Visual and Quantitative Analysis of Different Tastes in Liquids with Fuzzy C-means and Principal Component Analysis Using Electronic Tongue System

Joeng-Do Kim*, Dong-Jin Kim*, Hyung-Gi Byun**, Yu-Kyung Ham*, Woo-Suk Jung* and Dae-Won Choo*

Abstract - In this paper, we investigate visual and quantitative analysis of different tastes in the liquids using multi-array chemical sensor (MACS) based on the ion-selective electrodes (ISEs), which is so called the electronic tongue (E-Tongue) system. We apply the Fuzzy C-means (FCM) algorithm combined with Principal Component Analysis (PCA), which can be used to reduce multi-dimensional data to two- or three-dimensional data, to classify visually data patterns detected by E-Tongue system. The proposed technique can be determined the cluster centers and membership grade of patterns through the unsupervised way. The membership grade of an unknown pattern, which does not shown previously, can be visually and analytically determined. Throughout the experimental trails, the E-tongue system combined with the proposed algorithms is demonstrated robust performance for visual and quantitative analysis for different tastes in the liquids.

Key Words : MACS, ISE, Electronic Tongue, FCM algorithm, PCA

1. Introduction

A taste sensed by a human tongue can be said be qualitative data analyzed synthetically by a human brain indicating effects on taste buds of chemical components constituting a taste substance, not quantitative data indicating the contents of the chemical components. Of course, a human brain performs a quantitative analysis onchemical components according to the perceived intensity of a taste. However, a taste itself is a result of qualitative analysis of chemical components. Generally, tastes and flavors of foods or beverages are compared and determined through sensory evaluation but dose not produce numerical values being difficult to accurately quantify.

Conventional electrical taste evaluation methods are based on re-analysis of values measured using many Ion-selective electrodes (ISEs), color change measured using silicon chips and so on. Over the last decade several researchers have developed on "Electronic Tongue" which use an array of multi-selective chemical sensors based on ion-selective electrodes. [1,2,3] Ion-selective electrodes are membrane electrodes that exhibit selective membrane potentials to specific ion(s). Even through the ion-selective electrodes do not respond selectively to only one type of ions, they exhibit distinct to specific ions. [4,5] There are two main groups of ion-selective membrane electrodes : conventional ion-selective electrodes and solid-state electrodes. Unlike solid-state electrodes, conventional ion-selective electrodes require an internal reference filling solution between an ion-selective membrane and an internal reference metal electrode. In conventional ion-selective electrodes, an ion-selective membrane is fixed to a surface of the electrode so as not to be separated from the electrode. In solid-state electrodes, an ion-selective membrane is disposed over a surface of electrode without being fixed. In this respect, adhesion of an ion-selective membrane to an electrode surface is an important factor in determining electrochemical properties of an ion-selective electrode. The solid-state electrodes have the following advantages, and will likely be used in the development of industrial sensors associated with automated analysis equipment.

(a) Easy fabrication of thin electrodes due to the absence of an internal reference filling solution.

(b) Fabrication of multi sensors able to simultaneously detect different ions on one chip.

(c) Cost effectiveness due to mass production.

Following by those advantages, the "Electronic-tongue" system is used Multi-Array Chemical Sensors (MACS), which was commercialized by I-Sens, Inc. Korea (Fig. 1).

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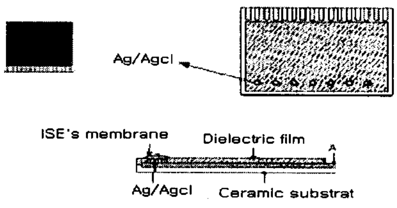

Fig. 1. Multi-Array Chemical Sensor(MACS).

