Smell Sensing and Classification by Machine Learning

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Abstract

This paper is concerned with smell sensing and classification using machine learning. Sensors used here is metal-oxide semi-conductor gas sensors and classification is machine learning. After explaining sensing principle, we show the classification results of coffee companies and kinds of coffees. Then their method apply to sensing and classification of human body smell so called Kunkun Body. The Kunkun Body can classify one of three human smells such as sweaty smell, middle-aged smell, and old-aged smell using four smell sensors. To train the Kunkun Body we gathered 2,100 persons who have one of three human body smells. We divide them into three groups according to each smell for human body and divide into 10 classes according to the density levels. The first stage for learning is to train the neural network of competitive learning to chemicals which are main components for human body smells. After pre-learning we settle the final values of weighting coefficients as the initial values. The real data for 2,100 persons are divided three groups for typical each smell and ten levels for strength. If the misclassification does not decrease, we adjust the structure of the neural network by increasing the number of neurons. When we can get high accuracy classification results, those weighting values will be stored and their values are used for Kunkun Body. Copyright © VBRI Press.

Keywords: Smell sensing, smell classification, machine learning, kunkun body, human body smells.

Introduction

The smell information has played an important role for our lives as being one of five senses. Human beings have done the culture or action by using those senses. In the course of evolution, those five senses have had different progresses. For example, in case of human beings, sight sense has been so much developed such that 90 % of our brain have been related to this sense. Compared with sight, hearing, and touching senses which appears as physical phenomena, smell and taste are chemical ones and they are not so easy to measure as physical values. Under such a situation, smell research has not been developed so much.

In 2004, R. Axel and L. B. Buck received "The Nobel Prize in Physiology or Medicine 2004" by discovering a large gene family, comprised of one thousand different genes (three per cent of our genes) that give rise to an equivalent number of olfactory receptor types [**1**]. Now smell sensors have been developed to detect the various smells. Two types of gas sensors have been focused. They are MOGSs and quartz crystal microbalance (QCM) sensors. They have been transformed from chemical phenomena into physical quantities based on the different principles. Former one is based on oxidation and reduction and latter one is frequency difference before and after of gas appearance.

Until now, many papers on electronic nose (E-nose) have been published. The author's group has considered E-nose from view point of sensor development and classification of odors [**2-5**]. Similar studies have been reported in [**6-9**]. Those researchers have been focused on mainly laboratory scale experiments. Thus, physical devises developed there are rather big and heavy. We have succeeded in developing the E-nose system, which is small size, light, and user friendly interface. My idea is to use a smart phone for the smell to make visible form (visualization of smell).

In this paper, we have used an array of the MOGSs to measure the smells. Furthermore, using learning vector quantization, we classify the smells into three typical smells of human body and show the results in visible form using a smart phone. We have named the hardware configuration as Kunkun (which means sniff-sniff in Japanese) Body.

Metal-oxide semi-conductor gas sensors

The MOGSs are the most widely used in order to make an array of artificial olfactory in the E-nose system. Those sensors are commercially available to detect some specific smells. Various kinds of metal oxide, such as SnO2, ZnO2, WO2, TiO2 are coated on the surface of semi-conductor. In this paper we select the metal oxide of SnO2. These metal oxides have a chemical reaction with the oxygen in the air and chemical reaction changes when the adsorbing gas is detected. The scheme of chemical reaction of the MOGS will occur as shown (1) and (2)

$$\frac{1}{2}O_2 + (SnO_{2-x})^* \rightarrow O^-ad(SnO_{2-x}) \qquad (1)$$

$$CO + O^-ad(SnO_{2-x}) \rightarrow CO_2 + (SnO_{2-x})^* \qquad (2)$$

where (·)* denotes burned active state, ad(·) means adsorbing state, and x = {0,1}.

When the metal oxide element on the surface of the sensor is heated at a certain high temperature such as 250 degrees Celsius, the oxygen is adsorbed on the crystal surface with the negative charge as shown in (1). In this stage the grain boundary area of metal oxide element forms a high barrier. Thus, the electron cannot flow the boundary, which means the resistance of the sensor becomes higher. When deoxidizing gas, for example, CO gas, is presented to the sensor, then there is a chemical reaction between negative charge of oxygen at the surface of the metal oxide element and deoxidizing gas as shown by the second chemical reaction in (2). The chemical reaction between absorbing gas and the negative charge of oxygen on the surface of MOGS reduces the grain boundary barrier of the metal oxide element. Thus, the electron can flow from one cell to another cell easier. This makes the resistance of MOGS lower by the changes of oxygen pressure. The relation has been shown in **Fig. 1**.

