

Fundamental Study on Chemical Data Analysis of Odors using Integrated Sensor Array and Machine Learning

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Thesis abstract

This thesis is devoted to a fundamental study on chemical data analysis of odors using integrated sensor array and machine learning. The chemical data analysis of odors plays an essential role in extracting crucial chemical information and monitoring physiology data for various applications in diverse fields such as the food industry, environmental monitoring, security surveillance, medicine, and healthcare which effectively improve the quality of the human lifestyle. However, although odor sensing-based integrated sensor arrays have demonstrated the feasibility of real-time monitoring of the above application, it is far from practical use, which will significantly restrict their further optimization and commercialization.

First, to extract the vast chemical information in odor, we present an automated method to identify multivariate chemo-/biomarker features of analytes in chromatography-mass spectrometry (MS) data by combining image processing and machine learning. Our approach allows us to comprehensively characterize the signals in MS data without the conventional peak picking process, which suffers from false peak detections. The feasibility of marker identification is successfully demonstrated in case studies of aroma odor and human breath on gas chromatography-mass spectrometry (GC-MS) even at the parts per billion level with a low error rate by comparison with the conventional method.

Second, by using the above approach, we demonstrate a preliminary study for the breath odor analysis and breath odor sensing-based individual authentication (fasting condition) using an integrated sensor array and machine learning. We successfully achieved a median accuracy of 96.4%. The impacts of several sensors (features) on the accuracy and reproducibility are demonstrated. However, the applicability of breath odor sensing in practical use needs to be justified.

Finally, we demonstrate a blood glucose prediction system by breath odor analysis. Multi-classification of blood glucose in a complex environment (fasting, drinking, exercise) can be achieved with high accuracy. Furthermore, recognizing different glucose spike patterns leads to blood glucose monitoring in daily life. Our findings in this study provide an essential foundation for a robust breath odor sensing-based integrated sensor array system in the predictable future