of 0.1 *times* 10 = 1 second. On the

Fig. 3. Numbering of the eight different sensors used in the experiments.

Fig. 4. Meeting of the 8 yogurts studied to create the data set for the validation of the methodology developed.

Table 2
Description of the type of yogurt in the data set recorded with the Palmsens 4 potentiostat and the MUX8R2 multiplexer.

ID	Yogurt	sample quantity
1	Feijoa	20
2	Strawberry	20
3	Peach	20
4	Blackberry	20
5	Kumis	20
6	Bebigurt Blackberry	20
7	Bebigurt Strawberry	11
8	Bebigurt Peach	20

other hand, the parameter *t interval* was set equal to 0.01 seconds, as shown in Fig. 6c). This parameter refers to the signal sampling step. In this case, a step has a duration of 0.1 seconds in a sampling step *t interval* = 0.01 seconds; hence there are 10 signal points per step. The number of points in the signal captured by each sensor is equal to 101 points since there are 10 steps and 10 points are taken per step.

Fig. 6 c) illustrates the response of the 8 sensors in an experiment performed on a feijoa yogurt in the PSTrace software. As shown in the *session data* panel, the 8 channels are listed, and a different color is assigned to each one. In this figure, the ordinate shows current values in mA and the abscissa time values in seconds. It is observed that the highest value on the x-axis is 1 second. Regarding the response signals obtained by the sensors, it should be noted that different responses are obtained due to the different materials of the working electrodes.

2.5. Data processing methodology for the classification of yogurts

Several stages comprise the signal processing methodology: a) data acquisition, b) data arrangement and unfolding, c) data normalization, d) dimensionality reduction, e) machine learning classification, and f) leave one out cross-validation. Following, the steps in the methodology are detailed:

1. Carry out the multi-step amperometry experiments and acquire the signals from the electronic tongue type sensor array. These signals are grouped in three dimensions i experiments $\times$ j sensors $\times$ k time instants.
2. Perform an unfolding process of the data according to the type E unfolding described in Westerhuis et al. (1999). In this way, the previous three-dimensional matrix is transformed into a two-dimensional matrix of size $i \times j{\cdot}k$.
3. Use the mean-centered group scaling MCGS Pozo et al. (2018) method which considers the magnitude variations captured by each working electrode of a different material.
4. Reduce the dimensionality of the data. In this work, two-dimensionality reduction methods were used to compare their behavior. These methods were PCA and t-SNE. Specifically, this methodology seeks to reduce the high dimensionality D of the data

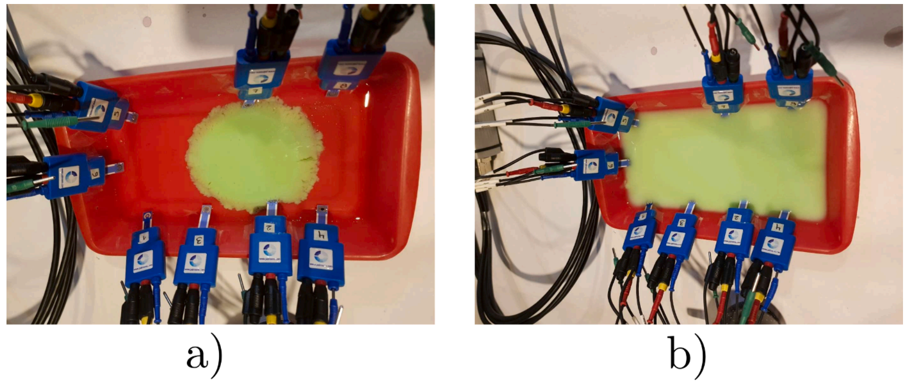

Fig. 5. a) Mixture of deionized distilled water and feijoa yogurt prior to mixing. b) Mixture of distilled deionized water and feijoa yogurt after mixing.

