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ORIGINAL ARTICLE

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Neuro-based olfactory model for artificial organoleptic tests

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Abstract Recently, the demand for odor processing apparatus in the fragrance and food industries has increased. In this article, we construct a neural network model of the olfactory system as the basis for artificial organoleptic tests that combine the advantages of both human sensory evaluation and machine olfaction. The simulation results indicate that the model can predict odor coding on the glomeruli by appropriately adjusting the parameters involved. Further, the model can simulate the feature extraction ability known as "attention".

Key words Neural network model · Olfactory system · Glomerular activity · Odor qualities

1 Introduction

Considerable evidence has been presented to show that odors have an effect on the memory and emotions,[1] and the importance of odors has begun to be recognized beyond their role as components of flavor. For this reason, the demand for odor processing apparatus in the fragrance and food industries is increasing.[2]

Two of the methods of odor assessment which have been developed to date are the sensory evaluation method and machine olfaction.[2] Generally, the sensory evaluation method is employed because it is based on the characteristics of human perception, although individual differences due to factors such as personal preference or physical condition can affect the evaluation results. Machine olfaction, in contrast, is an objective assessment method, but it tends to ignore the nature of odor perception. Accordingly, a novel odor assessment method is required which combines the advantages of both human sensory evaluation and machine olfaction, thus making it suitable for artificial organoleptic tests. To develop such a method, it is first necessary to predict how odorant information is coded in the brain to obtain the perception characteristics of animals. Then the mechanisms of feature extraction from the neuro-coded odor information must also be predicted. Although the ideal scenario would be to analyze the human olfactory system, current biological knowledge regarding the coding manner of odorant information in the human brain remains limited. Given this restriction, this study focuses on the olfactory system of mice.

An odor is a combination of more than 400 000 types of odorant molecule. Mice have approximately 1000 types of odorant receptor, each of which is responsible for detecting a specific group of odorant molecules.[3] The outputs of the receptor neurons evoke an odor-specific activity pattern on glomeruli.[4,5] As this activity pattern represents fundamental information for odor recognition, it is considered to be closely linked to the characteristics of perception. We constructed a neural network model[6] using biological data on glomerular activity patterns[5] as inputs, and attempted to simulate the perception characteristics of mice. The model also employed a feature extraction mechanism for "attention,"[7] in which the mice would focus on some of the most important molecules in odors. The results of the computer simulation were compared with those of behavioral experiments,[7] and it was confirmed that the model could predict the discrimination ability of mice. However, the scope of our model was limited to odorants with known glomerular activity patterns.

Here, we report on the extension of the model to enable the prediction of glomerular activity patterns from odorant

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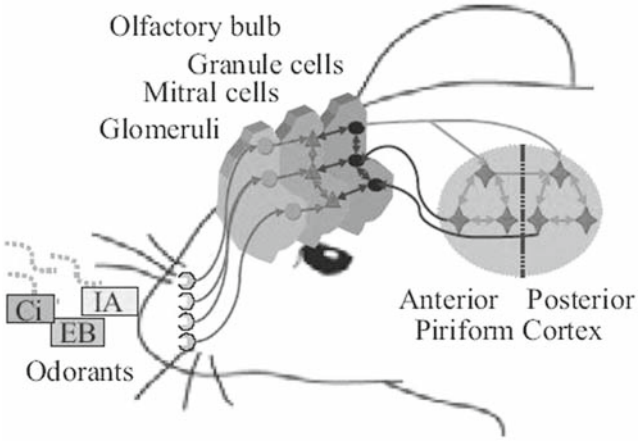

Fig. 1. The olfactory system of mice

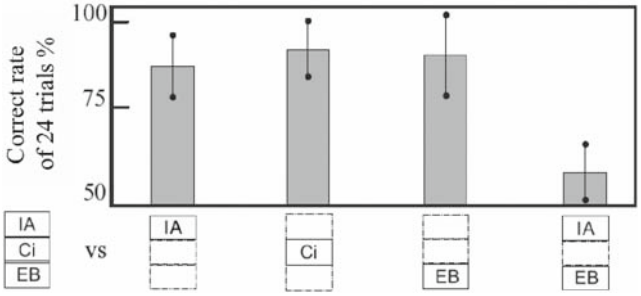

Fig. 2. Results of the odor discrimination experiment

properties. For this purpose, a 3-layered feed-forward neural network was added and trained by using a known biological data set. The predicted activity patterns were used as the input of the model for further "attention" processing. The simulation results were then examined through a comparison with the odor discrimination rates obtained from behavioral experiments on mice.