A taste sensory system transforms a taste of a liquid sample to an electrical signal measured by a sensor array composed of ion-selective electrodes. That is, a taste of a liquid sample is analyzed using a potential difference between a reference electrode and a detector electrode. Fig. 2 is shown a block diagram for "Electronic Tongue" system. Since the output signals from sensors are as low as several mV to several tens of mV, a bufferis introduced into a sensor input terminal so that a signal source is not affected by detection circuit. Signals that have passed through the buffer are filtered with a low-pass filter to remove high-frequency noise contained in the signal source. A multiplexer selectively receives input signals that have passed through respective filters of the sensors. Output signals of the multiplexer are input to an analogue and digital (A/D) converter via a buffer. The A/D converter has a 16-bit resolution and converts a measured data value to a digital value. Even though the A/D converter has a 16-bit resolution, a change of a reference voltage may lower measurement precision. In this regards, a voltage regulator that provides 0.1% voltage regulation is used to generate a reference voltage to be applied to the A/D converter. However, since 0.1% voltage regulation cannot achieve a precision corresponding to the 16-bit resolution, averaging of 200 or more received data per second is used. Therefore measured potential values have an error of less than 0.15mV. Data measured by A/D converters are transferred to one-chip microcontroller via Serial Peripheral Interface (SPI) communication and then to a PC via RS-232 communication.

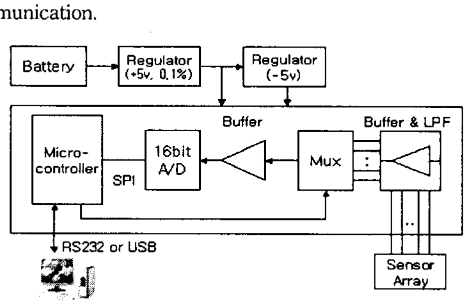

Fig. 2. Block diagram for "E-Tongue" system.

Even through the taste sensory system based on ion-selective electrodes has a good selectivity, analysis of signals generated in an array of membrane electrodes using an appropriate signal processing algorithm is required to detect a minute change in tastes of liquids. The principal component analysis (PCA), which is based on the Karhunen-Loeve (K-L) expansion [6], is a well-known statistical method for data projection, and widely used in data analysis. It is a linear orthogonal transformation from multi-dimensional input space to a two- or three-dimensional space, such that the coordinate of data in the two- or three-dimensional space are uncorrelated and maximal amount of variance from the original data are preserved by only a small number of coordinates. However, since the PCA is a visualization analysis technique, a separate method for quantitative or qualitative analysis of data is required. The k-means algorithm is a representative technique used to implement data for quantitative analysis and clustering. A fuzzy C-means (FCM) algorithm [7] is more intellectual clustering method then the k-means algorithm. The two algorithms are clustering methods using an unsupervised learning scheme but are methods of calculating the center of data cluster without reducing the number of dimensions. Since a human being generally depends on visual inspection for the determination of object features, the PCA or the generation of a Spider Map are most favorable for describing attributes or functions of objects in actual industrial fields. In this respect, the use of PCA is essential. However, quantitative description using the FCM algorithm is also necessary for automation of clustering or analysis, in addition to the PCA. If the PCA and the FCM algorithm are separately utilized, it is difficult to obtain a correlation between the data visually analyzed by the PCA and the data computed by the FCM algorithm since the dimensions of data in the PCA and the dimensions of data in the FCM algorithm are different. In this paper, we investigate a relationship between the PCA which is a visual analysis and the FCM algorithm which is a quantitative analysis. For our requirement, the three -dimensional principal components are calculated by PCA technique, and the FCM algorithm is implemented three-dimensionally using data dimensionally reduced using principal components. Therefore, the data which is newly introduced can be represented visually. Through the center of a cluster correlated with the visual data, membership grades which indicate the degree to which newly introduced input data belong to clusters can be determined. The superiority of the techniques proposed by this paper was demonstrated through experimental trails using an electronic tongue system based on selective electrodes sensors array for visualization and quantitative analysis of different tastes among the liquids, which is applicable to food and beverage industry.

2. The approach method

PCA is an algorithm for achieving dimensionality reduction mapping of multidimensional data into visually manageable two- or three-dimensional data according to eigenvectors, which correlated with the largest eigenvalues, as main components. It is enabled visual clustering, however, to quantitatively determine which newly introduced data are close to or belong to which cluster, a separate algorithm is required. If the PCA visual analysis and the k-means or FCM algorithm quantitative analysis are separately performed, it is difficult to find a correlation between the data visually analyzed using the PCA and data dimension in the FCM algorithm are different. However, the FCM algorithm based on the results obtained from the PCA can be used to determine the membership grades of newly introduced data in clusters using cluster centers correlated with the visually analyzed data obtained from the PCA. Throughout the suitable learning procedures with FCM algorithm, cluster centers of previously acquired data and a degree of membership of each pattern in a cluster is determined, then cluster centers are achieved. When the data of unknown samples are newly introduced, the cluster centers can be used to determine the membership grades of the unknown samples.

$$d_j = \|S - Z_j\| \tag{1}$$

where S is an unknown sample data, Zj is the center of j-th cluster (j=1,2,⋯,c)

The membership grades of unknown samples can be calculated by

$$V_j = \frac{1}{\sum_{l=1}^{n} \left[\frac{d_j}{d_l} \right]^2} \tag{2}$$

where Vj is the membership grade of a sample vector in the j-th clusters.