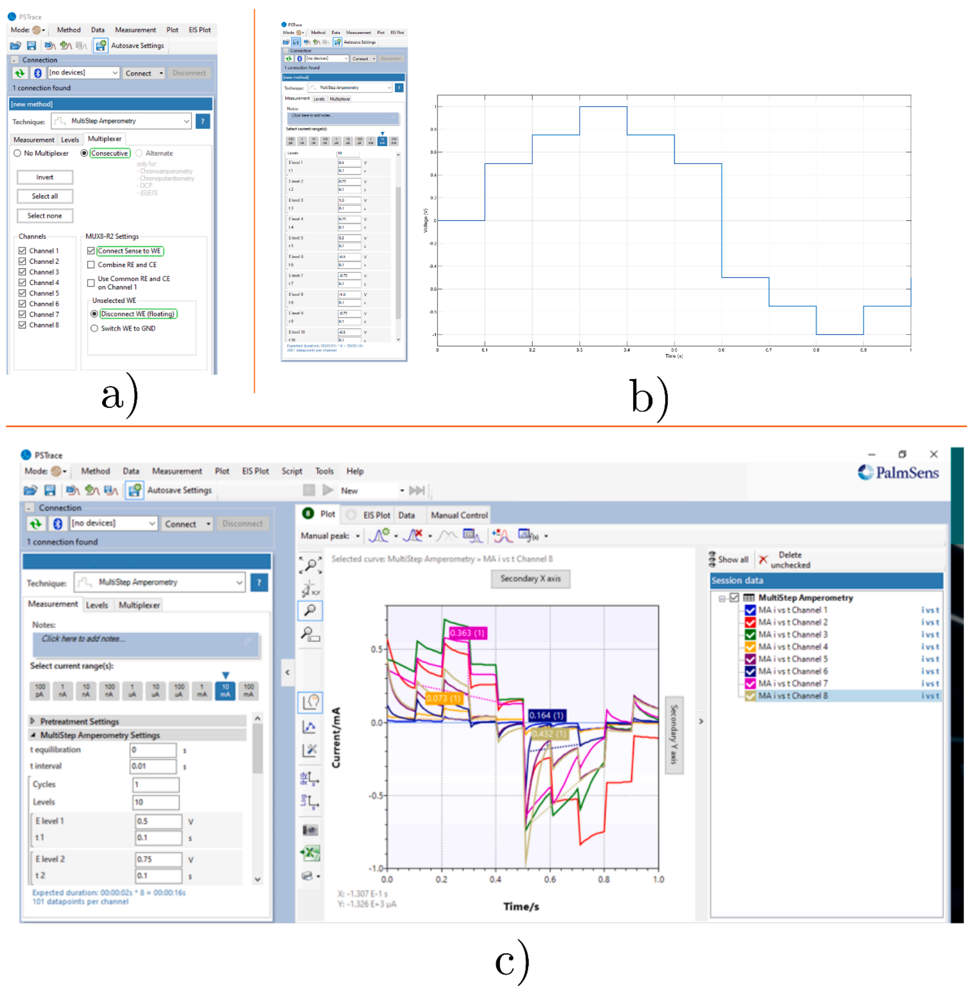

Fig. 6. a) Configuration of the MUX8R2 multiplexer in PSTrace Software for Performed multi-step Amperometry Experiments. b) Signal applied by the Palmsens 4 potentiostat to perform the pulse amperometry process. c) Capture the signals in a pulse amperometry experiment for one yogurt in the PSTrace software.

given by the product $j{\cdot}k = D$ and transform it into a low-dimensional space representation d. In this case $d < D$. As a result, a feature matrix is created with a column size significantly smaller than the original two-dimensional matrix.

5. The reduced feature matrix serves as input to a k-nearest neighbors classifier algorithm and a leave one out cross validation LOOCV is used to reduce the risk of overfitting and thus find the best k-NN classifier model.
6. An important parameter to tuning is the number of principal components in the PCA method and the number of target dimensions in the t-SNE algorithm. Therefore, a study of the behavior of the classification accuracy calculated in the added confusion matrix of the leave-one-out cross-validation process is carried out.

The steps that comprise the data classification methodology are summarized in Fig. 7. Besides, Fig. 8 describes the flowchart as pseudocode.

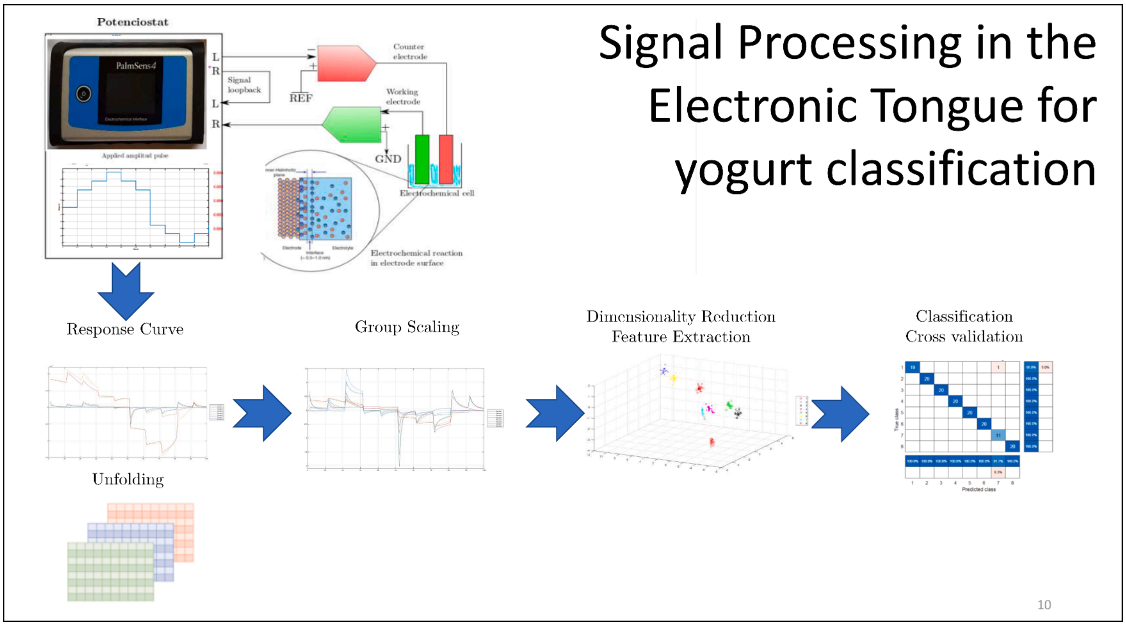

Fig. 7. Signal processing stages of the developed yogurt classification methodology.

The results and discussion section includes more details about the need for each step in the methodology.

3. Results and discussion

Following, a description of each step of the methodology and the results in its use are included.

3.1. Data unfolding

The first step for processing the signals obtained by the electronic tongue is the data unfolding. Originally, the raw data comes from a three-dimensional matrix *I experiments* × *J sensors* × *K measurement points*. To provide a data fusion of the data from the sensors, a data unfolding is performed, to produces a two-dimensional matrix *I experiments* × (*J sensors* ∗ *K measurement points*). This step allows for the analysis of the data as a unique sensor and facilitates the analysis for the next steps.

Since there are J=8 sensors used in the electronic tongue type sensor array, and K=101 data points per signal, thus, there are 8 × 101 = 808 points in the unfolded signal per experiment. The detail of the data unfolding carried out is illustrated in Fig. 9. This figure shows how the signals from each sensor are ordered one after the other for each experiment in the yogurt data set.

According to Table 2, a total of I=151 experiments were carried out in the total sum of the number of yogurt samples and the size of the unfolded matrix *X* is 151 × 808. Fig. 10 shows the unfolded signals of the 8 sensors for the first experiment of feijoa yogurt. This figure evidences the obvious difference between the signals captured by the silver sensors (#3 and #7). The results of scaling the signals are shown in Fig. 11. In contrast, a notable change can be observed, for example, in the magnitudes of the signals from the gold (#1), graphite (#4), and gold-platinum (#6) sensors. In general, after applying the scaling, the magnitude of the signals from the different sensors becomes homogeneous in such a way that none will prevail over the other.

