IEEE Access
Multidisciplinary ⋮ Rapid Review ⋮ Open Access Journal

Received January 9, 2020, accepted January 29, 2020, date of publication February 10, 2020, date of current version February 18, 2020.

Digital Object Identifier 10.1109/ACCESS.2020.2972946

A Perception-Driven Framework for Predicting Missing Odor Perceptual Ratings and an Exploration of Odor Perceptual Space

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This work was supported in part by the National Natural Science Foundation of China under Grant 61571140, and in part by the Guangdong Science and Technology Department under Grant 2017A010101032.

ABSTRACT There have been abundant research efforts on predicting verbal descriptions of odorants through the physicochemical features, physiological signals and E-nose signals. These approaches are interpreted as feature-driven methods in which the information about the inner links among different odor percepts is ignored. Different from that, we propose a perception-driven framework for predicting the missing odor perceptual ratings from other known odor percepts. Specifically, the work emphasizes pleasantness prediction based on level of importance in odor perception. In essence, this approach utilizes the relations among different odor perceptions, exploring the odor perceptual space subsequently. The missing perceptual ratings are predicted with an accuracy higher than 0.5 for more than half of the odor verbal descriptors, and almost half of the descriptors are predicted with a correlation higher than 0.8. The asymmetric clustering structure of odor perceptual space is revealed by feature selection for predicting the missing perceptual ratings. It is found that 'pleasantness' is primarily determined by 'sweet'.

INDEX TERMS Feature selection, perception-driven, perceptual ratings, pleasantness.

I. INTRODUCTION

Compared with vision and audition, the structure of olfactory perceptual space is a more challenging issue, which stems primarily from the more complicated physiology mechanism of olfactory perception [1], [2]. Besides the physiological complexity, olfactory perception is a comprehensive combination of genetic variation [3], individual experience [4], culture [5], [6] and psychology [7]; hence there is no general metric for quantifying it. To address the problem of olfactory perception description, a set of domain-specific odor verbal descriptors have been developed to profile the odorants [8], [9], such as 'sweet', 'fish', 'decayed'. These verbal descriptors, referred to as semantic attributes, can represent odorant perception reliably [10]. They constitute the odor perceptual space and can be considered as axises in the space [11]. However, the structure and dimensionality of odor perceptual space, as well as the relations among these descriptors, have been elusive [11]. The uncertainties of odor perceptual space are not obstacles for the practical use of odor descriptors, especially in perfume [12] and food industries [13].

There has been extensive demand in the industry for a systematic way to evaluate odor impression profiled by odor descriptors, leading to intense reasearch effort in the field. Due to the complexity of odor perception, numerous attributes and features have been used to predict odor impression. Chemical features, such as carbon chain length [14], [15] and molecular size [16] are correlated with odor impression. In addition to the single chemical feature, Keller *et al.* used thousands of chemical features to predict the perceptual ratings of 21 odor descriptors [17]. Nozaki *et al.* proposed an artificial neural network to predict the 138 odor descriptors of 999 odorants by mass spectrum [18]. Chang proposed a neural network for predicting odor perception by chromatography-mass spectrometry [19]. Due to the verbal representation of the odor perception, natural language

The associate editor coordinating the review of this manuscript and approving it for publication was Mehul S. Raval.

processing techniques are combined in olfactory perception and the distributional semantic representations of odor descriptors were used to predict odor perception [20], [21]. Among these odor descriptors, valence / pleasantness is the most salient one, so numerous works have focused on pleasantness prediction. Wu *et al.* proposed a convolutional neural network to predict the pleasantness of dozens of essential oils through the E-nose signals [22]. In addition to these physicochemical features, some physiological signals were also used to predict odor perception of odorants [23]–[26].

The research works described above adopt a similar approach – a set of highly efficient and effective odor identification algorithms using some kind of odorant's features or signals. These can be regarded as signal-driven or feature-driven methods, in which the relations among different odor percepts are not utilized and the information of odor perceptual space is not used. Moreover, most of these works just focus on a single odor descriptor's prediction such as pleasantness. There might be certain relations among different odor percepts, so some unknown odor percepts could be predicted by the other known odor percepts through the relations. For instance, if an odorant has a 'sweet' smell, it is more likely to be 'fruit' than 'garlic'. The relations among different odor percepts can reveal the structure of the odor perceptual space to some extent. For example, the distance between 'bakery' and 'sweet' should be closer than the distance between 'bakery' and 'decayed' in odor perceptual space. Motivated by these conceptions, we propose a perception-driven framework for predicting the perceptual ratings of a missing odor descriptor by the other known odor percepts through the relations among them, with the aim to reveal structure of the olfactory perceptual space. Particularly, our work emphasizes the prediction of pleasantness based on the level of importance in the odor perceptual space.

The main contributions of our work are summarized as follows.

1) A perception-driven framework for predicting the missing perceptual ratings over a set of descriptors is proposed. The predictions are not based on any odorant's features, but instead on the relations among these odor percepts. Considering the moderate size of the olfactory dataset, SVR is used. It is a machine learning method with moderate complexity for predicting perceptual ratings of the missing odor perception. A new metric called probability of error-ratio per sample is introduced to measure the performance of the predictive model.

2) Random forest (RF), LASSO, and Pearson correlation are applied to find the most important input features for prediction of missing perceptual ratings. The negative, positive and neutral effects of input features on the missing perceptual ratings are validated.

3) An exploration of the odor perceptual space is conducted. The asymmetric clustering structure of the odor perceptual space is revealed to some extent.

The remainder of this paper is as follows. Section II presents the related work of the representation and prediction of olfactory perception. Section III presents the method and material. The experiments and results are reported in Section IV. The discussion is presented in Section V. Finally, the conclusion and future work are shown in Section VI.

II. RELATED WORK

A. DESCRIPTION OF OLFACTORY PERCEPTION

There are two principal methods to characterize odors in practical applications: reference odorant methods [27] and semantic methods [28], [29]. Semantic methods are most frequently used for describing odor characters. Each odor descriptor can be expressed as a numeric rating [29] or a binary number [30], 1 representing the presence of odor descriptors, and 0 representing the absence.

Considering that odor description can be influenced by personal experience and subjectivity, resulting in bias in the assignment of odor profiles, the use of a panel is recommended [31]. There are hundreds of linguistic odor descriptors, so the fundamental problems to solve in odor representation are setting an appropriate number of odor descriptors and selecting the most important ones that correspond to primary odor descriptors. Consensus about these problems has not been obtained, and ranges of perceptual ratings are also diverse [17], [29].

B. THE PREDICTION OF OLFACTORY PERCEPTION

The datasets used to predict odor perception are composed of two parts: attributes of the odorants called stimulus features and the perceptual ratings of odor descriptors called perceptual features. The perceptual ratings of odor descriptors for odorant molecules are olfactory psychophysical datasets. Many odor attributes are used to predict the odor percepts, including GC-MS, E-nose signals, mass spectrometry, electroencephalogram (EEG), functional magnetic resonance imaging (fMRI), chemoinformatic features, etc. The main drawback of the datasets used for odor perception prediction is the small scale. Each dataset contain only hundreds of samples. Also, most of the odor compounds are mono-molecular and the amounts of odorants are not the same in different datasets [17], [29].