2 Biological insights

2.1 Olfactory system of mice

Figure 1 shows the basic structure of the olfactory system in mice, which consists of three parts: receptor neurons, the olfactory bulb, and the piriform cortex. Receptor neurons that are distributed on the surface of the nasal chamber express a single receptor from among 1000 different ones, and bind to specific odorants.[3] When odorant molecules bind to the receptor, its neurons are activated and sends signals to the olfactory bulb. The axons from the receptors that express the same gene terminate at the same point on the surface of the olfactory bulb.[4] The terminals of these axons form a small, round cluster called a glomerulus. A 2D map of glomerular distribution can be associated with receptor genes as well as odorants, and is therefore called an odor map.[4]

As well as the glomeruli, mitral cells and granule cells are the principal neurons in the olfactory bulb. Signals from the glomeruli are input to the mitral cells, which are interconnected via the excitatory synapse. The granule cells receive inputs from the mitral cells and send inhibitory signals back. In general, the olfactory bulb is considered to perform feature extraction.[8]

The mitral cells transmit the signal to the pyramidal cells in the piriform cortex, which then transmit signals back to the granule cells in the olfactory bulb and indirectly inhibit the mitral cells. The piriform cortex is divided into the anterior piriform cortex (APC) and the posterior piriform cortex (PPC); the division of their functions remains slightly unclear. Generally, the piriform cortex is believed to be responsible for the identification of odors.[9]

2.2 Attention mechanism in the olfactory system

Okuhara and Nakamura[7] conducted a series of odor discrimination experiments on mice. First, the mice were trained to select a rewarded odor, such as [IA, Ci, EB], composed of three types of odorant. They were then required to discriminate among other odors that contained elements in odor [IA, Ci, EB], such as [IA] or [IA, EB]. Figure 2 outlines the results of the odor discrimination experiment performed with 10 mice, and indicates that most of them had difficulty in discriminating between [IA, EB] and [IA, Ci, EB]. This implies that they focused on a combination of the odorants [IA] and [EB] when learning the odor [IA, Ci, EB]. This mechanism is called "attention", and contributes significantly to the odor perception characteristics of mice, as described above.

3 Model of the olfactory system of mice

3.1 Structure of the proposed model

Figure 3 shows the structure of the proposed neural network model, which consists of three parts: odor reception, the olfactory bulb, and the piriform cortex. The odor reception model is a feed-forward neural network of 3 layers, which are the preprocessing layer ($l = 1$), the odorant layer ($l = 2$), and the receptor layer ($l = 3$). The neuron populations for each layer (${}^{l}N$) are ${}^{1}N = 80$, ${}^{2}N = 500$, and ${}^{3}N = 1805$. The olfactory bulb model consists of the glomerular layer ($l = 4$), the mitral layer ($l = 5$), and the granule layer ($l = 6$). The neuron populations in the olfactory bulb are ${}^{4}N = {}^{5}N = {}^{6}N = 1805$. These populations were determined based on the actual number of glomeruli distributed on the olfactory bulb.[10] The piriform cortex model consists of an APC layer ($l = 7$) and a PPC layer ($l = 8$) corresponding to the anterior piriform cortex and the posterior piriform cortex, respectively. The neuron populations of the APC and the PPC layers are ${}^{7}N = 1000$ and ${}^{8}N = 100$, respectively.