3.2. Data scaling

Fig. 12 depicts the signals captured by each of the 8 sensors for a feijoa yogurt experiment. It can be observed that the platinum sensors 2, 5, and 8 obtain similar signals. Furthermore, it is evident that there are differences between the magnitudes of the signals obtained by each sensor due to the different materials from which they are made. Therefore, signal scaling is used based on the Mean Centered Group Scaling (MCGS) Anaya et al. (2017) method. In the MCGS method, the variables are divided into a predefined number of blocks of equal size, in this case, the blocks are the number of sensors *J*. Standard deviations of each variable in a block are calculated, and the average of these standard deviations is used to scale all columns in the block Leon-Medina et al. (2019). This is done for each sensor *J*.

The results after scaling the signals are illustrated in Fig. 13, evidencing the change that leads to a similar scale in all the signals and to no particular sensor that prevails among the others. It is important to highlight the numerical change in the ordinate axis of Figs. 12 and 13. In Fig. 12, the silver sensors (3 and 7) register quite high current values with respect to the other sensors, reaching values on the ordinate axis of $1 \times 10^4 \mu A$. In contrast, the ordinate values in Fig. 13 are in a range from -2 to 1.5, thus evidencing the effect of applying the MCGS scaling method. This step allows normalizing all the data from the different sensors to be compared in the same manner in the sensor data fusion analysis.

3.3. Dimensionality reduction using principal component analysis

The next step in the yogurt classification methodology is the reduction of the dimensionality of the data. This step is a need because of the multivariate nature of the data. The aim of this step is the reduction of the size of the data to work with the most relevant information captured by the sensors. For this purpose, the PCA Tibaduiza et al. (2013) algorithm was used, which allows the feature extraction process to be carried out. The results of the first 3 principal components after applying the PCA algorithm to the yogurt data set are evidenced in the scatter diagram of Fig. 14. The data for the different yogurts are grouped in such a way that each class differs from the others. There is no evidence of data mixing between classes in the representations of the scatter diagrams.

The PCA yields the fraction of variation in the data for each of the resulting 150 principal components. The accumulated variation of the first 22 principal components and their behavior as a fraction of accumulated variation is illustrated in Fig. 15. These first 22 principal components represent an accumulated variation of 99.96% which is a

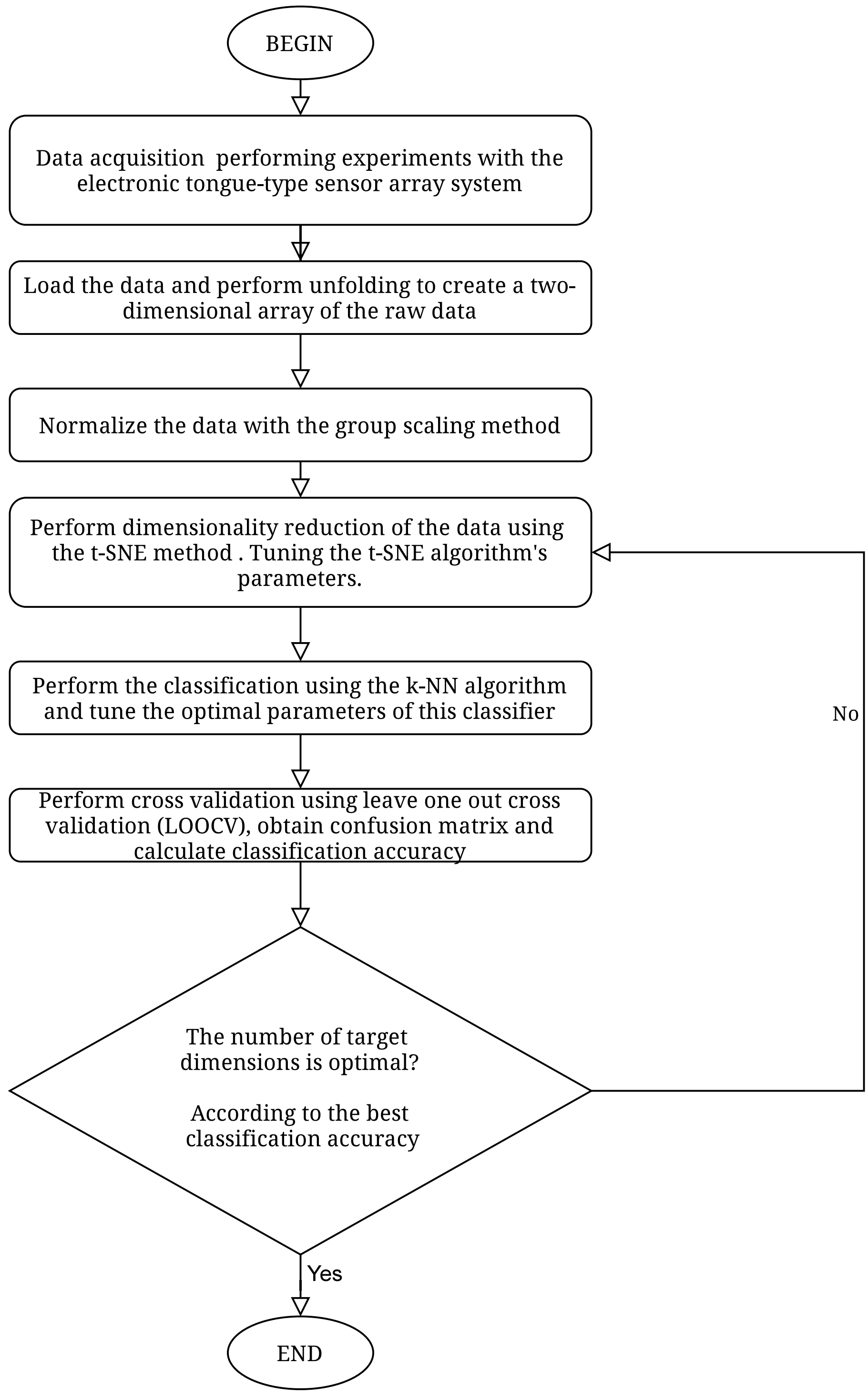

Fig. 8. Flowchart of the yogurt classification methodology.

relevant value and indicate that most of the variation in the data can be represented by these components.