Many statistic methods and machine learning approaches are applied in prediction of odor perception. Haddad *et al.* proposed a three-layered BP neural network to predict pleasantness ratings of 123 odorants through E-nose signals with above 80% similarity to average human ratings [32]. Support Vector Machine (SVM) was used to classify pleasant and unpleasant odors through EEG signals [26]. In both of these works, only pleasantness is predicted. Gutierrez *et al.* applied a semantics-based approach to infer the perceptual ratings of a large set of verbal descriptors, in which elastic net regression model was used to predict the perceptual ratings [33]. The linear model cannot reflect the non-linear relations and the semantic representations of the odor descriptors are not biased in any way to include more or less olfactory

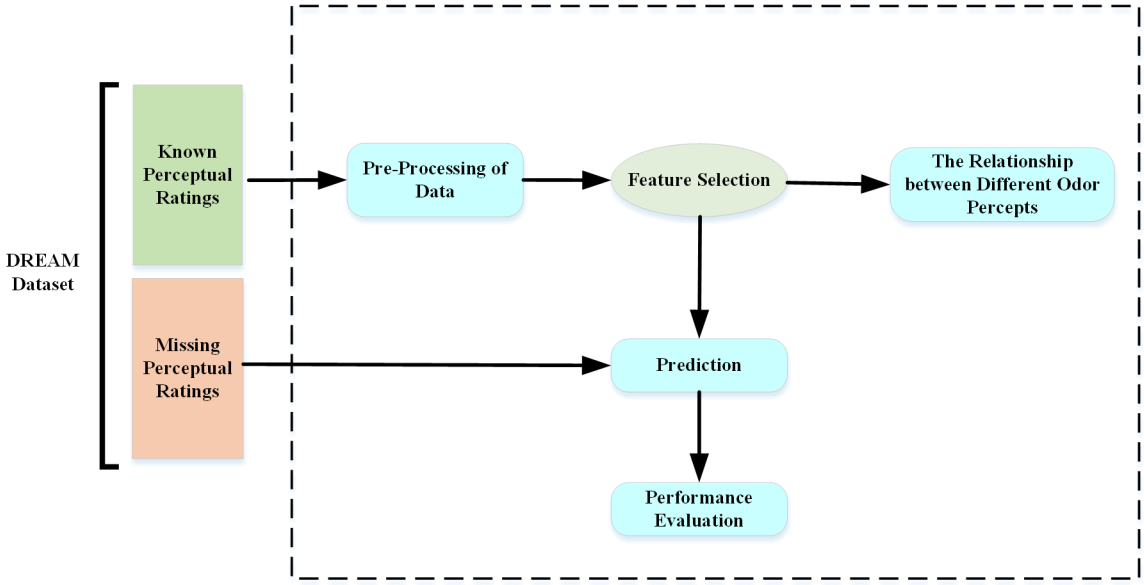


FIGURE 1. The framework for the prediction of missing odor perceptual ratings and exploration of odor perceptual space.

perceptual information. Li *et al.* applied a RF model to predict the perceptual ratings of 21 odor descriptors for both population and individual perception from large-scale chemoinformatic features, and found that just a small set of physicochemical features were necessary for odor perception prediction. The correlation was no more than 0.6 and RF was used as both the feature selection model and regression model [34]. These methods succeeded in predicting odor perception; however, they only focused on stimulus, information of different odor percepts' correlation was not utilized.

C. OLFACTORY PERCEPTION SPACE

Odor perception space is viewed as a high dimensional space and the basic perceptual dimensions of olfaction remain unclear. There is no consensus on its dimension and structure, and it has been an extensively discussed issue. It is widely accepted that pleasantness or hedonic valence is the primary axis of the odor perceptual space [35]. Khan *et al.* applied principal component analysis (PCA) to reduce the dimensionality for both odor percepts and physicochemical descriptors and claimed that pleasantness was the primary axis of odor perception space [36]. Because PCA algorithm changes the original axis of the input space, pleasantness is not exactly the primary axis and the precise name of the primary axis is not well-defined. Kepple and Koulakov generated a perceptual space, in which a molecule's location defined its percept, by computing the geodesic distance between all molecule pairs and embedding with ISOMAP, but the olfactory space obtained from the five datasets was slightly different from each other [37]. Koulakov investigated the structure of olfactory space based on the Atlas of Odor Character Profiles (AOCP), which was a database of sensory responses of human observers to an array of odorants, and found that odorants in human olfactory space accumulated near a 2D curved manifold, a curved surface that could be locally approximated by a plane [38]. The natural system of coordinates of the 2D surface was used to equilibrate the density of odorants, but they did not correspond to any concrete odor perception. These studies of odor perceptual space can not be used directly to profile the odor in the industry due to their ambiguous meanings.

III. METHOD AND MATERIAL

We adopt the DREAM or Vosshall dataset for missing odor percept prediction [17]. Support Vector Regression (SVR) is conducted as the regression model for the prediction of the missing perceptual ratings. RF, LASSO, and Pearson correlation are applied to perform input feature selection. Due to the salient feature selection capability of RF, RF will be combined with SVR to predict the missing perceptual ratings. The relations among different odor descriptors and the structure of odor perceptual space are explored through these three feature selection approaches. The framework is shown in Fig. 1.

A. ODOR PERCEPTION DESCRIPTION DATASET

We use the DREAM or Vosshall dataset which is a psychophysical dataset. 21 perceptual attributes or descriptors are used to profile the odor impression. The 21 verbal descriptors are sweet, bakery, fruit, fish, garlic, spices, cold, sour, burnt, acid, warm, musky, sweaty, ammonia / urinous, decayed, wood, grass, flower, chemical, intensity / strength,

and valence / pleasantness. There are 476 different monomolecules in the DREAM dataset, and their odor perceptual ratings of 21 verbal descriptors range from 0 to 100, where 0 is 'extremely weak' and 100 is 'extremely strong' for intensity; 0 is 'extremely unpleasant' and 100 is 'extremely pleasant' for pleasantness; 0 is 'not at all' and 100 is 'very much' for 19 semantic attributes.

The perceptual-rating dataset forms a 476 × 21 matrix. This psychophysical matrix can be interpreted in two different ways. From a descriptors-as-points view, each column can be interpreted as the characterization of the given semantic descriptions by several stimuli, which are vectors of 476 dimensions; from a stimuli-as-points view, each row can be treated as the characterization of a stimulus by several verbal descriptors, which are vectors of 21 dimensions. Each row also reflects the relations among these odor percepts.

B. PRE-PROCESSING OF DATA

One of the 21 odor descriptors is taken as the 'missing odor perception' and the rest are the ' known odor perceptions'. The perceptual ratings of missing odor perception are the targets for prediction. The perceptual ratings of 20 known descriptors are treated as input features. They are scaled to values between 0 and 1. The preprocessing formula is given as:

$$\mathrm{x}' = \frac{\mathrm{x} - \mathrm{x}_{min}}{\mathrm{x}_{max} - \mathrm{x}_{min}} \tag{1}$$

where x is the original values and x′ is the scaled values. x_{min} and x_{max} are the maximum and minimum of each input feature, respectively.

C. FEATURE SELECTION

1) RANDOM FOREST

Random forest (RF) is an ensemble machine learning algorithm for classification and regression, which contains numerous decision trees. RF is also a feature selection algorithm for obtaining the importance index of each input feature, and it makes the most important feature prominent. To obtain the importance index of each known feature, RF is trained on the DREAM dataset of 476 molecules. The input for the RF model is the perceptual ratings of 20 known odor percepts and the output is the perceptual ratings of the missing odor percept. Then the out of bag error of each known input feature for each decision tree is calculated. The out of bag error of j_{th} decision tree for k_{th} input feature is given as:

$$errOOB^{j}_{1k} = \frac{1}{m}\sum_{i=1}^{m}\left(\|y^{(i)} - \hat{y}^{(i)}\|\right)^2 \tag{2}$$

where m is the total number of the samples out of bag, $y^{(i)}$ is the label of i_{th} sample, and $\hat{y}^{(i)}$ is the prediction of i_{th} sample.

