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Environmental odor detection and classification with electronic nose system

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ABSTRACT

A prototype of an electronic nose (e-nose) system integrating a set of general-purpose gas sensors, an electronic module, and signal processing and classification methods has been designed and implemented to detect certain environmental odors that might pose a risk to human health. The proposed device explores the filter diagonalization method (FDM), an advanced signal processing technique for accurate spectral estimation, to detect the presence of odors together with random forest (RF), a popular machine learning algorithm, to classify the features of such spectra. Experimental results show that the proposed FDM-RF approach can recognize the targeted odors with an accuracy of 96.4%.

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1. INTRODUCTION

Mimicking human olfaction, which involves replicating the ability to detect and identify distinct odors, can be achieved using electronic noses (e-noses). E-noses encompass various sensors that detect and measure odors in their surroundings, each sensor responding differently to create unique patterns or "footprints" for each odor. Machine learning algorithms can then be trained on these footprints to recognize different odors.

E-noses have emerged as valuable instruments in various applications, from quality control in the food and wine industry to agriculture and environmental monitoring [1]-[3]. In particular, the scope of this technology in environmental monitoring is vast and fast-growing:

a. Air quality assessment: E-noses have been used to track air quality, detecting harmful pollutants like carbon monoxide, nitrogen dioxide, and volatile organic compounds (VOCs), among others [4], [5]. They also assist in tracking pollution levels, providing pertinent data for urban air quality management [6].
b. Water quality monitoring: E-noses can detect contaminants in water bodies by identifying odors associated with organic and chemical pollutants [7], [8].
c. Industrial emissions control: E-noses can assist in detecting fugitive emissions and leakage points ensuring compliance with environmental policies and regulations [9], [10].

d. Landfill monitoring: landfill sites emanate various odors that can be potentially pollutant and risky to human health. E-noses assist in detecting and monitoring these emissions, ensuring they remain within safe limits [11], [12].
e. Disaster response: in the event of chemical spills or natural disasters, e-noses can provide rapid assessments of air and water quality, guiding emergency response efforts better and faster [13], [14].

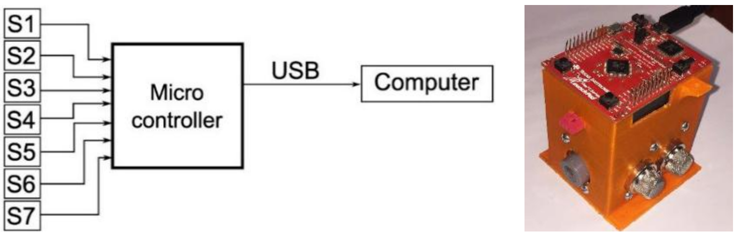
This work overviews the design and prototyping of a novel e-nose system devoted to air quality monitoring that exhibits some interesting features such as low cost and high portability. The prototype is capable of detecting certain odors that might pose a threat to human well-being such as smoke, combustible gas, methane, alcohol, hydrogen, and several organic gases. Moreover, our work explores the filter diagonalization method (FDM), a powerful spectral estimation technique that obtains reliable footprints from the odor temporal signals, together with random forest (RF), a robust machine learning technique to classify such footprints and recognize odors accurately.

The remainder of the paper is organized as follows: section 2 introduces the e-nose prototype, describes its associated methods (FDM and RF), and details the methodology used for the experimentation. Section 3 presents and discusses the findings of the study. Finally, section 4 concludes the paper by highlighting the main contributions and outlining perspectives for future work.

2. METHODS

2.1. Prototype

Figure 1(a) provides a system architecture overview of the proposed e-nose system. It encompasses seven different types of metal oxide semiconductor (MOS) sensors (S1-S7), a 32-bit microcontroller in charge of the sensors' signal acquisition and USB data transmission, and a computer, responsible for signal processing, classification, and data visualization. Figure 1(b) shows the prototype developed. It consists of a 3D-printed plastic case that hosts the set of sensors together with the electronic module and electrical connections. It is portable (mass: 500 g, dimensions: 6.5×5×7 cm) and low-cost (150 USD) [15]. Table 1 summarizes the target detection odors by each of the seven sensors in the device. Note that sensors react to a target odor but are also sensitive to secondary odors.