3.4. k-NN Classification and LOOCV cross validation

The next stage in the data processing methodology refers to the use of a supervised machine learning classifier algorithm. Due to the small number of experimental samples contained in the dataset with a total of 151 samples. It is decided to use the algorithm *k*-NN Vitola et al. (2017) as classifier. This algorithm is also used due to the behavior exhibited by the data of each class in the representation in the low-dimensional space where each class is properly grouped and each class is separated from each other, so the use of the nearest neighbors indicator leads to proper classification.

To find a final classification accuracy and also due to the small number of samples in the dataset, the leave one out cross-validation (LOOCV) technique was selected.

The parameter *k* selected in the *k*-NN algorithm was tuned performing a variation from 1 to 15. As is shown in Fig. 16, there is a tendency to decrease the classification accuracy as the parameter k

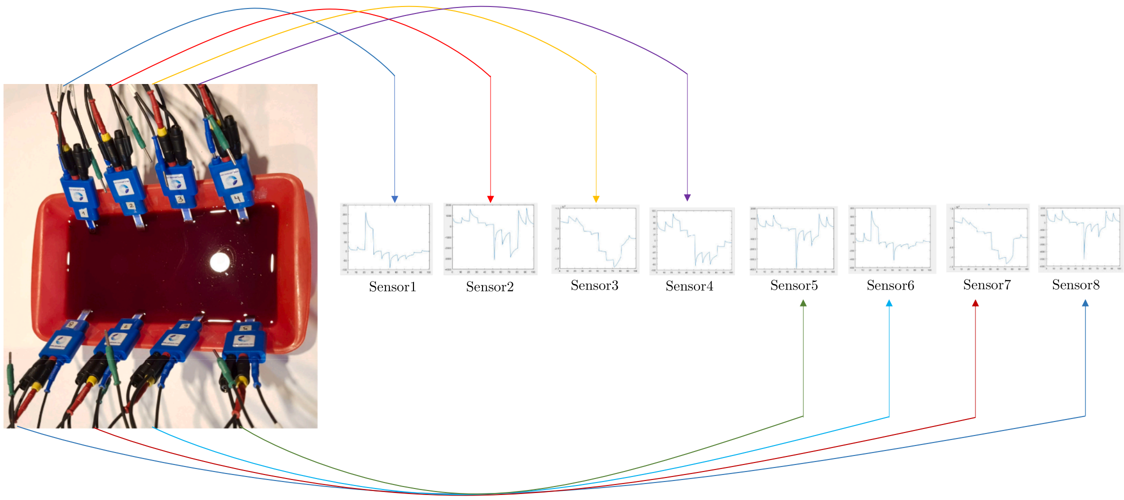

Fig. 9. Process of unfolding the signals obtained by each sensor to form the two-dimensional array *X*.

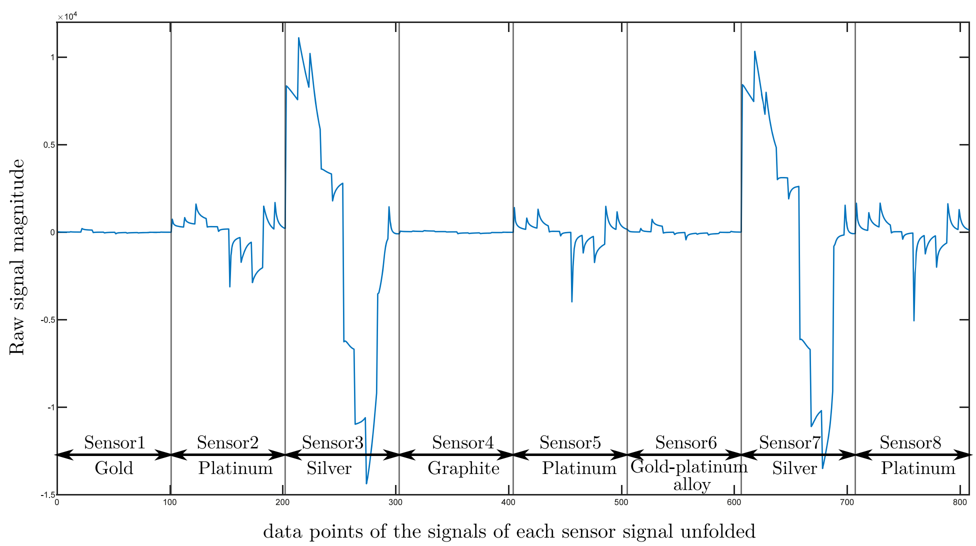

Fig. 10. Unfolded raw response signal of the 8 sensors for experiment #1 of feijoa yogurt.

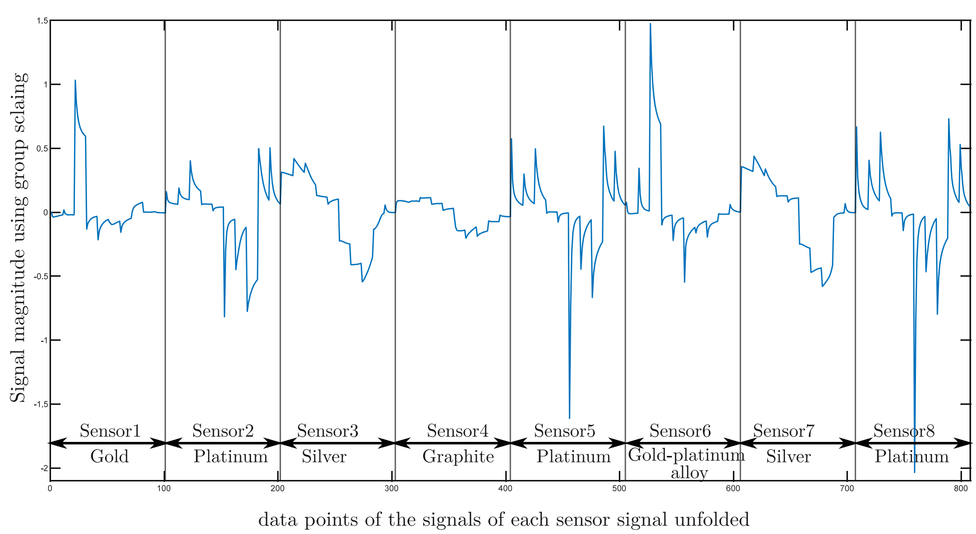

Fig. 11. Unfolded response signal of the 8 sensors after applying group scaling for experiment #1 of feijoa yogurt.

