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Predicting odor mixture's responses on machine olfaction sensors

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ABSTRACT

One of the challenging issues in current research on machine olfaction devices, which are often called electronic noses (e-noses), is how to approximate or predict the sensor response to odor mixtures. When each odor is produced by its own unique set of odorant compounds, combinations of these unique odorant sets create a sensing challenge for the e-noses with a limited number of elements in its sensing array. One possible approach proposed in the literature is based on an "additive law of mixing" model but it fails in a complex odor mixtures. Another method adopted a specific hardware solution called odor recorder developed by using active odor sensing system. In this study, signal decomposition/reconstruction based on wavelet analysis and support vector regression are adopted to predict a sensor's response to mixtures of odors. The prediction results of our method are investigated and compared with the real sensor responses collected from a commercial e-nose machine, the AppliedSensor NST 3320. We find that the proposed method provides good prediction when applied to different mixing ratios of some coffees and green tea.

1. Introduction

The field of artificial olfaction has been steadily developed over the last three decades. Many new technologies involved in this field have been implemented by a number of researchers and commercial organizations around the world. In addition, these devices, called electronic noses (e-noses) implementing these new technologies have been demonstrated successfully in a wide range of applications. For example, they can be applied for medical diagnostics [1], for environmental control [2,3], and for quality assessment of beverage products [4,5]. Typically, the e-nose system consists of three main functional components [6]: a sampling unit, a signal processing unit, and an odor classification unit.

Originally, in most published research reports, odor sensing systems (e-noses) were designed to deal with the odor classification and quantification problems. However, in recent years, these systems have been extended into new areas of application. Some of the most interesting are e-commerce, telemedicine, games, and reproducing odor in virtual environments. [7]. Although digital odor manipulation (storage, compression, and reformatting) has been attempted in the same manner as for other physical senses (vision and audition), odor reproduction technology still lags far behind. An example of an interesting application of odor digitization defined by Harel et al. [8] is called the odor communication system. The function of this system is to control an output device (whiffer) to produce an imitation of an odor sensed by a distant input device (sniffer). Basically, the sniffer is designed to digitize the smell in a way that preserves informative features, called the odor recipe, of the original odor input. Therefore, an e-nose can be used as the sniffer which is specifically implemented to this scheme. Once the odor recipe of the target odor is determined, it can be transmitted through the network and then be reproduced anytime using the odor blender contained in the whiffer. The whiffer consists of a set of palette odors and the odor blender used to mix them in proper manner. This concept can be extended to any system needing arbitrary odor reproduction. A developed version based on this model is implemented in [9] for odor communication, called mix-to-mimic algorithm (M2M).

Moreover, a few groups of researchers have tried to extend the application of e-noses to mixture analysis [10,11]. A challenging issue in current e-nose research is to generate a sensor's response waveform for a target odor mixture from measurements of that sensor's response to individual components of the mixture. One of the successful approaches that mimics the citrus flavor has been developed by Wyszynski et al. [12]. Their device is called an odor recorder (see Fig. 1) and is based on an active-sensing system (an e-nose they designed for this purpose) used for quantifying the mixing components [10,12–14].

The operation of the odor recorder system in Fig. 1 follows this sequence. First, the target odor is exposed to the array of sensors

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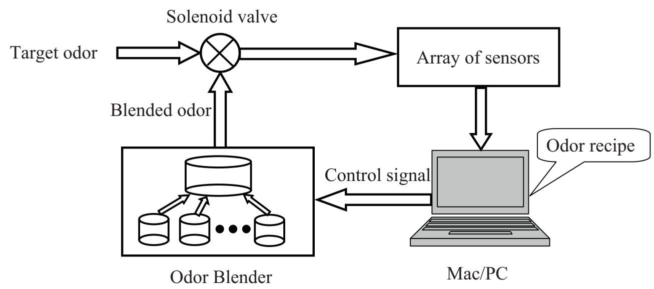

Fig. 1. Block diagram of odor recorder system.

and the target odor's response waveform is recorded by a computer. Then, a synthesized mixed odor obtained by combining several compounds using an odor blender is exposed to the array of sensors. Typically, the closest estimated responses to the target odor are chosen as the synthesized responses. The general approach used to estimate these responses is based on the superposition principle [14]. However, this principle provides large deviation from the actual ones due to the inherent properties of the sensor. After that, the odor response waveform from the estimated blended odor is compared with that from the target odor. Subsequently, the blended odor waveform is iteratively adjusted by changing the ratio of the mixing compounds so that the difference between the two odor response waveforms is minimized. Finally, the target odor is "quantified" by recording the ratio parameters used in the odor blender. Thus, an odor recipe is obtained. This approach provides good results if one has prior information regarding the target mixture ingredients. However, this approach requires ample time to carry out the experiment and to reach computational convergence.