After obtaining the out of bag errors of the k_{th} input feature for all decision trees, random noise is added to the k_{th} input feature. Then the out of bag error of each decision tree for all input features after adding noise is calculated. The out of bag error of j_{th} decision tree for k_{th} input feature after adding noise is given as:

$$errOOB^{j}_{2k} = \frac{1}{m}\sum_{i=1}^{m}\left(\|y^{(i)} - \hat{y}^{(i)}_{n}\|\right)^2 \tag{3}$$

where m, $y^{(i)}$ are defined as above, and $\hat{y}^{(i)}_{n}$ is the predicted value of i_{th} example after adding noise.

The importance index of k_{th} input feature can be obtained from $errOOB^{j}_{1k}$ and $errOOB^{j}_{2k}$. The importance index of k_{th} input feature is given as:

$$IM_k = \frac{1}{N}\sum_{j=1}^{N}\left(errOOB^{j}_{2k} - errOOB^{j}_{1k}\right) \tag{4}$$

where N is the total number of decision trees.

2) LASSO REGRESSION

LASSO regression is one of the most classical regression algorithms. L_1 norm is the regularization term, which forces some of the feature coefficients to be 0. The sparse constraint results in dimension reduction or feature selection. The perceptual ratings of 20 known odor percepts are the input of the LASSO model. The perceptual ratings of the missing odor percept are the output target. The cost function is given as:

$$\mathcal{L}(\mathrm{w}, \lambda) = \frac{1}{M}\sum_{i=0}^{M}\left(y^{(i)} - \mathrm{w}^{\mathrm{T}}\mathrm{x}^{(\mathrm{i})}\right)^2 + \lambda\|\mathrm{w}\|_1 \tag{5}$$

where M is the size of training dataset, w is the weight vector, and λ is the regularization coefficient.

This is a convex optimization problem equivalent to:

$$\begin{aligned} &\min_{\mathrm{w,b}} \frac{1}{M}\sum_{i=0}^{M}\left(y^{(i)} - \mathrm{w}^{T}x^{(i)}\right)^2 \\ &s.t.\ \|\mathrm{w}\|_1 \le C \end{aligned} \tag{6}$$

where C is the radius of a L_1 norm ball. By optimizing (6), weight vector w is obtained.

3) PEARSON CORRELATION

To estimate the relations among different odor percept pairs, Pearson correlation coefficients are calculated pairwise between every two 476-dimensional perceptual vectors. Pearson correlation coefficient is defined as:

$$\rho_{ij} = \frac{(\mathrm{p}_i - \bar{\mathrm{p}}_i)\,(\mathrm{p}_j - \bar{\mathrm{p}}_j)}{\|\mathrm{p}_i - \bar{\mathrm{p}}_i\|_2\|\mathrm{p}_j - \bar{\mathrm{p}}_j\|_2} \tag{7}$$

where p_i, p_j are 476-dimensional perceptual vectors, and $\bar{\mathrm{p}}_i$, $\bar{\mathrm{p}}_j$ are the means of p_i, p_j respectively, and $\|\mathrm{p}_i - \bar{\mathrm{p}}_i\|_2$, $\|\mathrm{p}_j - \bar{\mathrm{p}}_j\|_2$ are L_2 norm, respectively. After calculating all the correlation coefficients between every two 476-dimensional odor perceptual vectors, a 21 × 21 symmetric Pearson correlation matrix is obtained.

D. SUPPORT VECTOR REGRESSION (SVR)

SVR is applied as the regression model to predict the missing odor perceptual ratings through the other known perceptual ratings. Twenty known perceptual ratings, as the input features, are denoted as $\mathrm{x} = [x_1, x_2, x_3, \ldots x_{20}] \in \mathcal{R}^{20}$. The missing perceptual ratings, as the target output, are denoted as $y \in \mathcal{R}$. The goal is to train the function to map the known input perceptual ratings x to the target missing perceptual ratings y. The model is expressed as:

$$f(\mathrm{x}) = \mathrm{w}^T \Phi(\mathrm{x}) + \mathrm{b} \tag{8}$$

where w is the weight vector, b is the bias, $\Phi(\mathrm{x})$ is called the kernel function and the Gaussian kernel is adopted. It is given as:

$$\Phi(\mathrm{x}) = e^{-\frac{\|\mathrm{x}-\mathrm{x}'\|^2}{2\sigma^2}} \tag{9}$$

where σ is the bandwidth controlling the local scope. The parameters of SVR are optimized by the following expression:

$$\begin{aligned} \min_{\mathrm{w},\mathrm{b},\xi_1,\xi_2} \ & \frac{1}{2}\|\mathrm{w}\|^2 + C\sum_{i=1}^{M}\left(\xi_i - \hat{\xi}_i\right) \\ s.t. \ & f(\mathrm{x}_i) - y_i \le \epsilon + \xi_i \\ & y_i - f(\mathrm{x}_i) \le \epsilon + \hat{\xi}_i \\ & \xi_i > 0, \ \hat{\xi}_i > 0 \qquad i = 1, 2, \ldots M \end{aligned} \tag{10}$$

where C is the regularization term, ϵ is the insensitive loss, and ξ_i, $\hat{\xi}_i$ are slack variables.

Considering that y_i is the perceptual rating, $f(\mathrm{x}_i)$ is the prediction of y_i, so it should satisfy the following constraint:

$$0 \le f(\mathrm{x}_i) \le 100$$

Finally, parameters of SVR are determined through optimizing (10).

E. PERFORMANCE METRICS

Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), R^2, Pearson correlation r are adopted as the performance metrics. RMSE is defined as:

$$\mathrm{RMSE}(\mathrm{x}, f) = \sqrt{\frac{1}{M}\sum_{i=1}^{M}\left(\hat{y}_i - y_i\right)^2} \tag{11}$$

where M is the total number of samples, y_i is the label of i_{th} sample, and $\hat{y}_i$ is the prediction of i_{th} sample.

MAE is defined as:

$$\mathrm{MAE}(\mathrm{x}, f) = \frac{1}{M}\sum_{i=1}^{M}\left|\hat{y}_i - y_i\right| \tag{12}$$

where M, y_i and $\hat{y}_i$ are defined as above.

R^2 is defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^{M}\left(\hat{y}_i - y_i\right)^2}{\sum_{i=1}^{M}\left(y_i - \bar{y}_i\right)^2} \tag{13}$$

where M, y_i and $\hat{y}_i$ are defined as above, and $\bar{y}_i$ is the mean of the target labels.

Pearson correlation coefficient is defined as:

$$r = \frac{\sum_{i=0}^{M}\left(y_i - \bar{y}_i\right)\left(\hat{y}_i - \bar{\hat{y}}_i\right)}{\sqrt{\sum_{i=0}^{M}\left(y_i - \bar{y}_i\right)^2}\sqrt{\sum_{i=0}^{M}\left(\hat{y}_i - \bar{\hat{y}}_i\right)^2}} \tag{14}$$

where M, y_i, $\bar{y}_i$ and $\hat{y}_i$ are defined as above, and $\bar{\hat{y}}_i$ is the mean of the prediction values.

Besides those metrics above, a novel metric is proposed: the probability within 5% range of error-ratio per sample($\mathrm{PERPS}_{5\%}$).

1) THE PROBABILITY WITHIN 5% RANGE OF ERROR-RATIO PER SAMPLE($\mathrm{PERPS}_{5\%}$)

First, error-ratio per sample of i_{th} sample is defined as:

$$\mathrm{ERPS}_i = \frac{|y_i - \hat{y}_i|}{y_i} \tag{15}$$

Then, $PERPS_{5\%}$ is defined as:

$$\mathrm{PERPS}_{5\%} = \frac{M_{5\%}}{M} \times 100\% \tag{16}$$

where the $M_{5\%}$ is the number of samples whose ERPS_i are within 5%, M is the total number of samples. Different from the metrics above, $\mathrm{PERPS}_{5\%}$ can reflect the details of error per sample, and complements the other metrics. The probability within 10% range of error-ratio per sample and the probability within 20% range of error-ratio per sample can be defined in the same way.