MOGSs need to be operated at high temperature. Thus, they consume a little higher power than the other kinds of sensors. The reliability and sensitivity of MOGSs are provided to be very good to detect volatile organic compounds, combustible gas, and so on. Generally, the commercial MOGSs respond to various odors in different ways. In this paper we combine various MOGS as a sensor array of the E-noses.

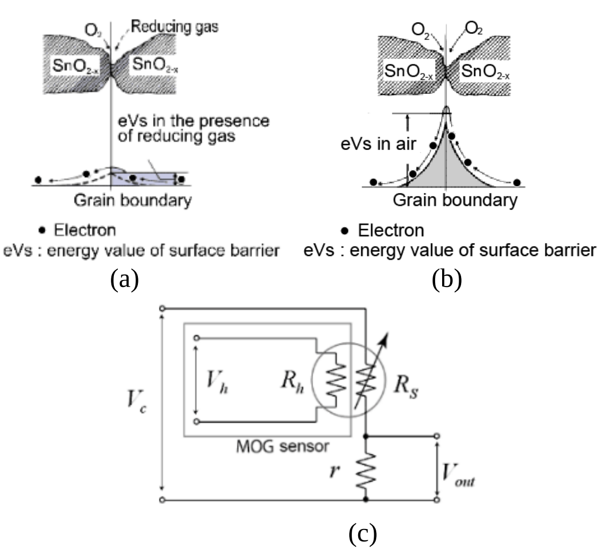

Fig. 1. Oxidation (a), reduction (b), and sensing circuit (c).

Smell sensors and sensing system

We have prepared many smell sensors as shown in **Table 1**. Each sensor can detect different kinds of gases although each sensor may detect different kinds of gas. The voltage signal for the heater and the circuit is equal to 5 [V]. We have used the same sensors in order to check the accuracy of TGS826 and TGS816.

Table 1. Sensor symboland main detection samples.

Symbol	Sensor model	Main detecting smells
Sensor 1	TGS 2600	Tobacco, Cooking odor
Sensor 2	TGS 2602	Hydrogen sulfide, Ammonia, VOC
Sensor 3	TGS 2610	LP gas, Butane, Propane
Sensor 4	TGS 2611	Methane
Sensor 5	TGS 2620	Alcohol, Organic solvent
Sensors 6,7	TGS 826	Ammonia, Amine compounds
Sensors8,9	TGS 816	Methane, Propane, Butane
Sensor 10	TGS 821	Hydrocarbon gas
Sensor 11	TGS 832	Chlorofluorocarbon gas
Sensor 12	TGS 825	Hydrogen sulfide
Sensor 13	TGS 830	Chlorofluorocarbon gas
Sensor 14	TGS 822	Alcohol, Organic solvent

The sensing system is shown in **Fig. 2** where Pemeater is a special measurement apparatus to control flow, mixing gases temperature, and humidity. Smell sensors are made in Figaro Inc., Japan.

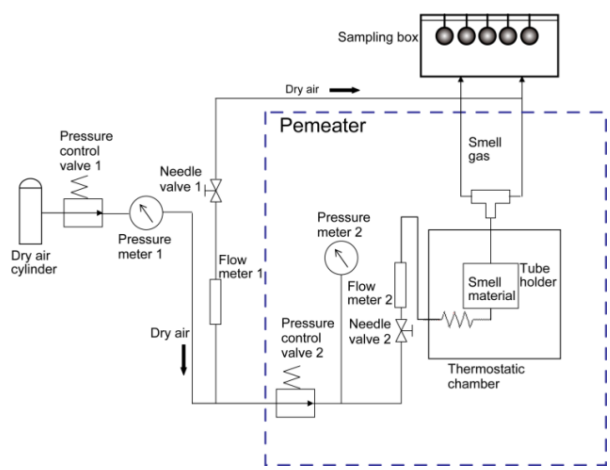

Fig. 2. Smell measuring scheme.

Sample paths using sensors

The sample paths by sensors in **Table 1** are shown in **Fig. 3**. Those sample paths shows six times repetition which is almost all similar patterns for each iteration. From these results, we could trust the sensor accuracy. Sensing interval is separated into two parts. One is for 900 [s] and another is for 300 [s]. The first one is to measure smell and the second one is to measure carrier gas (dry air). This cycle has been repeated six times.

In order to find features of the tested smell for each sensor, we must take some preprocessing. Before measuring the tested smell, it is necessary to measure the data of each sensor for carrier gas since each sensor shows the different value. We denote smell data at time

t of sensor $i(=1,2,\ldots,14)$ by V_{it} and the differenced voltage v_{it}, we have

$$v_{it} = V_{it} - V_{i0} \tag{3}$$

where sampling interval is one second.

Then the measurement data for coffee are shown in **Fig. 3** where A: Blendy AGF, B: Maxim AGF, C: Coffee break AGF, D: Excella, Nestle, E: Gold blend, Nestle, and F: Gold blend mocha, Nestle.