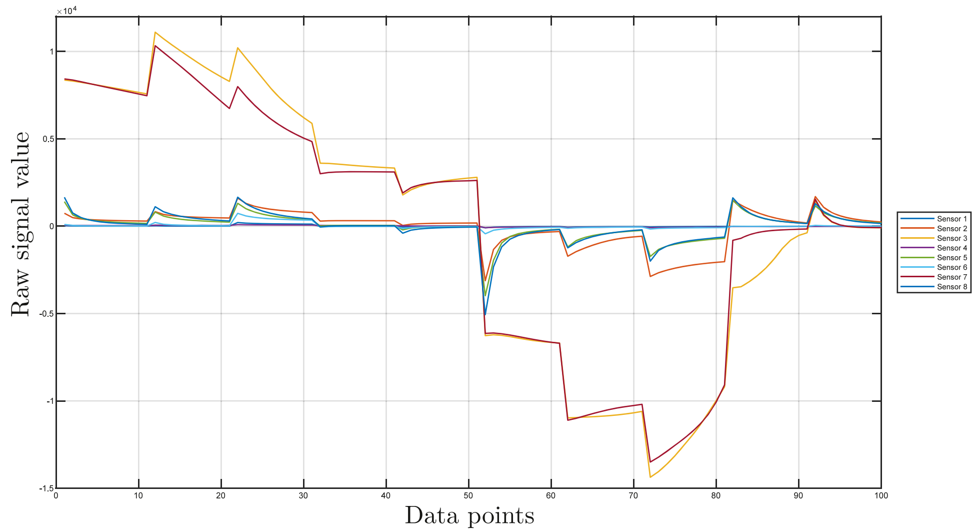

Fig. 12. Raw response signals from the 8 sensors for experiment #1 of feijoa yogurt.

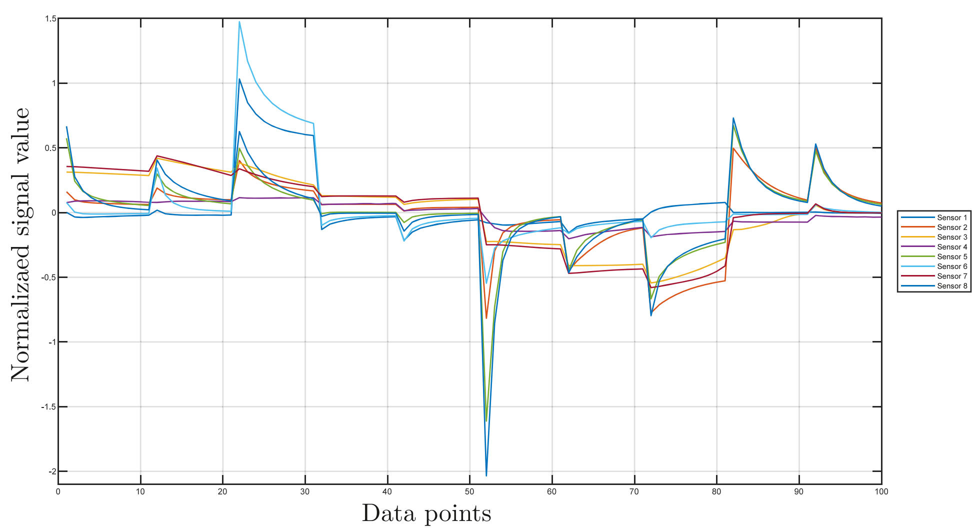

Fig. 13. Normalized response signals of the 8 sensors after applying group scaling for experiment #1 of feijoa yogurt.

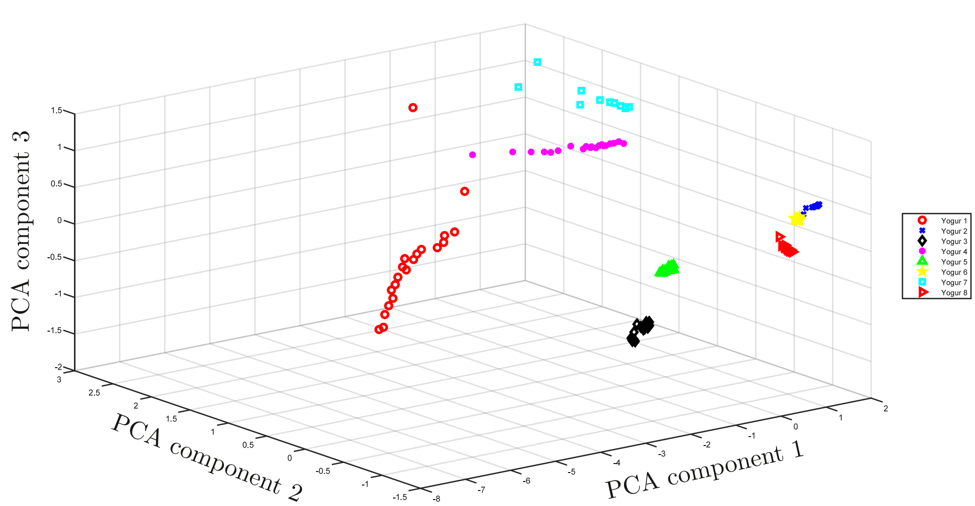

Fig. 14. Three-dimensional scatter plot for the first three principal components obtained after applying PCA to the yogurt data set.