IV. EXPERIMENTAL RESULTS

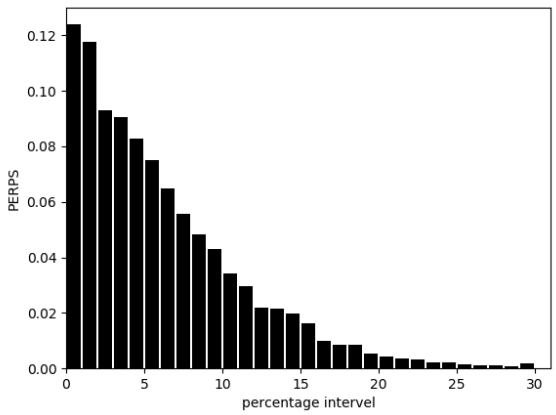
In this section, extensive experiments are conducted for predicting each missing odor percept with and without feature selection. Experimental settings are presented in Subsection A, the prediction of pleasantness ratings without feature selection is presented in Subsection B, feature selection for pleasantness prediction is presented in Section C, the prediction of pleasantness ratings with feature selection is presented in Subsection D, the predictions of the perceptual ratings of all the odor percepts without feature selection are presented in Subsection E, the predictions of the perceptual ratings of all the odor percepts with feature selection are presented in Subsection F, and an exploration of odor perceptual space is presented in Section G.

A. SETTINGS OF EXPERIMENT

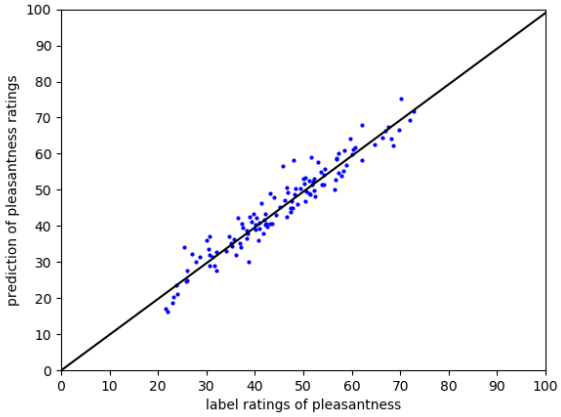
In the experiments, each known perceptual rating is first normalized into a value range from 0 to 1. In addition, ten-fold cross-validation is implemented. The detailed configuration of each base line is presented as follows.

1) For RF, 1000 estimators are used, iterating for 20 times to obtain a stable result of feature importance indices.

2) For LASSO, hyper parameter λ is searched in set $\{0.005, 0.001, 0.01, 0.1, 1\}$.



(a) PERPS of pleasantness prediction



(b) Pearson correlation of pleasantness prediction

FIGURE 2. PERPS and correlation of pleasantness prediction.

3) For SVR, it is implemented with the Gaussian kernel function. We take grid search for the best hyperparameters C and $\frac{1}{\sigma}$. The parameter C is searched in set {0.1,1,10,100,200}. The parameter $\frac{1}{\sigma}$ is searched in set {0.0001,0.001,0.1,1}. The number of iterations is 50.

B. THE PREDICTION OF PLEASANTNESS RATINGS WITHOUT FEATURE SELECTION

Due to the importance of pleasantness in odor perception, the pleasantness prediction is examined emphatically. To investigate whether pleasantness perceptual ratings could be inferred from the other 20 known odor perceptual ratings, all 20 known odor perceptual ratings are first used to predict the pleasantness ratings. SVR is adopted as the predicting model without feature selection and the predicted ratings of pleasantness are clamped within the range of 0 to 100. The results are reported in Table 1. The prediction of pleasantness rating has an R^2 around 0.92, a correlation around 0.96. The $PERPS_{5\%}$ is above 50% and the $PERPS_{10\%}$ is almost 80%. The detailed probabilities of ERPS are shown in Fig. 2, as well as the scatter diagram of the test dataset. To demonstrate the stability of the results, 50 iterations were implemented and the results are shown in Fig. 3. The results indicate that pleasantness can be inferred from other odor percepts. In other words, there are intrinsic connections among different odor percepts.

TABLE 1. The results of pleasantness prediction through 20 known odor percepts.

RMSE	MAE	R^2	correlation	$\mathrm{PERPS}_{5\%}$	$\mathrm{PERPS}_{10\%}$
3.53	2.69	0.92	0.96	51.5%	79.9%

C. FEATURE SELECTION FOR PLEASANTNESS PREDICTION

Although perceptual ratings of pleasantness are predicted very well by all the 20 known perceptual ratings, it is

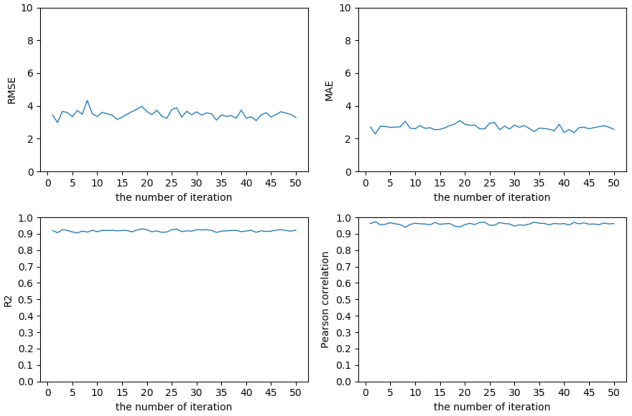
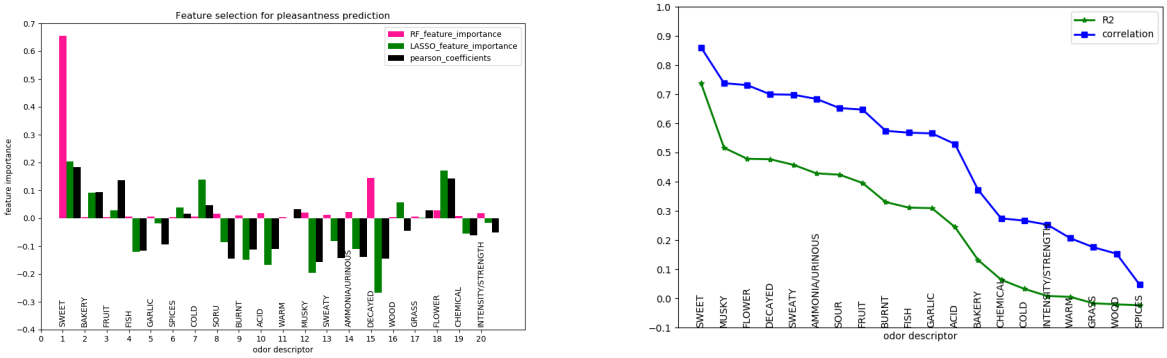


FIGURE 3. The performance of pleasantness prediction along with the iterations.

of interest to find out how many and which of them are essentially necessary for pleasantness prediction. To investigate this problem, we implemented feature selection by RF, LASSO, and the Pearson correlation matrix, with the aim to find the most important features for pleasantness prediction. The feature importance indices obtained by the three methods are shown in Fig. 4 (a), as well as the performance of pleasantness prediction through perceptual ratings of single known odor percept shown in Fig. 4 (b).