The connections between each layer in the olfactory bulb model and the piriform cortex model are set up based on the structure of the olfactory system described in Sect. 2.1,

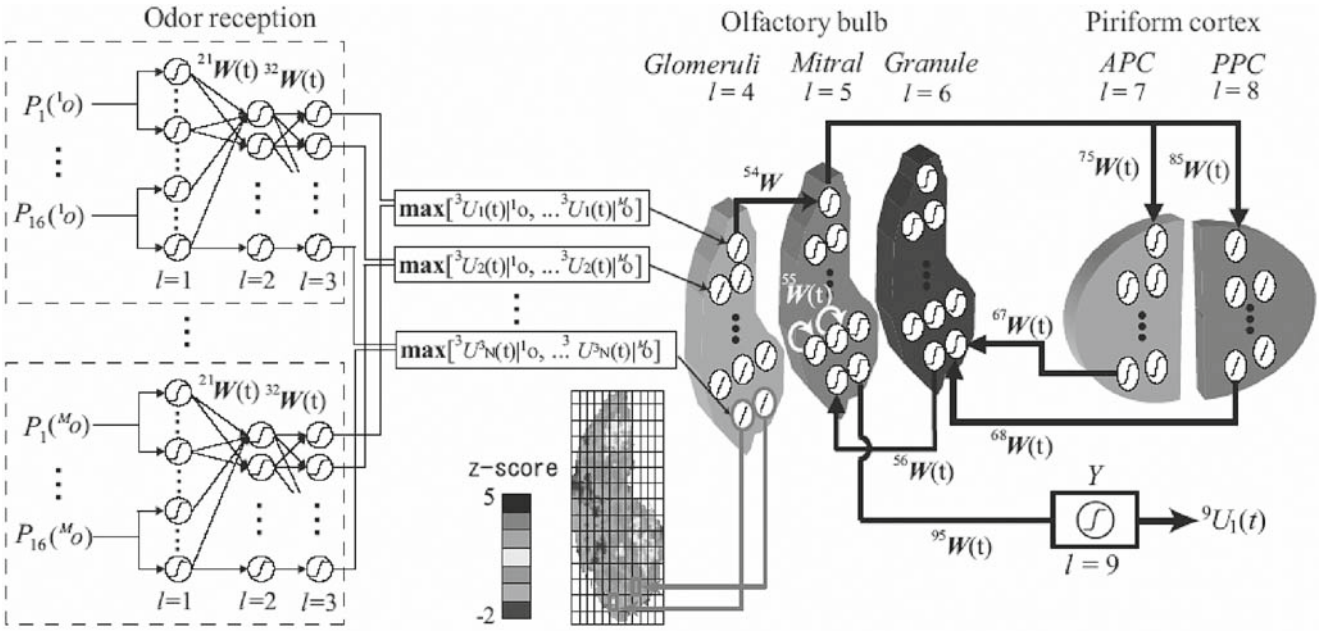

Fig. 3. Structure of the proposed model. The activity pattern of glomeruli is cited from Johnson and Leon[5]

with the exception that, for simplicity, the interconnections in each layer are not included in the model. In addition, a single neuron layer Y ($l = 9$) is artificially introduced as the output of the model.

The model takes the odorant properties as the input from the *preprocessing* layer. Since there are approximately 400 000 types of odorant (forming extremely high-dimensional information), it is impossible to input the odorant information to the model through binary coding. The properties of each odorant are therefore broken down into 16 numeric properties, as listed by Leon and Johnson,[11] along with their corresponding activity patterns.

In order to normalize the properties with different units and orders, the preprocessing layer converts the value of the properties into activated neuron numbers. This method is introduced based on the concept of population coding.[12] The neurons in the preprocessing layer are divided into 16 groups, each of which receives a different type of odorant property. The input to the neurons in the preprocessing layer is given by the equation

$$ {}^{1}u_s(t) = P_i({}^{m}o), \quad (s = (i-1)K + k, k = 1, 2, \ldots, K), \tag{1} $$

where ${}^{1}u_s(t)$ is the input to the s-th neuron in the preprocessing layer ($l = 1$) at time step t, ${}^{m}o$ is the m-th odorant in odor O, Pi is the i-th numeric property of the odorant mo, and K is the maximum number of neurons responsible for property P_i. The activities of the neurons are given by the sigmoid function

$$ {}^{1}U_s(t) = \frac{1}{1 + \exp\left(-{}^{1}\varepsilon_s\left({}^{1}u_s(t) - {}^{1}\theta_s\right)\right)}. \tag{2} $$