(a) (b)

Figure 1. E-nose system: (a) architecture and (b) prototype developed

Table 1. List of the MOS sensors in the device

Sensor	Target odor	Secondary odors
S1	Combustible gas	H_2, LPG, CH_4, CO, alcohol, and propane
S2	Alcohol	CO and H_2
S3	Methane	Propane and butane
S4	Carbon monoxide	H_2, LPG, and CH_4
S5	Hydrogen	CO
S6	Air quality	NH_3, NOx, alcohol, benzene, smoke, and CO_2
S7	Organic gases	acetone, alcohol, toluene, and hydrogen

The output signal from each sensor i is converted into a sinusoid $g(t)$ with variable frequency proportional to the odor concentration present at the time t, that is (1):

$$g_i(t) = sin\,[2\pi(f_0 + \Delta_i(t))t] \quad (1)$$

where f_0 is the carrier frequency of the signal (f_0=1 Hz) and $\Delta_i(t) = 0.1R$ is a variable term with R being a resistive proportionality constant that relates the odor concentration found in the sensor i at a given time t.

As example, Figure 2 shows the responses $g_i(t)$ of all seven sensors to butane. According to (1), the response will be a sinusoid of 1 Hz with amplitude 1 that increases its frequency according to the sensor's sensitivity to the odor. Note that sensor S1 is practically insensitive to butane while S3 is the sensor that exhibits the highest sensitivity to this odor.

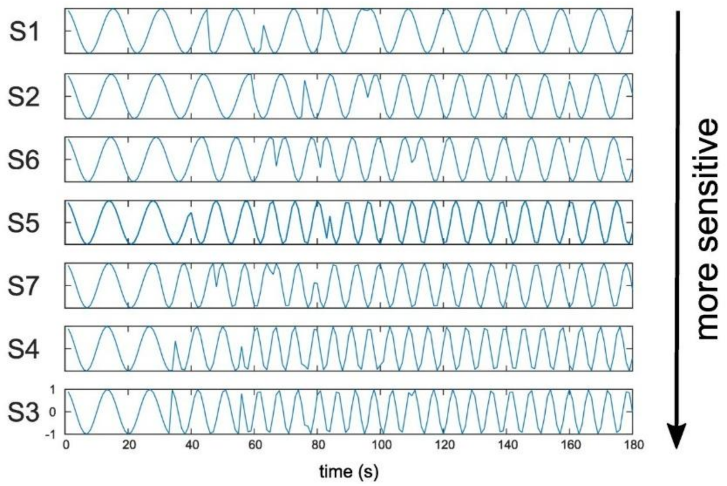


Figure 2. The sensors' response to butane

2.2. Filter diagonalization method

This research explores the use of the FDM to transform the signals obtained from the set of sensors into the frequency domain. We have previously demonstrated in [16] that FDM outperforms Fourier algorithms by providing more accurate spectra especially when using datasets with a limited number of samples. The application of FDM in e-noses represents a novel contribution, as this method has traditionally been used in quantum mechanics [17], magnetic resonance machines [18], and leak detection in pipelines [19].

FDM is a two-step technique that extracts the most important features from a signal. In the first step, an autocorrelation matrix constructed from the signal is diagonalized. This process involves finding a transformation matrix that converts the autocorrelation matrix into a diagonal matrix containing eigenvalues, each representing a frequency component of the signal. In the second step, a filter is applied to the eigenvalues of the diagonal matrix to retain only those that represent the most significant harmonics of the signal.

Let us address the method by considering a complex signal $c_n = c(n\tau)$ where $n\tau$ are equidistant-time values with n=$0, 1, \dots, N-1$. The FDM represents signal c_n as a sum of damped sinusoids, as shown in (2):

$$c_n = \sum_{k=1}^{K} d_k e^{-jn\tau\omega_k} \quad (2)$$

where d_k are the corresponding amplitudes and $\omega_k = 2\pi f_k - j\gamma_k$ are the complex frequencies of the signal with γ_k being the harmonic decay. To solve (1), the FDM uses the Hamiltonian operator $\hat{\Omega}$ to construct a correlation function with complex eigenvalues $\{\omega_k\}$, thus yielding (3):