As shown in Fig.4 (a), for RF, the most important feature for pleasantness prediction is 'sweet', followed by 'decayed', 'flower', 'ammonia / urinous', 'musky', 'acid', etc. Except for 'sweet' and 'decayed', the importance of other odor perception all become rather faint, that is, the most salient features for pleasantness prediction are 'sweet' and 'decayed', but whether a feature selected by RF has a positive or negative effect on pleasantness prediction is not clear. For LASSO, the most important six features are 'decayed', 'sweet', 'musky', 'flower', 'acid' and 'burnt' in order. The coefficients of 'sweet' and 'flower' are positive whereas



(a) The results of three feature selection methods for pleasantness prediction (b) R^2 and correlation of pleasantness prediction by single known percept

FIGURE 4. The results of three feature selection methods for pleasantness prediction and R^2, correlation of pleasantness prediction through single known percept.

TABLE 2. Three odor-descriptor categories of pleasantness prediction.

categories	odor descriptors
positive category	sweet, flower, fruit, bakery
negative category	decayed, musky, sweaty, acid, sour, ammonia / urinous, fish, garlic, burnt
neutral category	chemical, intensity / strength, grass, cold, warm, wood, spices

the other four are negative. It follows intuition. It means that 'sweet' and 'flower' smell would make people pleasant, on the contrary, 'decayed', 'musky', 'acid' and 'ammonia / urinous' are offensive. Only the coefficient of 'warm' equals to 0. The coefficients of the rest odor percepts are not 0, and the magnitude of more than half of them are rather large. It shows that the results of LASSO are not sparse enough for feature selection, which means that it cannot pick the most important features while not suppressing the influence of each odor percept. Moreover, it should be pointed out that the signs of LASSO coefficients do not always indicate the positive or negative effect on odor perception prediction. For Pearson correlation, the six most important features are 'sweet', 'musky', 'decayed', 'sour', 'flower' and 'sweaty'. As expected, 'sweet' and 'flower' are positively correlated with 'pleasantness' while the other four are negatively correlated. According to Pearson correlation coefficients, these descriptors are classified into three categories based on their impact on pleasantness prediction. They are negative, positive, and neutral categories. The results are shown in Table 2. 'Sweet', 'flower', 'fruit' and 'bakery', which have correlations with pleasantness higher than 0.4, belong to positive category; 'decayed', 'musky', 'sweaty', 'acid', 'sour', 'ammonia / urinous', 'fish', 'garlic', 'burnt', which have correlations with pleasantness lower than -0.4, belong to negative category; 'chemical', 'intensity', 'grass', 'cold', 'warm', 'wood' and 'spices', which have a correlation with pleasantness between -0.3 and 0.3, belong to neutral category, having little effect on pleasantness prediction. Similar to LASSO, the results of the Pearson correlation are not sparse enough for pleasantness prediction. Moreover, the Pearson correlation matrix is symmetric, which does not agree with the criteria of odor perception. Meanwhile, pleasantness prediction through a single known odor percept is conducted and the results are shown in Fig. 4 (b), which coincides with the results of feature selection, that is, the odor percepts belonging to a strong positive or negative category for pleasantness prediction have better prediction performance, while the single-known odor percepts belonging to the neutral category have R^2 below 0.1, correlation below 0.3.

From the analysis above, it is concluded that RF is the most effective method for feature selection due to its sparsity and effectiveness. Combining RF, LASSO, and Pearson correlation, the relation between pleasantness and the other odor percepts could be revealed in details.

D. THE PREDICTION OF PLEASANTNESS RATINGS WITH FEATURE SELECTION

In this section, we combine RF and SVR to implement the prediction for perceptual ratings of pleasantness by using RF as the feature selection model and SVR as the regression model. The importance indices of the input features are determined by RF in order, then SVR is implemented as the feature number increases from 1 to 20. The results are shown in Table 3. When the number of known odor descriptors is more than two, the performance of pleasantness prediction tends to be flattened, especially when the number of input features is more than six. The performance smoothness implies that the perceptual ratings of pleasantness could be predicted precisely only through the combination of one positive and one negative odor percept. To demonstrate this hypothesis, another nine experiments were conducted, and the results are shown in Fig. 5. Fig. 5 (a) shows that the performance of pleasantness predictions of all the four positive descriptors are rather smooth, indicating that they are similar to each other, i.e. they belong to the same cluster or they are in vicinity in odor perceptual space. Similar conclusions are derived

TABLE 3. The performance of pleasantness prediction along with the increasing number of odor descriptors.

the number of features	descriptor added each time	RMSE	MAE	R^2	r	$PERPS_{5\%}$	$PERPS_{10\%}$
1	SWEET	6.58558	5.20970	0.71385	0.85078	0.28823	0.52185
2	DECAYED	4.84442	3.79263	0.82942	0.91900	0.39034	0.65168
3	FLOWER	4.79165	3.68649	0.84530	0.92731	0.39454	0.65252
4	AMMONIA	4.35725	3.39118	0.87042	0.93928	0.43193	0.70420
5	MUSKY	4.08901	3.19921	0.88789	0.94314	0.43067	0.72269
6	ACID	3.87929	3.06885	0.89475	0.95428	0.44496	0.75000
7	INTENSITY	3.85863	3.02489	0.89997	0.95094	0.44748	0.74369
8	SOUR	3.76617	2.97708	0.90243	0.95324	0.46975	0.76050
9	SWEATY	3.76563	2.96588	0.90191	0.95443	0.44118	0.76933
10	BURNT	3.56244	2.76081	0.90730	0.96024	0.48949	0.77899
11	CHEMICAL	3.55781	2.74985	0.91100	0.96095	0.48328	0.77941
12	GRASS	3.62111	2.78658	0.91009	0.95841	0.49323	0.78655
13	GARLIC	3.55640	2.75296	0.91082	0.96000	0.49697	0.78529
14	FISH	3.64993	2.83437	0.91113	0.95997	0.49731	0.76092
15	COLD	3.58608	2.75717	0.91104	0.95815	0.49622	0.77479
16	WOOD	3.58468	2.75871	0.91322	0.96038	0.50857	0.78235
17	SPICES	3.58524	2.80361	0.91728	0.95591	0.50826	0.78151
18	BAKERY	3.57322	2.74740	0.91984	0.95835	0.51299	0.79453
19	FRUIT	3.55711	2.71229	0.91789	0.95848	0.51470	0.79915
20	WARM	3.53370	2.69496	0.92054	0.95909	0.51513	0.79983

from the negative category and neutral category. Besides, the performances of the positive or negative category are much better than that of the neutral category. The R^2 of neutral category increases from 0.05 to 0.3, this index is too lousy for the prediction of the pleasantness, but the amount of increase indicates that there may be a great distance among those neutral descriptors so that this diversity forms a complementary for each other and an increasing performance through the combination of them is achieved. Fig. 5 (b) and (g) are the results of combining positive descriptors with negative descriptors for pleasantness prediction. The results of four positive descriptors combining with each one of the negative descriptors are shown in Fig. 5 (b). The result curves in Fig. 5 (b) show that a significant improvement in the performance of pleasantness prediction is achieved only by the combinantion of one positive descriptor and one negative descriptor except for the combination of 'bakery' and 'acid'. In Fig. 5 (g), the result curves are overall flattening, indicating that a positive descriptor combining with one or two negative descriptors can almost reach optimal performance and the other negative descriptors are redundant. Notably, the combination of 'sweet' and 'decayed' outperforms other combinations and these two descriptors are exactly the first two important features the RF has sought out. It is demonstrated that RF is a powerful algorithm for feature selection.

