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FEATURE EXTRACTION AND SUPERVISED LEARNING FOR VOLATILE ORGANIC COMPOUNDS GAS RECOGNITION

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Abstract
The emergence of advanced technologies, particularly in the field of artificial intelligence (AI), has sparked significant interest in exploring their potential benefits for various industries, including healthcare. In the medical sector, the utilization of sensing systems has proven valuable for diagnosing pulmonary diseases by detecting volatile organic compounds (VOCs) in exhaled breath. However, the identification of the most informative and discriminating features from VOC sensor arrays remains an unresolved challenge, essential for achieving robust VOC class recognition. This research project aims to investigate effective feature extraction techniques that can be employed as discriminative features for machine learning algorithms. A preliminary dataset was used to predict VOC classification through the application of five supervised machine learning algorithms: k-Nearest Neighbors (kNN), Random Forest (RF), Support Vector Machines (SVM), Logistic Regression (LR), and Artificial Neural Networks (ANN). Ten feature extraction methods were proposed based on changes in sensor response as inputs to classify three types of gases in the dataset. The performance of each model was evaluated and compared using k-Fold cross-validation (k=10) and metrics derived from the confusion matrix. The results demonstrate that the RF model achieved the highest mean accuracy and standard deviation, with values of 0.813 ± 0.035, followed closely by kNN with 0.803 ± 0.033. Conversely, LR, SVM (kernel=Polynomial), and ANN exhibited poor performances when applied to the VOC dataset, with accuracies of 0.447 ± 0.035, 0.403 ± 0.041, and 0.419 ± 0.035, respectively. Therefore, this paper provides evidence that classifying VOC gases based on sensor responses is feasible and emphasizes the need for further research to explore sensor array analysis to enhance feature extraction techniques.

Author Keywords
feature extraction; Gas classification; Supervised machine learning; VOC Sensor; Volatile Organic Compound

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