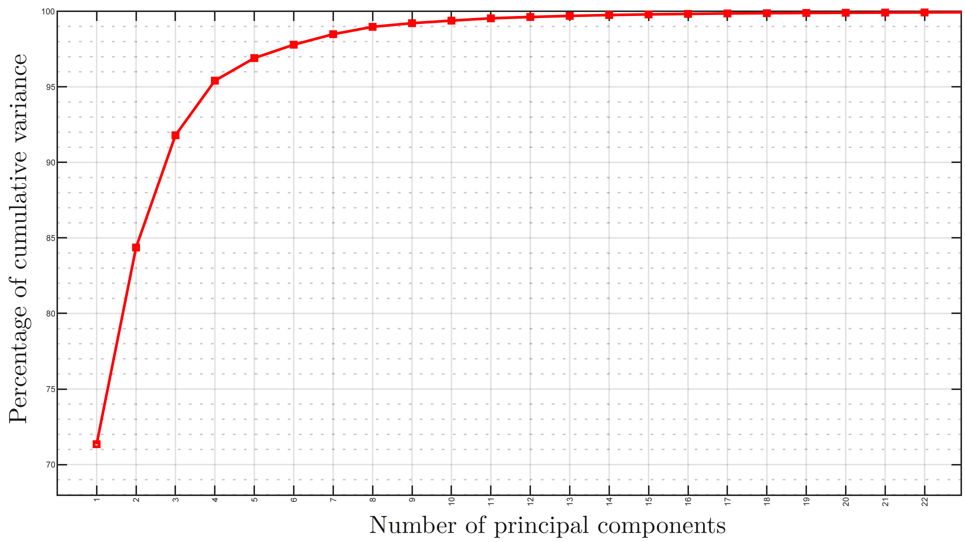

Fig. 15. Cumulative variation of the first 22 principal components.

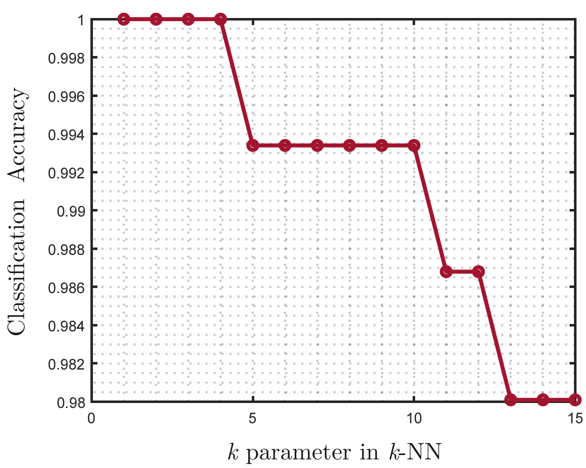

Fig. 16. Classification accuracy behavior when varying the number of k neighbors parameter of the k-NN classifier algorithm.

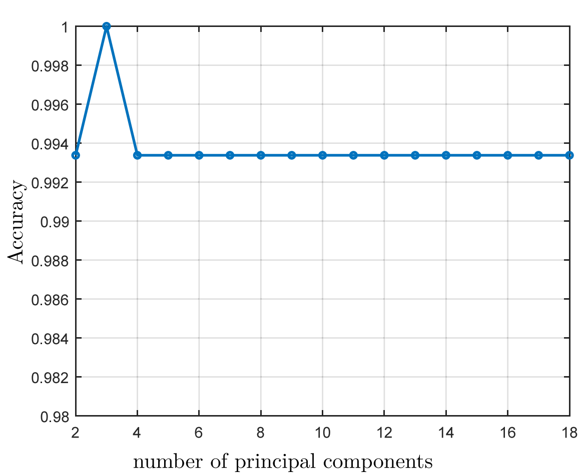

Fig. 17. Behavior of the classification accuracy when varying the number of components at the input of the classifier algorithm k-NN.

increases. Thus, the k parameter =1 was selected as the best to perform the experiments.

To define the number of principal components required for the feature matrix at the input of the k-NN classifier, a study was carried out changing the number of components vs. the classification accuracy obtained by the k-NN algorithm. As observed in Fig. 17, the accuracy behavior tends to remain constant at a value of 99.33%. Only when the first 3 principal components were selected, a classification of 100% of the yogurts was achieved.

Fig. 18 shows the results of the confusion matrix for the accuracy of 99.33%. In this case, class 1 has a single classification error. This means that from the total of 151 samples, 150 were properly classified.

3.5. Dimensionality reduction using t-SNE algorithm

As an alternative method for dimmensionality reduction, *t*-SNE Van der Maaten and Hinton (2008) algorithm was used to perform the feature extraction process. The parameter to configure in the *t* -SNE method was the perplexity, which was set at 38.

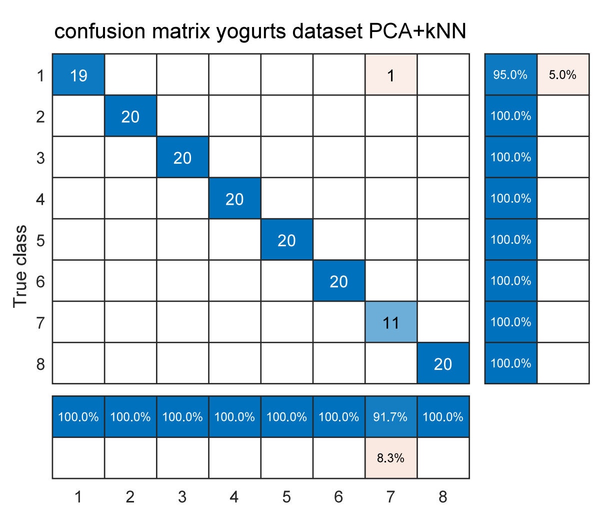

Fig. 18. Confusion matrix resulting from leave one out cross validation after applying the PCA + k-NN algorithms to the yogurt data set. Accuracy value = 0.9933 obtained by taking into account the first two principal components at the input of the classifier algorithm k-NN.