3. Result and Discussions

Input data for liquid samples detected by taste sensory system are presented in Table 1 below, and are simulated by the PCA.

The three-dimensional pattern-clustered data by feature extraction from the seven-dimensional input data with PCA are presented in Fig. 3.

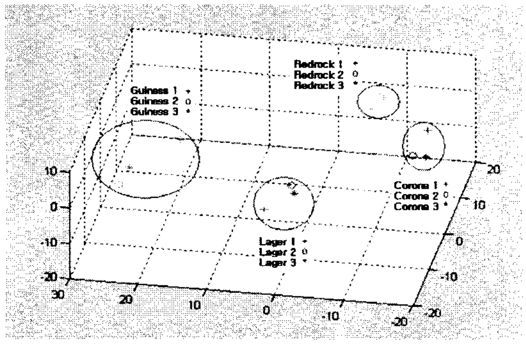

Fig. 3. PCA analysis result for samples. The visual distinct data clustering is shown for liquids samples using PCA.

The data mapped to a lower dimension using the PCA technique were used as input data for the FCM analysis. Therefore, the center values of input data and the membership grades of the input data based on the center values could be identified numerically. Table 2 presents centers of clusters for input data using FCM and table 3 presents membership grades represented by distances between the input data and the centers. As shown in table 3, membership grades of the input data for centers from liquids samples can be numerically identified and the degree of membership can be easily determined.

Table 1. Input data for liquids samples.

Sample	Sensor 1	Sensor 2	Sensor 3	Sensor 4	Sensor 5	Sensor 6	Sensor 7
Lager 1	46.5	-61.4	-52.3	-89.0	-16.5	228.5	178.9
Lager 2	39.8	-59.7	-53.4	-85.3	-18.4	217.0	179.7
Lager 3	41.5	-63.7	-51.1	-93.3	-19.4	221.7	180.6
Corona 1	41.4	-49.4	-51.1	-91.8	-12.5	191.5	170.6
Corona 2	40.4	-47.1	-48.3	-87.5	-14.6	189.6	178.3
Corona 3	41.2	-46.7	-49.3	-89.8	-13.5	189.4	177.8
Guiness 1	26.6	-58.5	-38.5	-79.0	-11.6	208.4	174.3
Guiness 2	24.2	-54.1	-32.8	-76.8	-12.4	224.9	182.3
Guiness 3	20.9	-53.4	-35.7	-77.2	-13.1	222.7	179.1
Redrock 1	32.9	-64.2	-46.5	-95.4	-16.2	196.2	171.4
Redrock 2	34.6	-64.6	-45.2	-92.5	-16.1	195.3	172.2
Redrock 3	33.2	-65.7	-47.0	-94.4	-15.9	198.6	173.8

Table 2. The numerical presentation of cluster centers for liquids samples.

Sample	Main component 1	Main component 2	Main component 3
Lager	313.98	0.41914	-3.3531
Corona	285.26	14.035	10.132
Guiness	303.22	-22.905	2.5512
Redrock	291.25	9.0387	-8.5773

Table 3. Membership grades for liquids samples using FCM algorithm based on the PCA.

	Distance from cluster center											
	Lager 1	Lager 2	Lager 3	Corona 1	Corona 2	Corona 3	Guiness 1	Guiness 2	Guiness 3	Redrock 1	Redrock 2	Redrock 3
Lager	0.813	0.955	0.991	0.010	0.003	0.002	0.021	0.060	0.010	0.001	0.002	0.005
Corona	0.036	0.009	0.001	0.911	0.981	0.986	0.010	0.042	0.007	0.002	0.008	0.013
Guiness	0.091	0.023	0.004	0.015	0.004	0.003	0.949	0.814	0.966	0.001	0.004	0.012
Redrock	0.059	0.011	0.002	0.063	0.010	0.008	0.018	0.082	0.014	0.994	0.983	0.970

Fig. 4 illustrates three-dimensional FCM results based on the PCA using the distances (membership grades) between the centers and the input data. Hitherto, the seven-dimensional input data were reduced to the three-dimensional input data using the PCA and then visualized. The membership grades of the input data were quantitatively represented using the FCM algorithm.