The outputs of sigmoid neurons in other layers are also calculated using Eq. 2. The threshold ${}^{1}\theta_s$ and the gradient ${}^{1}\varepsilon_s$ of the sigmoid function are determined according to the corresponding property by the equations

$$ {}^{1}\theta_s = k\frac{(P_{i,\max} - P_{i,\min})}{K}, \tag{3} $$

$$ {}^{1}\varepsilon_s = C_s\frac{(P_{i,\max} - P_{i,\min})}{K}, \tag{4} $$

where $P_{i,\max}$ and $P_{i,\min}$ are the maximum and minimum values of the property P_i in an odorant data set, respectively, and C_s is a constant.

The output of the preprocessing layer ($l = 1$) is input to the odorant layer ($l = 2$) through a connective weight matrix ${}^{1}\mathbf{W}(t)$. The input to the odorant layer is given by the equation

$$ {}^{2}u_n(t) = \sum_s {}^{21}w_{ns}(t)\,{}^{1}U_s(t), \tag{5} $$

where ${}^{2}u_n(t)$ is the input to the n-th neuron in the odorant layer, and ${}^{1}w_{ns}(t)$ is the connective weight between neuron units n and s, which is an element in the connective weight matrix ${}^{21}\mathbf{W}(t)$.

The output of the odorant layer is input to the receptor layer ($l = 3$) through ${}^{32}\mathbf{W}(t)$ in the same manner as Eq. 5.

The output of the receptor layer ($l = 3$) is passed to the glomerular layer ($l = 4$). According to Lin et al.,[13] the glomerular activity of an odorant mixture O can be represented by binary addition of the activities evoked by its odorant components. Thus, the input and output of the glomerular layer are determined by the equation

$$ {}^{4}u_e(t) = \max\left[{}^{3}U_r(t)\big|_{{}^{1}o} \ldots {}^{3}U_r(t)\big|_{{}^{M}o}\right]. \tag{6} $$

The output ${}^{4}U_e(t)$, which is calculated by Eq. 2, is an element in the activity pattern vector ${}^{4}U(t)$. Each element corresponds to a divided lattice of the activity patterns provided by Johnson and Leon,[5] as shown in Fig. 3.

The output of the glomerular layer is input to the mitral layer on a one-to-one basis. The detailed structure of the

olfactory bulb and piriform cortex part is described in our previous paper,[6] where the inputs and outputs of each layer are determined in the same manner as described above.

The inputs of the newly introduced Y (l = 9) layer represent the output of the model. Its output is determined by the input from the mitral layer, as the equation:

$$ {}^{9}U_1(t) = \frac{\exp\left(-{}^{9}\varepsilon_1\left({}^{9}u_1(t) - {}^{9}\theta_1\right)\right)}{1+\exp\left(-{}^{9}\varepsilon_1\left({}^{9}u_1(t) - {}^{9}\theta_1\right)\right)}. \tag{7} $$

To predict the glomerular activity patterns and perception characteristics affected by attention, the connective weights appearing in each equation must be appropriately adjusted. The next subsection describes the learning algorithm of the model.

3.2 Algorithm of the learning phase

The learning algorithm consists of two steps, whose details are described in this subsection.

3.2.1 The first step of the learning phase

In the first step, the connective weights ${}^{21}\mathbf{W}(t)$ and ${}^{32}\mathbf{W}(t)$ are adjusted for an accurate prediction of the activity patterns of the glomerular layer from the input odorants' properties as given by the training set. The connective weights are adjusted to minimize the error energy E:

$$ E = \frac{1}{2}\sum_{i}^{{}^{4}N} e_i = \frac{1}{2}\sum_{i}^{{}^{4}N}\left({}^{4}U_i - a_i\right)^2, \tag{8} $$

where e_i is the mean square error (MSE), ${}^{4}U_i$ is the output of the glomerular layer, and a_i is the activity of actual glomeruli in the i-th lattice. For the implementation of weight adjustment, the RPROP algorithm proposed by Riedmiller and Braun[14] is utilized. This algorithm allows fast error convergence with a reasonable computer memory requirement. The connective weights are iteratively adjusted until a preset maximum iteration number is reached.