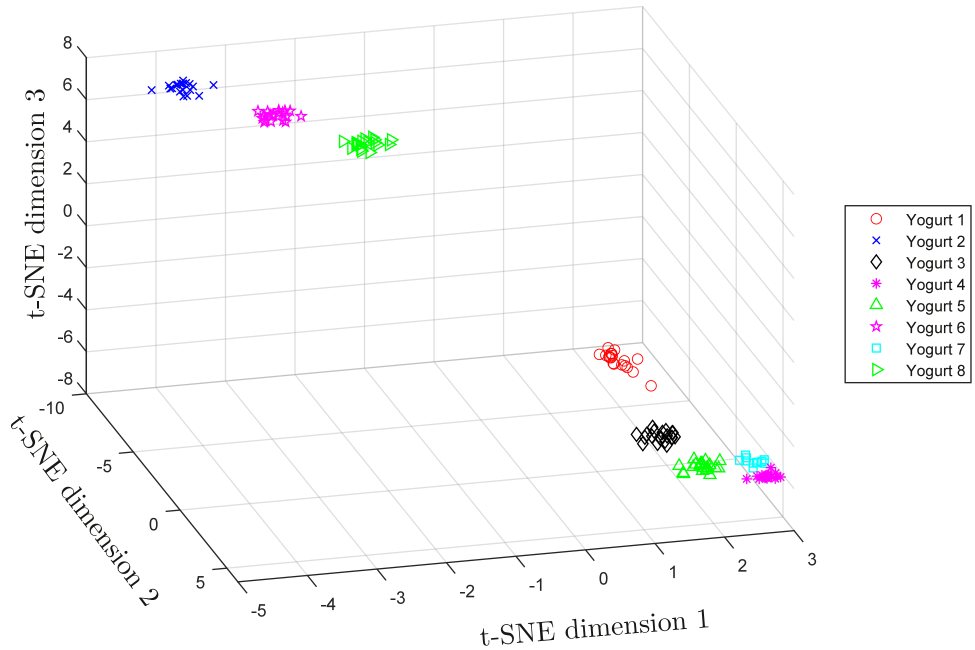

Fig. 19. Scatter diagram of the first three components resulting from applying the t-SNE method to perform dimensionality reduction.

The results of the first three dimensions after applying the manifold learning algorithms to the yogurt dataset are evidenced in the scatter diagram in Fig. 19. This method allows evidence of a clear separation between the eight classes.

3.6. Classification results using t-SNE and k-NN

The algorithm *t*-SNE needs the definition of the target dimension. To find this parameter, a study was carried out of the change of the target dimension d vs. the classification accuracy obtained by the algorithm k-NN with $k = 1$ and Euclidean distance. The cross-validation process executed was leave one out cross validation (LOOCV) due to the small number of samples in the yogurt dataset. This procedure uses different data in an iterative manner for training and testing. This means that the number of experiments in the dataset defines the total number of iterations. In each iteration, one experiment was defined as a test set, while the rest of the experiments were used to form the training set Leon-Medina et al. (2022). As shown in Fig. 20, the accuracy behavior tends to increase with d up to a maximum of $d = 5$ for classification accuracy of

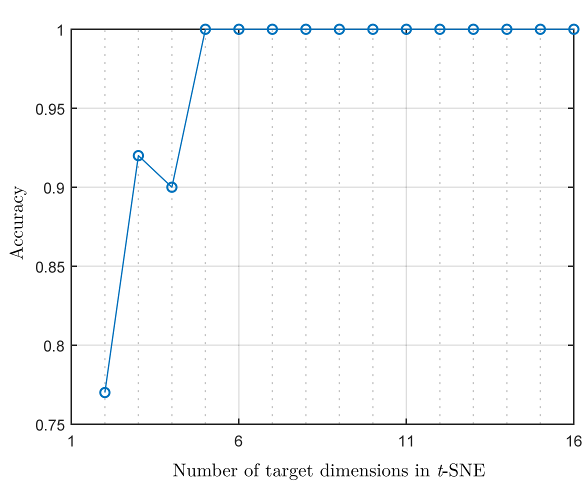

Fig. 20. Accuracy behavior when varying the number of dimensions obtained with the *t*-SNE method at the input of the *k*-NN algorithm.

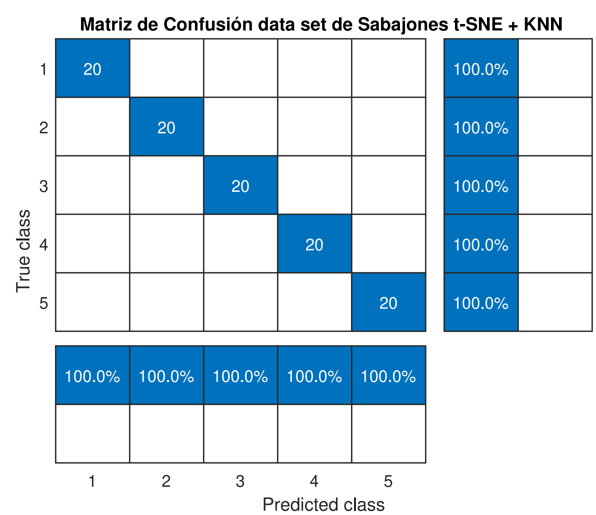

Fig. 21. Confusion matrix resulting from using t-SNE + *k*-NN and LOOCV in the yogurt dataset, taking into account 5 dimensions at the input of the algorithm *k*-NN.

100%. This is why $d = 5$ was selected as the optimal dimension; therefore, the size of the characteristics matrix at the input of the *k*-NN classifier algorithm is equal to 100×5.

Fig. 21 shows the confusion matrix results when the first five dimensions obtained by the algorithm *t* -SNE are taken into account, thus getting a classification accuracy of 100%.

3.7. Classifier comparison

This section presents the results of the evaluation of different machine learning methods to show the relevance of our methodology. For this comparison, in additional to k-NN the following methods are considered: Linear Discriminant Analysis (LDA), Classification trees, Naive Bayes and Support Vector Machines (SVM). The comparison is made in terms of classification accuracy and calculation time. The results of this comparison are shown in Tables 3 and 4.

Table 3
Classification accuracy obtained by different machine learning classifiers and dimensionality reduction methods.