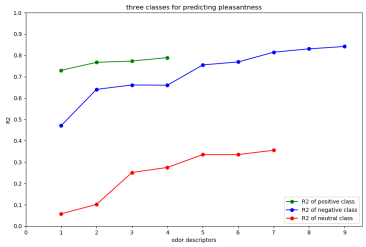
Fig. 5 (c) and (f) show the performance of pleasantness prediction of the combination of positive and neutral descriptors. Fig. 5 (c) shows the results of four positive descriptors combined with only one neutral descriptor. Fig. 5 (f) shows the results of four positive descriptors combined with neutral descriptors whose number of members change from 1 to 7. Prediction smoothness of all these curves reveals that the neutral descriptors have little impact on pleasantness prediction. Fig. 5 (e) and (h) show the results of combining negative and neutral descriptors, the similar conclusion can also be derived from the smoothness of these curves. It means that the combination with neutral descriptors has little performance improvement. On the contrary, the combination of positive and negative descriptors could improve the prediction performance remarkably, as shown in Fig. 5 (b), (d), (g) and (i). These results demonstrate the validity of RF feature selection and reveal the relations between these odor percepts and pleasantness to some extent.

E. THE PREDICTIONS OF THE PERCEPTUAL RATINGS OF ALL THE ODOR PERCEPTS WITHOUT FEATURE SELECTION

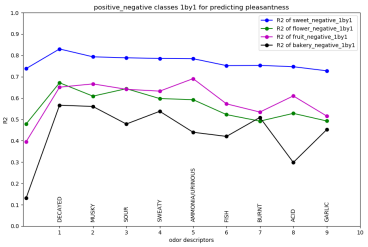
In this section, the predictions of the perceptual ratings were implemented for each of the odor descriptors by SVR through the other odor perceptual ratings without feature selection. The results are shown in Fig. 6. These results can be classified into three categories. The top team which has a R^2 higher than 0.8, r higher than 0.9, includes 'sweet' and 'pleasantness'. The medium team, which has a R^2 between 0.5 and 0.8 includes 'fruit', 'chemical', 'musky', 'sweaty', 'acid', 'sour', 'decayed', 'bakery', 'flower', 'garlic', 'ammonia / urious' and 'fish'. The bottom team, which has a R^2 lower than 0.5, includes 'burnt', 'intensity / strength', 'warm', 'wood', 'spices', 'cold' and 'grass'. It should be noted that all the correlations of the perceptual rating prediction of 21 odor descriptors are higher than 0.5. It means that they are not independent points and some of them can be inferred from the other odor perceptual descriptions precisely. Those with a R^2 less than 0.5 can be interpreted as independent points due to the feeble prediction through other odor percepts.

F. THE PREDICTIONS OF THE PERCEPTUAL RATINGS OF ALL THE 21 ODOR PERCEPTS WITH FEATURE SELECTION

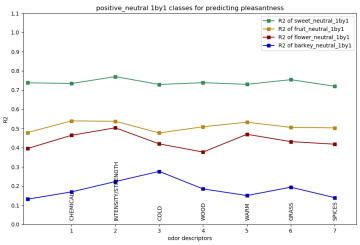
To investigate the relations among different odor percepts and seek the most important features for the prediction of the missing odor perception, RF was implemented for all odor percepts as a feature selection technology. Then SVR was applied to predict the missing perceptual ratings. The results are shown in Fig 7. It is shown that all the curves are rather flattening at the tail, that is, only less than four features are important for the missing percept prediction and particularly most of the missing percepts are determined



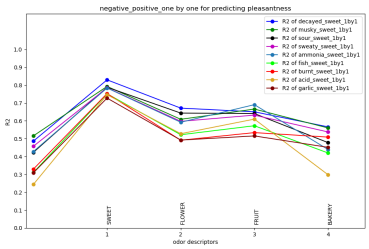
(a) The performace of the combination of each class



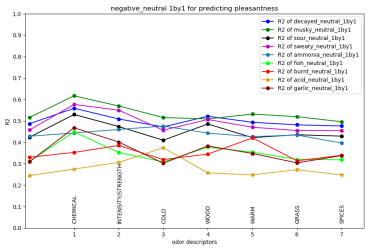
(b) Positve-plus-negative 1by1



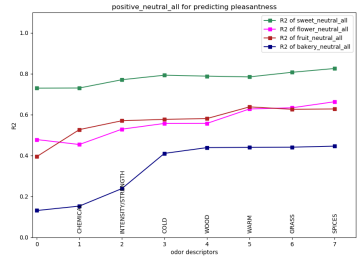
(c) Positive-plus-neutral 1by1



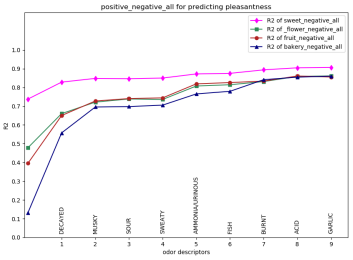
(d) Negative-plus-positive 1by1



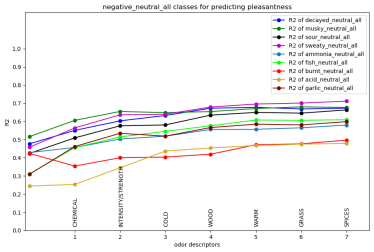
(e) Negative-plus-neutral 1by1



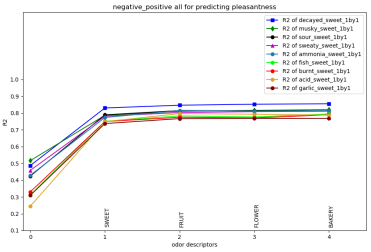
(f) Positive-plus-neutral all



(g) Positive-plus-negative all



(h) Negative-plus-neutral all



(i) Negative-plus-positive all

FIGURE 5. **The performance of different combination among three categories for pleasantness prediction.**

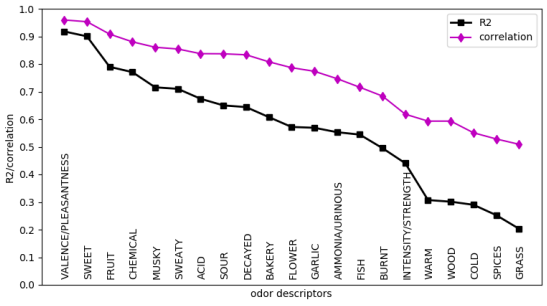


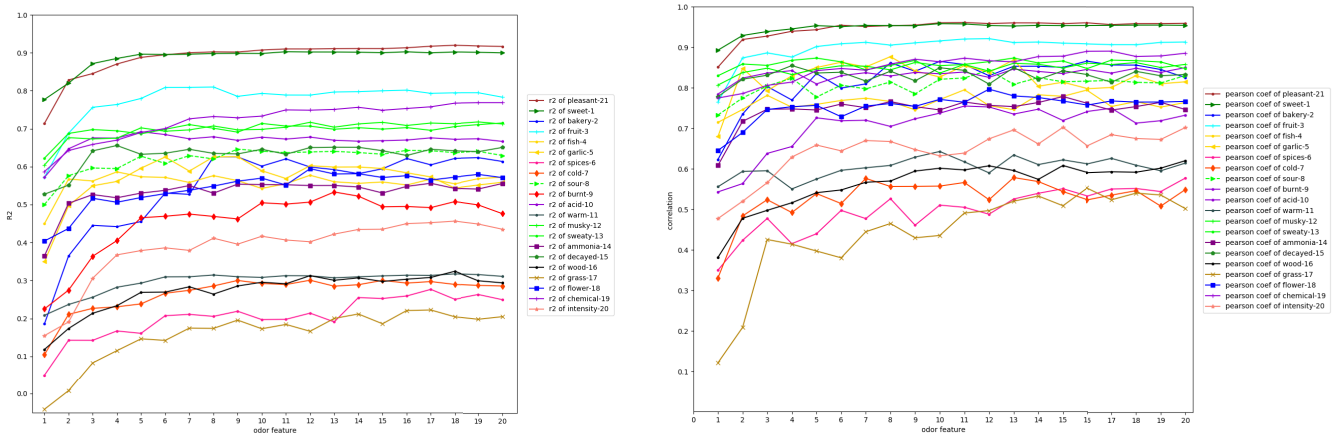
FIGURE 6. **The performance of 21 percepts prediction without feature selection.**

by only one or two input features. Notably, the perceptual ratings of 'pleasantness' and 'sweet' are predicted with R^2 above 0.9. The top three curves correspond to 'pleasantness', 'sweet' and 'fruit' with R^2 above 0.79. 15 out of the total 21 odor descriptors are predicted with correlations above 0.7.