3.2.2 The second step of the learning phase

In the second step, the connective weights in the olfactory bulb and piriform cortex are modulated based on the algorithm proposed by Soh et al.[6] Since most of the computational functions of the olfactory system, especially the connection from the piriform cortex to the olfactory bulb, are not yet clearly understood, signal transduction or connective weight modulation are hypothesized based on the odor discrimination experiment outlined in Sect. 2.2.[7] We assume that the connection from the piriform cortex to the olfactory bulb plays a role in extracting the most activated regions in the glomeruli. With regard to these assumptions, we propose a learning algorithm that consists of the three steps outlined below.

In the first step, the connective weights ${}^{75}\mathbf{W}(t)$ and ${}^{67}\mathbf{W}(t)$ are modulated to subtract the background activity from the activated part of the mitral layer using the equations

$$ {}^{75}W_{zb}(t+1) = \alpha\,{}^{75}W_{zb}(t) + \beta\,{}^{5}U_b(t)\big|_{{}^{A}O}\,{}^{7}U_z(t)\big|_{{}^{A}O}, \tag{9} $$

$$ {}^{67}W_{gz}(t+1) = \alpha\,{}^{67}W_{gz}(t) + \beta\,{}^{7}U_z(t)\big|_{{}^{A}O}\,{}^{5}U_b(t)\big|_{\text{back}}. \tag{10} $$

This adjustment enables the model to compare the features of the memorized odor to the input odors using the comparison algorithm described in the next subsection.

3.3 Comparison algorithm

In the comparison phase, an arbitrary odor B is input to the model. The input to the Y layer can be calculated as follows:

$$ \begin{aligned} {}^{9}u(t)\big|_{{}^{B}O} &= \sum_{b}{}^{95}w_{1b}(t)\,{}^{5}U_b(t)\big|_{{}^{B}O} \\ &= \sum_{b}{}^{5}U_b(t)\big|_{{}^{A}O}\,{}^{5}U_b(t)\big|_{{}^{B}O} \end{aligned}. \tag{11} $$

Accordingly, calculating the input to the Y layer is equivalent to calculating the correlation between the current output ${}^{5}U_b(t)|^{B}{}_{O}$ and the memorized output ${}^{5}U_b(t)|^{A}{}_{O}$ of the mitral layer. The correlation is then converted to an index of dissimilarity by Eq. 7. It can be assumed that the mice tend to make wrong decisions when the outputs of the mitral layer are similar. Accordingly, the output of the model is considered to correspond with the results of the odor discrimination experiments on mice.[7]

4 Simulation

This section describes the simulations performed based on the algorithm described in the previous section.

4.1 The first step of the simulation

First, data on 70 odorants were selected from the 365 odorants provided by Leon and Johnson[11] as a training data set. Then, three odorants with identical structures but different carbon numbers were chosen and added to the set.

Figure 4 shows the outputs of the model after the training is completed. In Fig. 4, the molecules in the uppermost row are the input odorants followed by the actual activity patterns,[5] the output of the model, and a graph of the mean square errors (MSEs). The odorants with a gray background are included in the training set, while those with no background color are untrained odorants. This figure indicates that the model successfully predicted the activity patterns in the training data set with a prediction error MSE of below 0.002. The predicted activity patterns of untrained odorants were also close to the actual activity patterns, with MSEs ranging from about 0.007 to 0.015. Consequently, the model is capable of predicting the tendency for the activated parts of glomeruli to shift continuously along with the carbon number.[5]