	LDA	Classification trees (C4.5)	Naive Bayes	k-NN	SVM
PCA	1	0.9934	0.9603	0.9934	0.9934
t-SNE	0.9934	0.9868	0.9934	1	0.9934

Table 4
Time calculation (seconds) obtained by different machine learning classifiers and dimensionality reduction methods.

	LDA	Classification trees (C4.5)	Naive Bayes	k-NN	SVM
PCA	4.704	4.430	4.669	6.934	51.386
t-SNE	25.302	11.719	8.970	11.877	47.257

These analyses consider using PCA and t-SNE dimensionality reduction algorithms, where five dimensions are used at the input of each classifier. Results in Table 3 showed that each classifier obtained high values of accuracy. However, the best results of 100% of accuracy were obtained by the PCA dimensionality reduction method and LDA classifier combination and by the *t*-SNE dimensionality reduction method and *k*-NN classifier. Differences between the methods are in calculation time, where the classification by using LDA resulted in a faster method.

Table 4 lists the results of the calculation time needed to execute the classification after the LOOCV. From Table 4 is evident that the PCA dimensionality reduction method requires less execution time than *t*-SNE. Besides, the classifier that took the longest time to execute its job was SVM.

4. Discussion

Due to data acquired by the sensor array having a high dimensionality in the experimental tests, it was necessary to apply a dimensionality reduction method. The representation in a low-dimensional space of the data allows generating a matrix of new characteristics (features) that was later used at the input of a supervised machine learning classifier algorithm to perform the correct classification of yogurts. This work used Principal Component Analysis (PCA) as a linear dimensionality reduction method. The application of this method resulted in the extraction of relevant characteristics from the signals of all sensors in a multivariate analysis approach. The original data was projected into a new low-dimensional space defined by a number of principal components. The optimal number of principal components to be used in the input of a supervised classification algorithm must be determined. For this purpose, and to carry out its training, the fraction of variance explained by each principal component was determined, and the classification accuracy was evaluated by varying the number of principal components. It was found that, when taking into account the first three principal components, the classification accuracy reached a value of 100% in the dataset obtained in this article, with the substance classification system based on an array of the electronic tongue. On some occasions, the representation structures of the raw data present nonlinearities. For this reason, with the purpose of bringing the data to a new representation located in a low-dimensional space, $t-SNE$ can be used as a manifold learning algorithm to carry out this non-linear dimensionality reduction. The application of this algorithm was satisfactory in obtaining a correct representation of the data in a low-dimensional space, as it presents an additional configuration parameter that allows obtaining a different data model in this type of space. Therefore, the flexibility offered by this type of algorithm makes them ideal for finding the correct interclass separation of the data and obtaining adequate compactness between the data of each class.

5. Conclusions

This study presented an electronic tongue system to classify different yogurts by using a sensor array, a data acquisition system, and a pattern recognition unit. From the point of view of the sensor array and the data acquisition system, the used configuration allowed obtaining different signals for each one of the different materials of the working electrode of each sensor. As a result, signals were obtained by performing multi-step amperometry tests on eight different yogurts, using a Palmsens 4 potentiostat and MUX8R2 multiplexer equipment. Due to the results in the classification, it is possible to conclude that data from this system are satisfactory because, in all cases, the yogurt reached a high classification accuracy. Furthermore, an advantage observed during the work with the system is its portability, resulting in a portable and economical solution to classify liquids compared with other methods such as high-resolution liquid chromatography or the panel of experts.

Regarding the data pre-processing process, it was found that the information obtained required as a first step to be organized because of the need for sensor data fusion. This step, known as unfolding, allows obtaining a representation in two dimensions, thus forming a matrix of rows and columns. Specifically, the rows correspond to the # of samples and the columns to the product (#data points • # of sensors). This organization of the data allowed for satisfactorily carrying out the multivariate analysis of the data.

Since the signals came from different sensors in each experiment, a normalization method of the data was used to bring them to the same scale. The results showed good behavior when using the group scaling method. Furthermore, this method yielded better results in yogurt classification accuracy when compared with the methodology without data normalization. This is because the combination of the data from the sensors allows for the improvement of the pattern introduced to the classifier. However, due to the number of sensors and samples per sensor, a dimensionality reduction is a necessary step to eliminate possible noise and redundant information from the raw data that can increment the time for the classification. This is an important point because this kind of device requires the possibility of portability and real-time analysis for complex analysis where a huge number of sensors are used, and computation requirements can be constrained by the use of some embedded electronic systems or communication capabilities.

The classification accuracy reached a 100% value using PCA for dimensionality reduction and LDA as a classifier. A shorter execution time was evidenced for PCA and LDA compared to the results obtained with $t-SNE$ for dimensionality reduction and *k*-NN as a classifier. Each dataset is different, and the type of feature extraction method, whether linear or nonlinear, depends on the nature of the data. Therefore, a comparative study between different dimensionality reduction algorithms is required to determine which technique to use. In this article, the indicator used to select the best dimensionality reduction method was the classification accuracy calculated in the final confusion matrix when performing the LOOCV cross-validation process. Future work related to the use of an incremental learning approach that will allow updating the classifier with the arrival of new data will be taken into account.

CRediT authorship contribution statement

Jersson X. Leon-Medina: Conceptualization, Validation, Writing – review & editing. **Maribel Anaya:** Conceptualization, Methodology, Validation, Writing – review & editing. **Diego A Tibaduiza:** Conceptualization, Methodology, Validation, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

The authors are grateful with Administrative Department of Science, Technology and Innovation of Colombia—Colciencias with the grant 779—"Convocatoria para la Formación de Capital Humano de Alto Nivel para el Departamento de Boyacá2017" for sponsoring the research presented herein. This work was supported by FONDO DE CIENCIA TECNOLOGÍA E INNOVACION FCTeI DEL SISTEMA GENERAL DE REGALÍAS SGR. Jersson X. Leon-Medina is grateful with Gobernación de Boyacá and Colciencias for the PhD fellowship. J.X. Leon-Medina thank Prof. Miryam Rincón Joya from the Department of Physics of the National University of Colombia and Prof. Leydi Julieta Cardenas Flechas, for their introduction to the electronic tongue sensor array field of research.

Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.iswa.2022.200143.

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