$$c_n = \left(\Phi_0 \middle| e^{-jn\tau\Omega}\Phi_0\right) \quad (3)$$

The problem can be simplified to the diagonalization of the Hamiltonian operator $\hat{\Omega}$ or, as discussed in [20], to the evolution operator $\hat{U} = e^{-j\tau\Omega}$. Briefly, a symmetric internal product operator defined by (a|b)=(b|a) without the conjugate complex is considered, where Φ_0 is the initial state. Given that an orthonormal eigenvector set Y_k is used to perform the diagonalization of $\hat{U}$ as shown in (4):

$$\hat{U} = \sum_k u_k \,|Y_k)(Y_k| = \sum_k e^{-j\omega_k\tau}|Y_k)(Y_k| \quad (4)$$

and replacing (4) in (3), it yields (5):

$$d_k = (\Phi_0|Y_k)(Y_k|\psi_0) = (Y_k|\Phi_0)^2 \quad (5)$$

The resulting eigenvalues determine the harmonics' position and width while the eigenvectors define their amplitudes and phases. Assuming a set created from the Krylov vectors, generated by the evolution operator $\Phi_n = \hat{U}^n\Phi_0 = e^{-jn\tau\hat{\Omega}}\Phi_0$ and according to (5), it yields:

$$\left(\Phi_n \middle| \hat{U}\Phi_m\right) = \left(\Phi_n \middle| \Phi_{m+1}\right) = c_{m+n+1} \tag{6}$$

Given that the set is non-orthonormal, the overlapping matrix can be calculated according to (7):

$$\left(\Phi_n \middle| \Phi_m\right) = \left(\hat{U}^n\Phi_0 \middle| \hat{U}^m\Phi_0\right) = \left(\Phi_0 \middle| \hat{U}^{m+n}\Phi_0\right) = c_{m+n+1} \tag{7}$$

Notation U^0 can then be used, being this the overlapping matrix representation of dimensions M+1×M+1. Similarly, U^1 can be used for $\hat{U}$. To reformulate (2), it is then necessary to solve the generalized eigenvalues problem as shown in (8):

$$U^1 B_k = u_k U^0 B_k \tag{8}$$

where $u_k = e^{-jn\omega_k\tau}$ contains the lines of the spectrum and its corresponding widths. Eigenvectors B_k contain both amplitudes and phases.

To analyze the sensors' data with FDM, let us consider the sensors' readings as the signals c_n. Figure 3 shows the flowchart detailing the algorithm implementation.

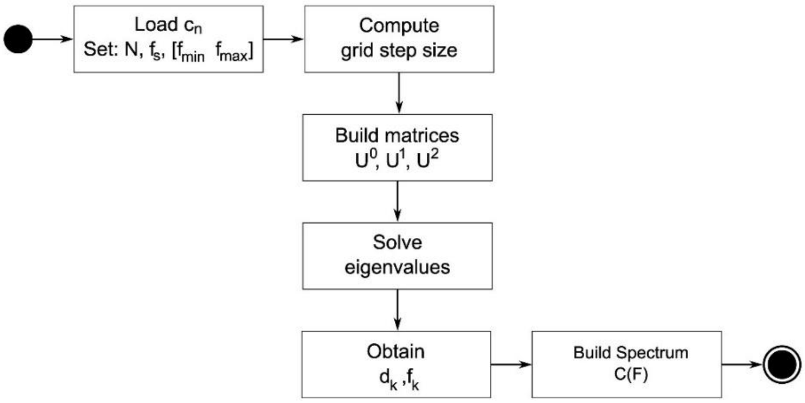


Figure 3. Six-step algorithm for the FDM implementation in the e-nose

a. After acquisition, signals c_n are loaded, N is their number of samples, and f_s is their sampling frequency. Finally, the frequency interval $[f_{min}\ f_{max}]$ in which the spectral analysis will be performed is selected.
b. The grid step size is created with angular frequency values $2\pi f_{min}<\varphi j<2\pi f_{max}$ with $j=0, 1, 2,\ldots, K_{win}$ and $K_{win} = \frac{N(f_{max}-f_{min})}{2\tau}$.
c. Three symmetric complex matrices $U^{(p)}$ of dimensions $K_{win}\ x\ K_{win}$, with $p=0, 1, 2$ are determined. In (9) is used to calculate the elements located in the diagonal:

$$U^{(p)}(\varphi, \varphi') = \sum_{n=0}^{2M}(M+1-|m-n|)e^{jn\varphi} \tag{9}$$

d. The generalized eigenvalues problem is solved with (8) and the QZ algorithm [21].
e. The complex amplitudes d_k are selected using (10):

$$d_k^{1/2} = \sum_{j=1}^{K_{win}} \boldsymbol{B}_{jk} \sum_{n=0}^{M} c_n e^{jn\varphi_j} \tag{10}$$

f. Resulting values ω_k and d_k are finally used to estimate the FDM spectrum $C(F)$ according to (11):

$$C(F) = -\sum_k Im\left\{\frac{d_k}{2\pi F-\omega_k}\right\} \tag{11}$$

2.3. Random forest

RF is a supervised learning model that combines multiple decision trees into a single model to reach a more accurate and stable prediction [22]. This algorithm was chosen because it is commonly used in classification tasks and is especially useful on large and complex datasets [23]-[25], such as the ones produced by the e-nose sensors. The process of building an RF model for odor classification is the following:

a. A subset of features from the FDM dataset is randomly selected.
b. These attributes are used to construct a decision tree.

c. Steps 1 and 2 are repeated several times to create a set of decision trees (a forest).
d. Each tree in the forest predicts an individual output (a class). The output of the RF model is the class selected by most trees.

Figure 4 shows the simplified structure of the RF model used for odor classification.

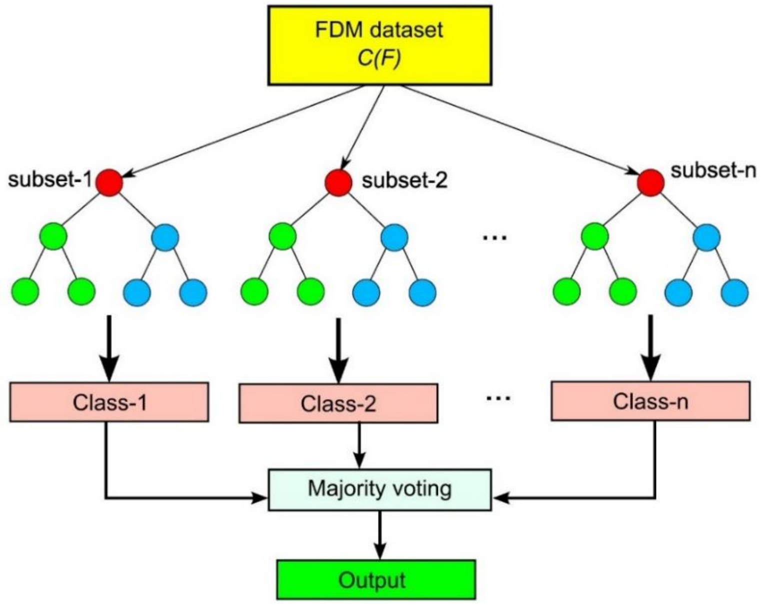


Figure 4. RF model implemented for the e-nose

2.4. Experimentation

To assess the performance of the FDM-RF approach a set of 224 trials was randomly performed in the following scenarios: i) presence of acetone, ii) presence of alcohol, iii) presence of butane, and iv) no odor (clean air). To ensure a proper odor distribution around the sensors, the e-nose was placed inside a hermetic acrylic enclosure. Outside the setup, an air pump was deployed to transport the odor samples to the acrylic cabinet via a hose. The experiment starts with the cabinet closed isolating the e-nose from the outside. For the first 20 seconds, all seven sensors acquire data from the air present in the cabinet (clean air). The pump is turned on and starts to draw the sample odor into the cabinet. For the next 30 seconds, the pump will remain activated ensuring that the acrylic cabinet is filled with the sample odor. The pump is then turned off and for the next 130 seconds, the odor will remain in the cabinet allowing the sensors to react. The experiment is concluded by opening the acrylic box and allowing the sample to dissipate in the environment. The sensors' collected data is sent to the computer for off-line analysis and classification.