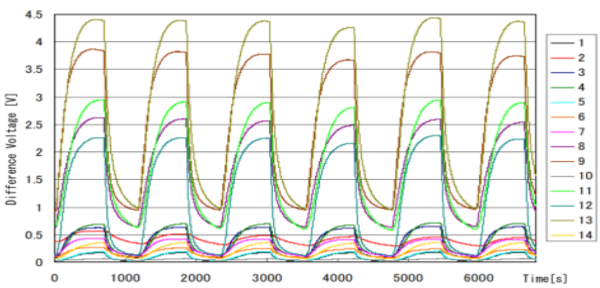

Fig. 3. Sample paths using sensors of Table 1.

Smell classification method

We have adopted learning vector quantization since the structure is suitable for hardware configuration and it attain the 100% classification rate for sample data theoretically. The algorithm is to find the minimum distance d_c between input $x = (x_1, x_2, \ldots, x_n)$ and $w_j = (w_{j1,}, w_{j2,\ldots,,}, w_{j1n})$

$$d_c = \min_i d_i\,,\quad d_i = \|x - w_i\|.$$

If x and $w_c(t)$ belong to the same class, then the next iteration of w_c becomes as

$$w_c(t+1) = w_c(t) + \alpha(t)\big(x - w_c(t)\big)$$

and if x and $w_c(t)$ belong to the different class,

$$w_c(t+1) = w_c(t) - \alpha(t)\big(x - w_c(t)\big)$$

as shown in **Fig. 4** where. $\alpha(t) \geq 0$ and t is iteration.

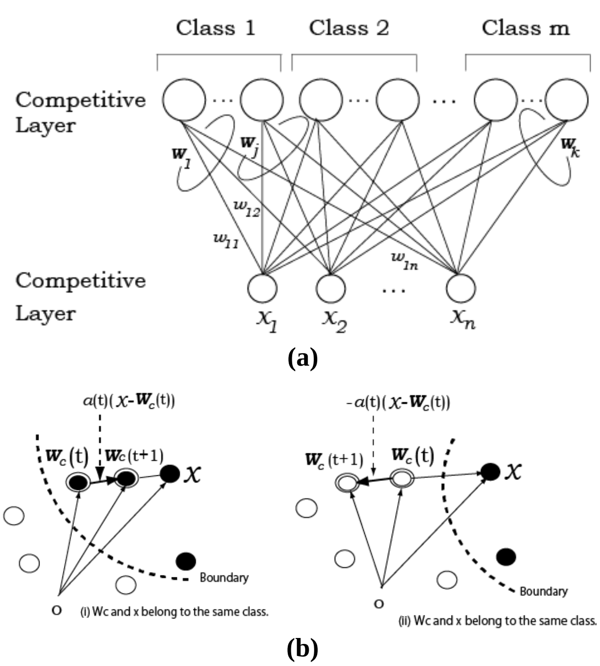

Fig. 4. Machine learning (a) learning vector quantization structure (b) learning principle.

Classification results

Using the data of **Fig. 3**, we 50 data were selected for training and after training to get 100%, test data of 450 data were classified. The results were shown in **Table 2**. A, B, and C are made of AGF company and D, E, and F were Nestle Company. Except for B and F, more than 92% of classification rates were obtained. B and F are very similar smell although they were produced different companies, to get more precise classification rates, we must more neurons in both Classes.

Table 2. Scattering matrix where left hand column shows sand the row shows classified results and correct RATE.

Symbols	Output results (numbers)						Correct rates (%)
	A	B	C	D	E	F	
A	476	23	0	0	1	0	95.2
B	2	330	0	0	29	139	66.0
C	0	7	486	7	0	0	97.2
D	0	0	0	500	0	0	100
E	13	24	0	0	461	2	92.2
F	0	101	0	0	0	399	79.8

Classification device for human body smells

Smell sensing and classification algorithm have been extended and new products have been developed. We will show Kunkun Body, which has been sold out from December in 2017. The total configuration is shown in **Fig. 5**, which has been developed by Konica-Minolta Company. It can sense and classify three smells of human body for twenty seconds. The length is one hundred millimeters, width is fifty three millimeters, height is twenty two millimeters mm and weight is one hundred grams. It works by a lithium-ion battery and has been connected through Bluetooth. According to the strength of each of three typical smells, sweat smell, middle-aged smell, and elderly-aged smell, Kunkun Body can indicate ten levels. Finally, it can show the value as one of hundred levels together with some comments about the smell of human body as shown in **Fig. 5**.

Fig. 5. Kunkun Body products with smart phone.