G. EXPLORATION OF ODOR PERCEPTUAL SPACE

21 odor descriptors can be interpreted as axes in the olfactory perceptual space and they are not isolated to each other. To investigate the relations among these odor percepts, RF, LASSO, Pearson correlations are calculated as shown in Fig. 8. The labels of 1 to 21 represent sweet, bakery, fruit, fish, garlic, spices, cold, sour, burnt, acid, warm, musky, sweaty, ammonia / urinous, decayed, wood, grass, flower, chemical, intensity / strength, and valence / pleasantness, respectively. The coefficients with the odor percept itself are all set to 1 in those three feature selection results, that is, all the elements on the diagonal are 1.

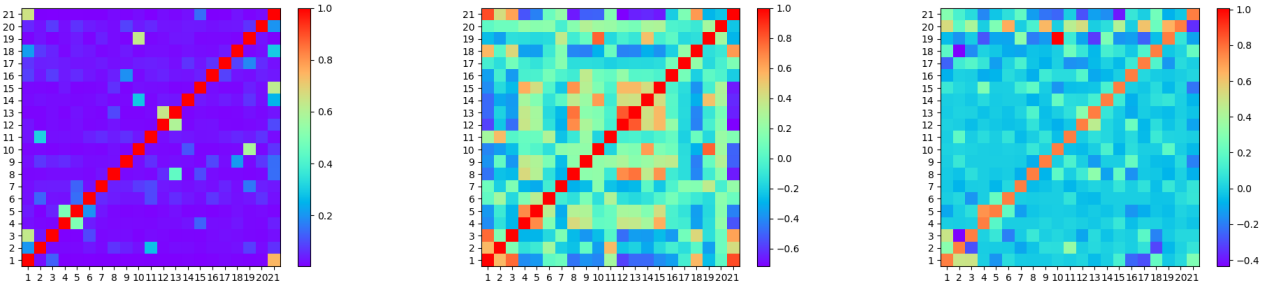
According to the previous analysis, the results of LASSO feature selection are not sparse enough and does not depress the effect of known perception belonging to the same cluster on missing odor perception prediction. Besides, it could not reflect the positive or negative effects on the prediction of the missing odor percepts. Pearson correlation determines the positive, negative or neutral effect on the missing odor prediction, but its symmetric property is not applied for the



(a) R^2 of the prediction of 21 odor percepts with feature selection

(b) Correlations of the prediction of 21 odor percepts with feature selection

FIGURE 7. The performance of the prediction of 21 odor percepts with feature selection.



(a) The results of RF feature selection

(b) The results of Pearson correlation feature selection

(c) The results of LASSO feature selection

FIGURE 8. The results of feature selection for all 21 odor percepts.

odor perceptual space and is not sparse. RF can find the most important features for the missing odor perception prediction, but it suppresses the effects of the features which is similar to the most important features for the prediction of the missing odors percepts and it could not confirm the positive or negative effect for the prediction of the missing odor percepts. Therefore, we combine the results of LASSO, RF and Pearson correlation, and take the sign of correlation coefficient as the sign of the importance indices of RF to obtain the ultimate feature importance with a positive or negative sign, as shown in Table. 4. At the same time, the results of LASSO are accounted for the features whose effects are suppressed by RF. Then we examine the relations among different odor percepts.

As shown in Fig. 8(a) and (c), the feature selection results are not thoroughly symmetric. For example, the RF importance index of 'sweet' for 'pleasantness' is 0.74416, while the RF importance index of 'pleasantness' for 'sweet' is 0.6541. This indicates that the relation between 'pleasantness' and 'sweet' is close, and could be clustered into one group, but their relation is not symmetric, that is, 'sweet' could predict 'pleasantness' more accurately than 'pleasantness' could predict 'sweet'.

In addition, it is found that, 'acid' and 'chemical' have high mutual importance indices, 0.5869 and 0.6341, and they can be predicted only by the other with a R^2 above 0.55. This indicates that 'acid' and 'chemicial' have a close relation with each other and can be clustered into one group, but the distance between them should be father than the distance between 'sweet' and 'pleasantness'. The mutual importance indices for 'fish' and 'garlic' are 0.5011, 0.4935. The mutual importance indices for 'sweaty' and 'musky' are 0.59587, 0.63915, therefore these odor descriptors can be clustered into the same groups. The importance of 'sweaty' for 'sour' is 0.4423, indicating that the distance between 'sour' and 'sweaty' are not too far. On the other hand, all the importance indices of 'burnt', 'intensity', 'warm', 'wood', 'cold', 'spices' and 'grass' are all below 0.3, and the sum of the first three importance indices is less than 0.5, resulting in the poor performance of their prediction, therefore these odor perceptual descriptors may be interpreted as independent points. Besides, The highest RF importance indices of 'bakery',

TABLE 4. The relations among different odor percepts.