Another approach to generate a sensor's response pattern is proposed by Carmel et al. [11] which is based on a simple additive law of mixing which can be expressed as follows:

$$S(o_1, o_2, \ldots, o_n; c_1, c_2, \ldots, c_n) = S(o_1; c_1) + S(o_2; c_2) + \cdots + S(o_n; c_n) \tag{1}$$

where o_i denotes an odor sample i. c_i denotes a concentration of an odor sample i. $S(o_i; c_i)$ is the sensor response of an odor sample (o_i) with c_i concentration. $S(o_1, o_2, \ldots, o_n; c_1, c_2, \ldots, c_n)$ is the sensor response to the mixture of $o_1, o_2, \ldots, o_n$ with $c_1, c_2, \ldots, c_n$ concentrations.

The generalized model of the additive law of mixing can be written as a linear law of mixing [11]:

$$\begin{aligned} &S(o_1, o_2, \ldots, o_n; c_1, c_2, \ldots, c_n) \\ &\quad = \alpha_1 \cdot S(o_1; c_1) + \alpha_2 \cdot S(o_2; c_2) + \cdots + \alpha_n \cdot S(o_n; c_n) \end{aligned} \tag{2}$$

where α_i denotes a mixing coefficient of $S(o_i; c_i)$.

The additive law model is designed for mixtures of non-interacting compounds. This condition is not satisfied in many e-nose applications since the components in an odor mixture may interact with each other resulting in a nonlinear change in the odor sensor's waveform. As a result, this model may provide poor prediction for some mixture odorant.

In general, the data acquisition cycle [15] used in many electronic nose devices to gather features from an odor sensor response is shown in Fig. 2. This cycle typically comprises three stages. The first stage of the process (the reference phase) is to flush a reference gas over the sensor to obtain its baseline value. Then, in the second stage (the sniffing phase), the sensor is exposed to an odor sample, which causes a change in the sensor response, driving it towards a steady-state. Finally (the recovery phase), the odor sample is flushed out of the sensing chamber by a washing agent to remove odor molecules that might remain adsorbed to the sensor's active surface area. In general, the features from an odor sensor response used in e-nose devices for classification are extracted on the reference phase and the sniffing phase. As a result, the approximation of the sensor response proposed in this study is approximated on those two phases only.

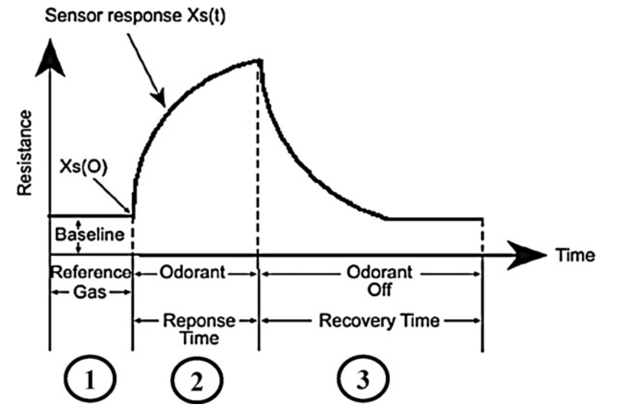

Fig. 2. Data acquisition phases of an e-nose sensor [after 15].

In this study, odor mixture data sets were collected using NST 3320 e-nose system which consists of metal oxide silicon field effect transistor (MOSFET) sensors and metal oxide (MOX) sensors with different sensitivities. Three types of odor samples used in evaluating our proposed algorithm are a common coffee blend, pure sumatra coffee, and pure green tea. The mixture of the odor samples are encoded as follows:

Let's define:
X – Regular coffee
Y – Sumatra coffee
Z – Green tea

The mixed odor sample is denoted as: X–Y–Z in which each numeric number of X, Y, and Z represents the amount of each in the mixture.

An example of sensor responses of mixed odor samples for MOX sensor is illustrated in Fig. 3 in which each sensor's waveform corresponds to different ratios of odor mixture.

Our goal in this study is to develop a prediction algorithm that can provide good approximation of an odor sensor's waveform without special apparatus but requires only some pre-measurement of the odor compound. The proposed approach is based on the combination between signal decomposition/reconstruction from wavelet analysis and support vector machine (SVM) to predict the waveform of the odor mixtures. The closeness between our prediction results and the measured sensor's waveform is used to evaluate the performance of the proposed method.

The remainder of this study is organized as follows. Section 2 describes a basic concept of discrete wavelet analysis and Support Vector Machine (SVM) for regression. The proposed prediction model of odor mixtures is presented in Section 3 and experimental results are demonstrated in Section 4. A discussion of the results and their implication are given in Section 5, and conclusions are drawn in Section 6.

2. Basic discrete wavelet analysis and support vector machine

In this section, we briefly explain the main points of discrete wavelet analysis and support vector machine which are necessary to understand the proposed approach in this study.