This experimental protocol was used to train the RF model. Once trained, it is possible to classify new samples. Each time a new sample is analyzed and classified; it is incorporated into the model thus gradually increasing its robustness.

3. RESULTS AND DISCUSSION

Following the experimental protocol described in section 2.4, let us analyze the results obtained for acetone. Figure 5 shows the sensors' temporal responses to such odor. As described by (1), the most sensitive sensors will be those that exhibit the sinusoids with the highest frequencies once the acetone fills the acrylic cabinet (t>50 s). This is the case for sensors S4 and S7.

The temporal signals are then processed by the algorithm detailed in Figure 3. Figure 6 shows the corresponding FDM spectra. Relevant features to discuss are: i) the green-dashed line in all seven spectra is the harmonic describing the 1 Hz carrier, ii) as the amplitude of the sinusoid signal is 1, the maximum value of *C(F)* is 0.5, iii) the sooner a harmonic appears in the spectrum, the greater the slope of the temporal signal meaning a higher concentration of the target odor, and iv) a group of closely located harmonics means the sensor is highly sensitive to the target odor (e.g., S7). Each of the seven spectra can be considered a unique footprint for acetone and all together will integrate the FDM dataset to be analyzed by the RF classification model.

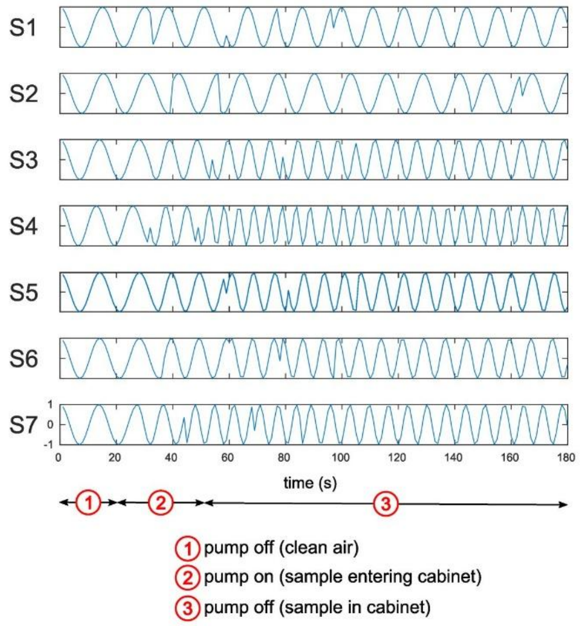


Figure 5. The sensors' response to acetone

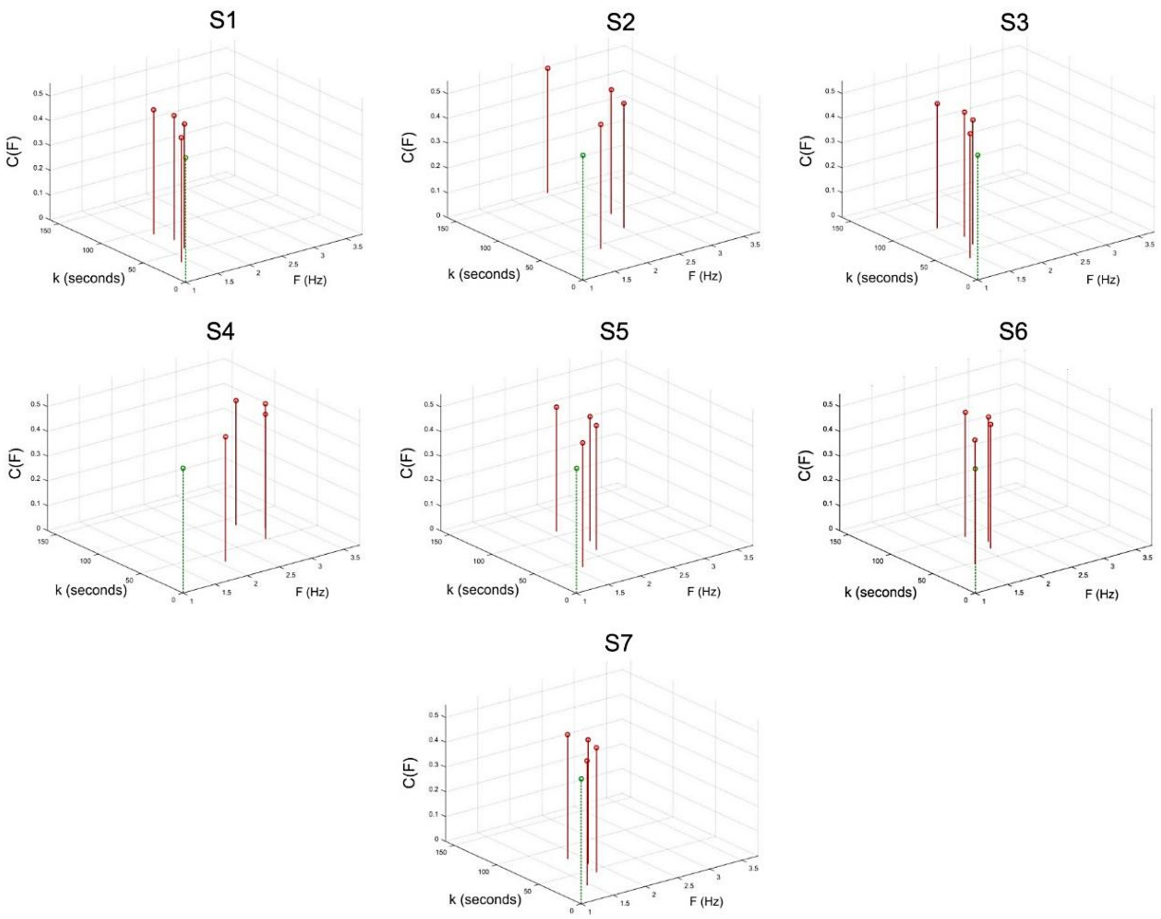


Figure 6. The FDM-based spectra for the signals collected by the sensors