	SWEET	BAKERY	FRUIT	FISH	GARLIC	SPICES	COLD	SOUR	BURNT	ACID	WARM	MUSKY	SWEATY	AMMONIA	DECAYED	WOOD	GRASS	FLOWER	CHEMICAL	INTENSITY	PLEASANTNESS	R^2
SWEET	1	0.0216	0.1273	-0.0045	-0.0063	0.0038	0.0048	-0.0044	-0.0039	-0.0034	0.0047	-0.0055	-0.0060	-0.0080	-0.0042	-0.0075	-0.0149	0.0103	-0.0067	0.0077	0.7442	0.9001
BAKERY	0.2055	1	0.0156	-0.0153	-0.0138	0.0307	-0.0158	-0.0684	0.0445	0.0238	-0.2758	0.0120	-0.0184	-0.0181	-0.0123	-0.0194	-0.0190	-0.0260	-0.0828	0.0179	0.0646	0.6076
FRUTI	0.6315	0.0327	1	-0.0059	-0.0066	-0.0943	0.0137	-0.0175	-0.0199	-0.0082	0.0179	-0.0135	-0.0091	-0.0113	-0.0101	-0.0182	0.0229	0.0200	-0.0125	0.0112	0.0231	0.7896
FISH	-0.0224	-0.0125	-0.0104	1	0.5011	0.0399	-0.0185	0.0141	0.0159	0.0139	0.0128	0.0199	0.0185	0.0284	0.1296	0.0208	-0.0187	-0.0321	-0.0149	0.0131	-0.0424	0.5442
GARLIC	-0.0371	-0.0057	-0.0458	0.4935	1	0.1977	-0.0322	0.0125	0.0104	-0.0119	0.0074	0.0140	0.0242	0.0086	0.0113	0.0074	-0.0132	-0.0238	-0.0147	0.0177	-0.0110	0.5689
SPICES	0.0244	0.1333	-0.0273	0.0245	0.1459	1	-0.0549	-0.0382	0.0290	-0.0293	0.0951	-0.0271	-0.0591	-0.0337	-0.0206	0.0709	-0.0388	-0.0251	-0.0318	0.0660	0.0247	0.2523
COLD	0.0221	-0.0382	0.0386	-0.0397	-0.1317	-0.0258	1	-0.0439	-0.0444	0.0762	-0.0956	-0.0339	-0.0299	0.0216	-0.0318	-0.0215	0.0489	0.0214	0.1598	-0.0426	0.0325	0.2898
SOUR	-0.0130	-0.0140	-0.0187	0.0186	0.0202	-0.0141	-0.0280	1	0.0157	0.0197	-0.0135	0.0583	0.4422	0.0107	0.0994	-0.0199	-0.0131	-0.0129	-0.0010	0.0124	-0.1455	0.6501
BURNT	-0.0222	0.0713	-0.0453	0.0564	0.0351	0.0187	-0.0208	0.0228	1	0.0187	0.0618	0.0175	0.0224	0.0208	0.0114	0.0925	-0.0213	-0.2081	0.0161	0.0727	-0.1441	0.4945
ACID	-0.0123	-0.0133	-0.0102	0.0152	-0.0098	0.0125	0.0107	0.0247	0.0109	1	-0.0163	0.0145	0.0122	0.1116	0.0111	0.0114	-0.0149	-0.0162	0.5869	0.0152	-0.0701	0.6740
WARM	0.0299	0.3095	0.0226	0.0249	0.0224	0.0424	-0.0585	-0.0389	0.0638	-0.0326	1	-0.0210	-0.0379	-0.0314	-0.0245	0.0262	-0.0374	0.0520	-0.0379	0.0686	0.0177	0.3071
MUSKY	-0.0293	-0.0097	-0.0197	0.0145	0.0234	-0.0116	-0.0153	0.0275	0.0127	0.0129	-0.0109	1	0.5959	0.0129	0.0240	0.0257	-0.0117	-0.0113	-0.0142	0.0200	-0.0969	0.7155
SWEATY	-0.0097	-0.0103	-0.0197	0.0099	0.0268	-0.0143	-0.0107	0.0933	0.0094	0.0087	-0.0162	0.6392	1	0.0094	0.0168	0.0131	-0.0103	-0.0121	-0.0253	0.0148	-0.0301	0.7099
AMMONIA	-0.0164	-0.0252	-0.0197	0.0190	0.0149	-0.0164	0.0276	0.0136	0.0138	0.2874	-0.0150	0.0340	0.0312	1	0.0334	0.0242	-0.0378	-0.0256	0.0663	0.0230	-0.2551	0.5529
DECAYED	-0.0153	-0.0128	-0.0107	0.0327	0.0098	-0.0111	-0.0138	0.0643	0.0099	0.0240	-0.0210	0.0194	0.0095	0.0123	1	-0.0211	-0.0114	-0.0116	-0.0441	0.0232	-0.6221	0.6438
WOOD	-0.0840	-0.0339	-0.0792	-0.0368	-0.0564	0.0331	-0.0213	-0.0426	0.1946	0.0172	0.0367	0.0471	0.0308	0.0282	-0.0442	1	0.0864	-0.0287	0.0218	-0.0431	-0.0339	0.3012
GRASS	-0.0706	-0.0427	0.0456	-0.0364	-0.0290	-0.0280	0.0363	-0.0224	-0.0261	-0.0399	-0.0439	-0.0381	-0.0222	-0.0685	-0.0321	0.0666	1	0.0875	-0.1824	-0.0574	0.0242	0.2032
FLOWER	0.2164	0.0752	0.0486	-0.0138	-0.0423	-0.0332	0.0130	-0.0192	-0.0354	-0.0131	0.0213	-0.0221	-0.0159	-0.0257	-0.0207	-0.0181	0.0353	1	-0.0121	-0.0216	0.2971	0.5718
CHEMICAL	-0.0090	-0.0277	-0.0081	-0.0193	-0.0381	-0.0102	0.0446	-0.0196	0.0086	0.6341	-0.0133	-0.0190	-0.0315	0.0326	-0.0124	0.0144	-0.0149	-0.0085	1	0.0276	-0.0063	0.7705
INTENSITY	0.0532	0.0272	0.0788	0.0223	0.0680	0.0402	-0.0301	0.0195	0.0881	0.0369	0.0524	0.0289	0.0270	0.0353	0.0349	-0.0243	-0.0306	-0.0329	0.0680	1	-0.2010	0.4404
PLEASANTNESS	0.6541	0.0045	0.0043	-0.0054	-0.0056	0.0045	0.0053	-0.0170	-0.0103	-0.0185	0.0039	-0.0213	-0.0126	-0.0234	-0.1449	-0.0045	0.0059	0.0276	-0.0085	-0.0182	1	0.9178

'flower' and 'ammonia / urious' are all less than 0.3, which means that they can be interpreted as independent points, but the sum of the first three importance is more than 0.5, which lead to R^2 of their prediction is above 0.5.

V. DISCUSSION

The aim of this paper is to explore the relations among different odor percepts and reveal the structure of the odor perceptual space. To this end, the predictive model is established, in which the known odor perceptual ratings are the input, and the missing odor perceptual ratings are the output.

The results in this paper indicate that the relations between different odor percepts are different and asymmetric. The different distances between odor percepts in odor perceptual space may imply that odor percepts which are in a vicinity could be clustered into the same group, and the asymmetric relations among different odor percepts may imply a hierarchical structure of the odor perceptual space. These findings are in consistent with those in [38]. Moreover, some odor percepts can be predicted precisely through the other odor percepts. Different from the previous feature-driven methods for predicting the target odor perceptual ratings [17]–[19], [22], [24]–[26], [30], [32]–[34], [36], [37], a perception-driven framework is proposed to predict the perceptual ratings of missing target odor percepts with a much better performance, and some rules of olfactory perception psychology are revealed to some extent, which could not be obtained though feature-driven methods.

In summary, these findings form the foundation of olfactory perception psychology, and they are important for the identification of primary odor percepts.

VI. CONCLUSION

This paper proposes a perception-driven framework for predicting the perceptual ratings of the missing odor percepts through other known perceptual ratings. This model comprises two parts: using RF to implement feature selection and using SVR to predict the missing perceptual rating. This approach can predict perceptual ratings through only the known perceptual ratings, without the need of any other physicochemical features nor a small set of general olfactory perceptual descriptors. This model can be extended to mixture odorants. The result is much better than that in [17], especially for 'sweet' and 'pleasantness', in which the R2 is higher than 0.9.

This paper also explores the structure of the odor perceptual space. The essence of this predicting approach is to exploit the relations among different odor percepts, so it can reveal the structure of the odor perceptual space to some extent. The present work demonstrates that the odor descriptors are clustered into different asymmetric categories. Also, it guarantees the axes of the odor perceptual representations is understandable by feature selection to reduce the dimension of input perceptual features. This result is useful for choosing the most appropriate general odor descriptors when launching odor psychophysical experiments for research or in the application in the industry, such as food, perfume odor test.

It is also beneficial for the identification of the primary odor descriptors.

Several limitations of the current approach need to be mentioned. In this paper, isolated odor descriptors are not predicted well enough. To address this, additional features could be used. The structure of the odor perceptual space is not adequately detailed, so more powerful model, such as deep neural network, could be applied. The number of odor descriptors necessary for constituting the odor perceptual space remains elusive. Natural language processing technique could be introduced to solve this problem. Despite these limitations, our work could be a solid foundation for these extensions.

ACKNOWLEDGMENT

The authors would like to thank IEEE Access journal and their respective Universities for their respective support.

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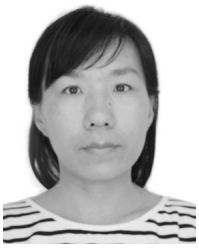

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