Principle of Kunkun Body classifier

The principle of Kunkun Body is based on learning vector quantization as stated above as shown in **Fig. 6**. The typical smells of human body are sweaty smell, middle smell, and well-aged smell, which are called three typical smells. Roughly speaking, the sweaty smell will start about 15 years old to 35 years old, middle smell will appear from 35 years old to 55 years old, and well-aged smell will appear above 55 years old. Those sweats include specific chemicals. The sweaty smell includes ammonium or iso-valerate, which is produced by metabolism and death of bacteria. The second smell is produced by di-acetyl, which occurs by metabolism and oxidation. The last one is 2-nonenal which occurs oxidation.

Konica-Minolta Company gathered the real human body smells of 2,100 persons who are classified into three smells clusters with 10 stages of the strength. In order to achieve high classification rate, every class included the same numbers, that is, 70 persons. They were selected by perfumers, very high level experts who could chemically mix perfume as a profession. Applying **Fig. 6 (a)** as the initial structure and weights for data of three smells of 2,100 persons, we checked the errors. In the beginning, we could not expect the correct results. The results were miserable since the situation was not the same for learning of **Fig. 6 (a)**.

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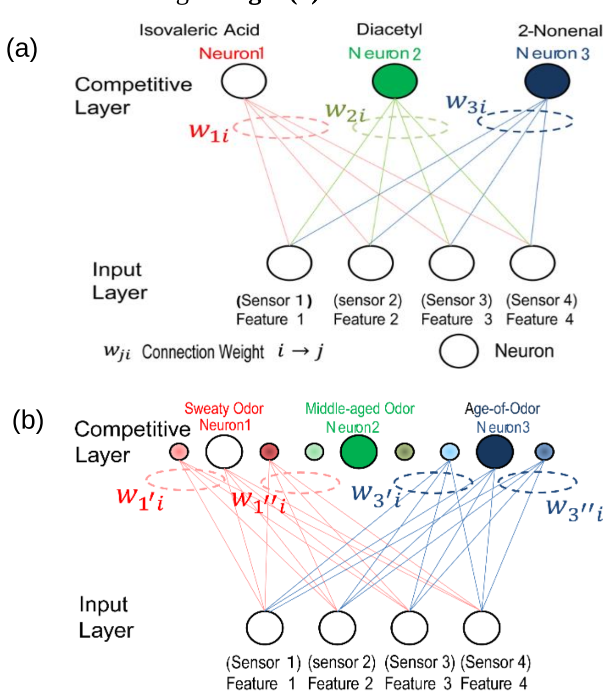

Fig. 6. Structure of Kunkun Body: (a) Chemical classifier (b) Real human body smell classifier.

The first trial to correct the errors was to increased the number of neurons of competitive layer. It is clear that if we select the number of 2,100 neurons in the competitive layer, we could get perfect classification rate, that is, 100%, theoretically. Therefore, starting the **Fig. 6(a)** structure, we extended the neurons in the competitive layer such that new connection weights were selected as the original weights plus random noise with small deviations as shown in **Fig. 6(b)**. Then we could obtain the 100% classification rate. To get such a result, we took two months by trial and error process.

Konica Minolta Company adopted to use cloud-funding approach. In the beginning, 2,000 devices were sold out suddenly. It was the first trial to realize the compact and beautiful style of Kunkun Body. It was broadcasted on TV and newspaper not only in Japan but also in the world. The development was successful and it is now best-selling product in Japan as the open innovation approach.

The Kunkun Body has been sold out now and some claim were sent back since the training data were limited. Those claims are helpful to improve the devise. We changed the software and the new version has been in the market as update. Therefore, Kunkun Body has become wiser and wiser based on those claims and advices.

Results and discussion

We have measured several smells and classified. In case of coffees smells, Measuring smells of coffees, we could classify into the name of coffees and produced company. Thus, similar smells could be classified rather precisely. But there are different thresholds to detect the smell by human nose. For example, a dog could detect the drugs very precisely compared with human being.

By using Kunkun Body If we limit some smells, for example, human body smells, then the smell could be classified into several classes.

But the strength follows logarithmic nature just like other senses such as sight, hearing, touching, taste senses.

Taking into consideration, we should take the log conversion in advance.

Within some clusters of smells we could assume we feel the smell strength according to the levels. This means that we could visualize the smells level using some indicators such as smartphone. In our case, we have developed using smartphone with Bluetooth to show the sensing levels graphically. We call this device visualization of smells although it might be over-advertised.

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We have proposed smell measurement and classification. Furthermore, we have developed Kunkun Body which enables us to measure and classify our human body smells in a visualizing way. From now on, we will concentrate to improve the classification and extend the method for breath classification.

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Author's contributions

Basically, all the part of the paper is written by me except for the open innovation part to make hardware device of Kunkun Body.

Supporting information

Supporting informations are available from VBRI Press.

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