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Thesis Outline

Olfactory perception from its chemoinformatic parameters such as mass spectrum of odorant molecules is an important topic in machine olfaction domain. Typical task of machine olfaction focused on odor classification and mixture identification. However, higher abstract levels of information such as linguistic information associated with odor impressions have been rarely studied.

In the domain of odor impression prediction, the important issue to be solved is the imbalance problem, i.e., that means the number of target odor descriptors (for example, peach odor descriptor prediction) we want to predict is much smaller than the negative samples (non-peach samples). Although we have found a very few papers related to solving imbalanced problems of odor prediction using oversampling techniques, prediction performance improvement was limited due to restricted artificial data. Creating artificial samples can duplicate samples from the negative class and this increases the likelihood of overfitting especially for high oversampling rates when class skew was severe. For this reason, we solve the imbalance problem for the mapping of the mass spectrum of odorant molecules into the binary odor perceptual space without generating the artificial samples. Although there are different algorithms for imbalanced binary data classification, we utilized the method of one class support vector machine because it does not require equal proportions of positive-negative samples & neural network trained with weighted neural network to handle these large numbers of negative samples with small target odors.

Perfumers usually use linguistic information to express odors. If we can automatically extract sensing data for an odor impression, it will be useful to create scents. After successfully predicting the odor descriptors from the mass spectrum, our next target is the inverse model, which means, the prediction of the sensing data (mass spectrum) for an intended binary scent impression. Our target is to extract the sensing data for a given odor descriptor that will help perfumers to create scent although one-to-one relationships are not usually guaranteed. Result shows that more than one mass spectra associated with the given odor descriptors can be extracted. This study is first report for predicting sensing data for a given binary scent impression.

After experimenting with single odor molecules, we predicted the odor impression from the mixed scent that are more complex than mono-molecule chemicals. Previous studies tried to solve the odor mixture perception using the physicochemical features as an input. But this method cannot guarantee the perception of mixed scent because if we add the physicochemical properties of two mono-molecule odorants, it will only be the sum of those features which can be very different from the mixture. Thus, we considered the blends of mass spectrum of odorant molecules to predict odor impression since linear superposition is valid in mass spectrum. In our previous work, we utilized the mass spectrum of chemical mixtures such as essential oils. Followed by that work, we used the binary mass spectrum mixture of two different group essential oils to predict the scent impression. As this is the first time, we reported the mixture odor prediction using mass spectrum, we only predicted the sweet odor impression.