Figure 7 shows the confusion matrix summarizing the RF model prediction accuracy. The rows correspond to the true class while the columns indicate the predicted class. Values on the diagonal represent (top) the number of times the odor was presented to the e-nose and (bottom) the corresponding recognition rate. For example, acetone was presented 51 times and was always recognized (recognition rate: 100%). Alcohol was presented 49 times out of which 47 times it was correctly recognized (recognition rate: 95.9%). The overall recognition rate across the 224 trials is 96.4% which suggests that RF is an adequate model to classify FDM footprints of odors.

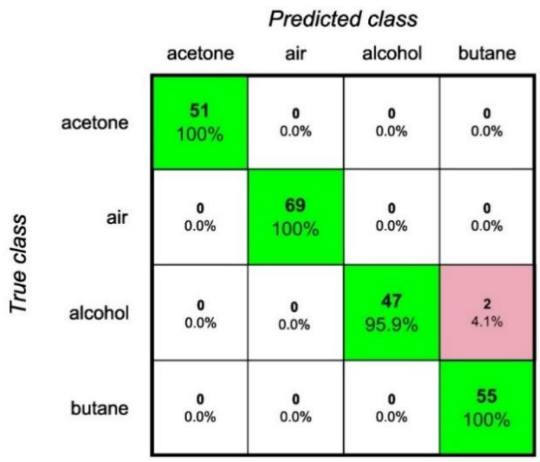


Figure 7. Confusion matrix of the RF model for odor classification

4. CONCLUSION

This paper has presented a prototype of a low-cost, compact e-nose system designed to detect specific environmental odors that may pose risks to human health. The system consists of seven gas sensors, an electronic unit, and dedicated software for signal processing and classification. The signal processing stage is based on the FDM, a novel non-Fourier data processing algorithm that provides spectra containing the most relevant features of the temporal signals. By calculating the FDM-based spectra for each of the seven signals provided by the sensors, reliable footprints can be established for target odors. The classification stage employs a RF model to identify the odors in the e-nose's surroundings. Experimental results show that the RF model achieves a 96.4% classification accuracy. To the best of our knowledge, the combined use of FDM and RF is a novel contribution to odor detection and classification, offering a promising approach for e-nose systems. Future work will compare the classification accuracy of the RF model with other models, such as neural networks, k-nearest neighbors, and support vector machine.

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