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Article / Book Information

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Title(English)	Exploration of Odor Components for Odor Reproduction Based on Mass Spectrometry
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論 文 要 旨

THESIS SUMMARY

系・コース： Department of, Graduate major in	Information and Communications Engineering	系 コース	申請学位（専攻分野）： Academic Degree Requested	博士 Doctor of	（Philosophy）
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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

Olfactory is one of the primary senses and plays an essential role in living organisms. It enables us to sense odorant stimuli which can cause a deep subconscious response of humans. Odorant stimuli are present in various ways and are indispensable in daily human life. It is widely known that humans can distinguish among around 10,000 with their roughly 400 types of olfactory receptors. Experts and people who work in an odorous environment can distinguish among more smells. Thus, there is a wide variety of odor-related samples available to be obtained. However, primary smells have not been known yet, unlike primary colors in vision. Hence, finding a set of odor components to cover a certain range of smells is indispensable for odor reproduction.

Odor reproduction can be achieved by blending different kinds of odor components to approximate the target odor. This odor reproduction method enables us to generate different odors by changing the blending recipe of odor components. The important point in odor reproduction is that the reproduced odor should be as close as possible to the target odor. The number of odor components should be as small as possible while it should cover a wide range of odors as possible.

On the other hand, unwanted compounds called fixatives used in odorant samples can also cause interference and contradictive results in odor component analysis. Such compounds appear in the odorant analysis, especially when using mass spectrometry, but the human nose cannot sense them. This causes a problem when we want to increase the odorant samples to be analyzed. Hence, a method for the removal of interference before odor component analysis is needed.

In the present study, mass spectra of 185 essential oils were analyzed for odor reproduction. Nonnegative matrix factorization (NMF) was utilized for odor component analysis, and the nonnegative least squares method was utilized to calculate the recipe for odor reproduction. Moreover, we regarded the small peaks that appear in the high m/z region (more than 150 m/z) of mass spectrometry as an important feature in the odorant analysis since humans tend to have high sensitivity to a slight change in the high m/z region. In this study, NMFs with Kullback-Leibler (NMF-KL) divergence and Itakura-Saito (NMF-IS) divergence as cost functions were compared. Both cost functions have different properties in treating small peaks. In addition, nonnegative least squares with IS divergence was utilized to calculate the recipe of odor reproduction based on NMF-IS, whereas ordinary nonnegative least squares method for was utilized NMF-KL. Furthermore, a sensory test was conducted to evaluate the result of both NMFs. Sensory test results revealed that approximated odor by NMF-IS was closer to the target one than the approximated odor by NMF-KL. Thus, the improvement of accuracy of odor approximation is possible when incorporating IS divergence as cost function with NMF than that of KL divergence.

Moreover, the study also presents a method to suppress interferences caused by unwanted compounds when we want to increase the number of odorant samples. Independent Component Analysis (ICA) was utilized on the mass spectra of odorant samples to remove the influence of unwanted compounds. The advantage of ICA in revealing independent components without apriori knowledge was utilized in this study. We applied ICA to mass spectra of essential oils and revealed that ICA could extract pure odor sample mass spectrum data without the influence of fixatives, even if the fixatives were added to the odor samples. Furthermore, we also applied ICA to the newly obtained 99 perfumes mass spectrum data where ICA could extract the pure perfume mass spectrum data without the influence of fixatives. The result also revealed the possibility to increase the number of odorant samples for odorant analysis without concern of interference by unwanted compounds. We also performed NMF analysis using the pure data extracted by ICA, which revealed the possibility of increasing the approximation accuracy due to the removal of interferences.

備考 ：論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。

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