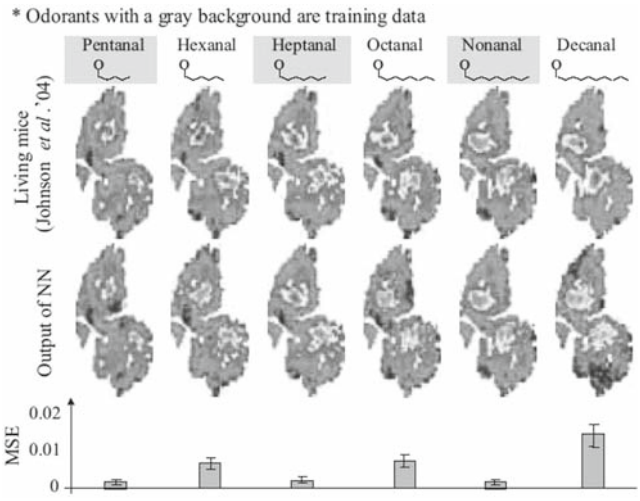

Fig. 4. Simulation results of aldehydes

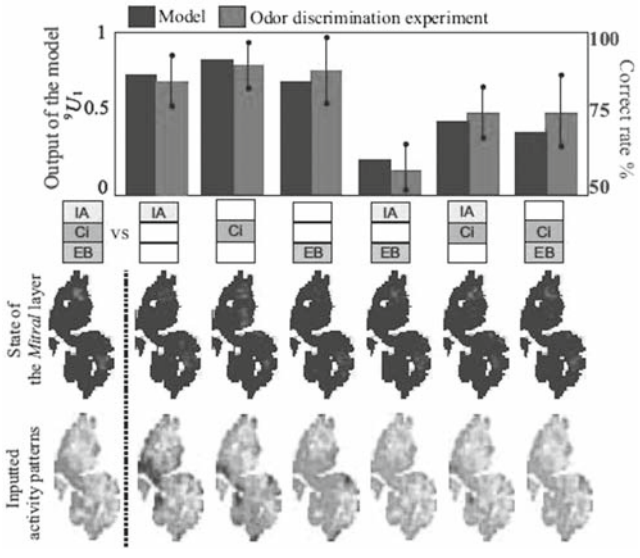

Fig. 5. Comparison between the results of the behavior experiments

4.2 The second step of the simulation

In the learning phase, an odor [IA, Ci, EB], representing an odorant mixture composed of isoamyl acetate, citral, and ethyl butyrate, is input to the proposed model. The connective weights are then adjusted according to the learning algorithm described in Sect. 3.2.2. The initial values of the connective weights are determined by uniform random values ranging between -10^{-5} and 10^{-5}.

After the learning phase, six different odors [IA], [EB], [Ci], [IA, EB], [IA, Ci], and [Ci, EB] are input to the model. Then the output of the neuron in the *Y* layer is compared with the correct rates in odor discrimination experiments on mice. In this step, the connective weights are fixed on the values determined in the first step of the simulation. The outputs of the glomerular layer to each odor are shown in the bottom row in Fig. 5.

The output of the mitral layer after the second learning phase is shown in the middle row, and the outputs of the neurons in the *Y* layer are plotted at the top. The discrimination rates obtained from the odor discrimination experiment on mice are also plotted beside the output of the *Y* layer.

Comparing the activity patterns of the glomerular layer with those of the mitral layer shows that the activated region becomes narrow, but its activity becomes stronger, which means that most activated regions in the glomerular layer were extracted. Figure 5 indicates a similar tendency between the correct rates and the output of the neurons in the *Y* layer; the higher the output, the higher the correct rate. From these results, we can conclude that the model is capable of accounting for the perception characteristics of mice to a certain extent through the assumed "attention" mechanism.

5 Conclusions

We have proposed a neural network model of the olfactory system of mice. Utilizing this model, we tried to predict the activity pattern in glomeruli evoked by odorants. The simulation results indicated that the model was capable of predicting the activity patterns of untrained odors with different carbon numbers, and showed consistency with those of odor discrimination experiments on mice. This ability to predict perception characteristics makes the model suitable as a basis for artificial organoleptic tests.

However, odors in nature are composed of odorants in different concentrations, which is not accounted for in the proposed model. Future studies must therefore include the odor coding manner for different concentrations. In addition, since the simulations were performed only with odorants [IA], [Ci], and [EB] using limited experimental data, further behavioral experiments and simulations need to be performed on other odorants to verify the ability of the model.

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