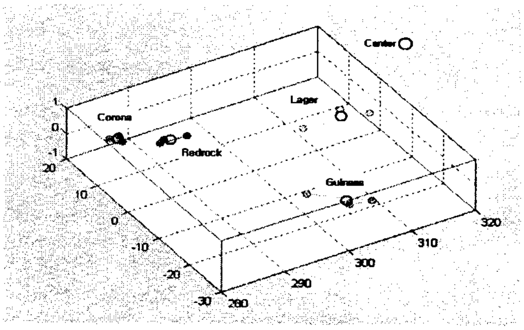

Fig. 4. The FCM result based on the PCA for liquids samples.

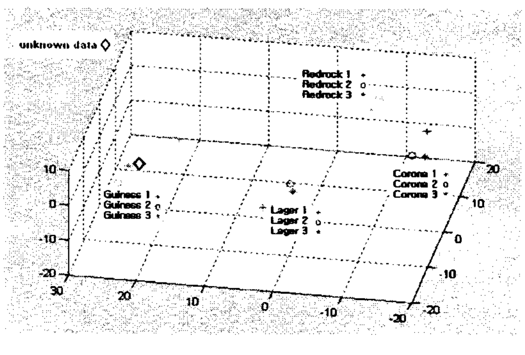

Fig. 5. PCA result for the previously unseen data.

Hitherto, standardized data for liquids samples were obtained from known data through the FCM algorithm based on the PCA. Based on the standardized data, the data cluster to which newly introduced unknown data belong can be determined by visualization using the PCA and then quantification using the FCM algorithm. From the fig. 5, the cluster to which the unknown data belong can be visually identified. The PCA result for the unknown data was expressed numerically using the FCM algorithm in the table 4 and the showed the fig. 6.

Table 4. Membership grades for the previously unseen data using FCM algorithm based on the PCA.

	Lager	Corona	Guiness	Redrock
Unknown data	0.0032207	0.0011879	0.99392	0.001667

The FCM algorithm combined by the PCA results showed visually and quantitatively that the newly introduced unknown data being to the Guiness class.

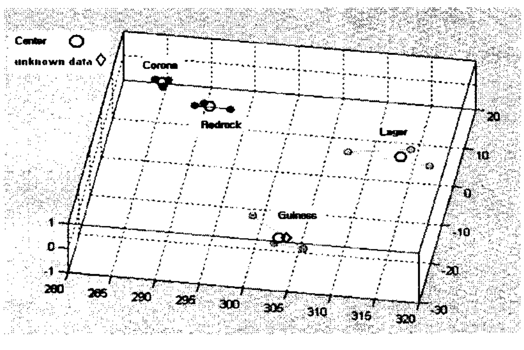

Fig. 6. The FCM results based on the PCA for the previously unseen data.

3. Conclusion

A taste sensory system, which is called "Electronic Tongue" system"is implemented using multi-array chemical sensors to the mimicking of human tongue which responds to distinct tastes. The data acquired by the electronic tongue system including a sensor array based on the ion-selective electrode principal and a 16-bit A/D converter are clustered by visual analysis of the PCA and quantitative analysis of the FCM algorithm. The input data are reduced to three-dimensions using the PCA technique so that features of the input data can be visually identified. To overcome the disadvantage of the PCA, which dose not provide the numerical values for data attributes, the input data are quantitatively analyzed using the FCM algorithm to determine the membership grades of the input data based on cluster centers. The developed electronic tongue system can be widely used for a various industrial applications including food, liquids, cosmetics, environmental monitoring. Also, it is applicable when direct tasting by human is unnecessary or difficult such as toxic and hazard environments. However, determination of the membership grades of input data by standard data density and an embodiment of an electronic tongue system that is not affected by an ambient environment still remain as future development tasks.

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