Semi-supervised Gas Detection Using an Ensemble of One-class Classifiers

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***Abstract*—Detecting chemical compounds using electronic noses is important in many gas sensing related applications. Existing gas detection methods typically use prior knowledge of the target analytes. However, in some scenarios, the analytes to be detected are not fully known in advance, and preparing a dedicated model is not possible. To address this issue, we propose a gas detection approach using an ensemble of one-class classifiers. The proposed approach is initialized by learning a Mahalanobis-based and a Gaussian based model using clean air only. During the sampling process, the presence of chemicals is detected by the initialized system, which allows to learn a one-class nearest neighbourhood model without supervision. From then on the gas detection considers the predictions of the three one-class models. The proposed approach is validated with real-world experiments, in which a mobile robot equipped with an e-nose was remotely controlled to interact with different chemical analytes in an open environment.**

***Index Terms*—metal oxide semiconductor sensor, electronic nose, gas detection, gas sensing, open sampling systems**

I. Introduction

Portable, low-cost electronic noses (e-noses) are widely used to perform gas sensing in many applications, among others environmental monitoring, gas leakage detection, exploration of toxic or explosive areas. Gas detection is a fundamental step in gas sensing tasks, which allows to indicate a significant event such as the presence of new chemical compounds, or a noteworthy change of concentration levels. Gas detection in complex environments is carried out with Open Sampling Systems (OSS), which pose different challenges than using gas sensors in laboratory set-ups, where the gas sensors are hosted in a chamber to interact with chemical compounds at a constant concentration over a prolonged time. In a continuous sampling process in uncontrolled environments, the concentration levels reflected by the sensor readings are often fluctuating due to the turbulence and advection in gas dispersal or the movement of the sensing platform, which prevents the applicability of the well-established three-phase sampling strategy [1]. Moreover, when an OSS is deployed to an unknown environment, accurate concentration estimation in absolute gas concentration units, e.g. ppm, could be infeasible, especially if the gases present are not known in advance. In such cases, gas detection is addressed by finding specific patterns in instantaneous responses caused by the presence of gas in an array of metal oxide (MOX) sensors [2]. A typical strategy is to model the MOX sensor response. For example, the approach reported in [3] can overcome the slow recovery time of MOX sensors. This approach is based on the knowledge of the nature of the target gas, and requires a corresponding pre-calibration of the detection system. In [4], the authors modeled the MOX sensor responses as a piecewise exponential signal to detect change points as the junctions between consecutive exponentials. Although [3] and [4] achieve success in detection performance, both approaches are supervised in the sense that they rely on some prior knowledge on the response pattern of the target analyte. This drawback cannot be avoided by model-free methods either. For instance, Smulko and co-authors used regression to estimate concentration levels as the basis of gas detection in [5]. Their approach is sufficient to predict gas concentrations with acceptable accuracy, but its model training requires measurements of the target analytes at various concentration levels.

In some scenarios, e.g. emergency responses, OSSs have to deal with unknown chemicals, or there is not sufficient time to prepare a supervised gas detection model. In such cases, the applicability of the aforementioned gas detection approaches is limited. One work that partially overcomes this problem is an adaptive classification model based on the artificial immune system proposed by Martinelli and his co-authors [6]. Their classification model is learned from unbalanced data and without prior assumption on the drift model, which significantly reduces the dependence on training data. However, their work is not a direct approach for gas detection as its purpose is sensor drift mitigation. In this paper, we propose a semi-supervised gas detection approach that does not assume the response patterns of the target analytes are known. Our approach can be initialized with clean air measurements only, and then learns an unsupervised model of gas exposure from the acquired measurements. We validated the proposed approach with real-world experiments.

II. Method

Using an ensemble of diverse classifiers aims to improve the detection performance [7]. We propose an ensemble one-class classification system that consists of three models, namely, a Mahalanobis-based One-Class Model (MOCM) and a One-Class Gaussian Model (OCGM) together to model baseline responses, and a One-Class Nearest Neighbor model (OCNN) to model gas exposure. Since the MOX sensors are usually partially sensitive to various chemical compounds, the Mahalanobis-based MOCM is applied to consider the correla-

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tions of the sensor responses. Since we do not have accurate prior information of the correlation between the sensors when they are exposed to the target analytes, the OCGM is included to compensate the MOCM model as the OCGM does not take the correlation into account.

As shown in the block diagram in Fig. 1, the model learning of the ensemble system is as follows: first, the MOCM and the OCGM model are learned with an amount of baseline responses $\mathbf{B}$ in the beginning of a gas sensing task. This training phase takes place when the e-nose is ensured to interact with clean air. As predictive models, the OCGM and the MOCM estimate test measurements with two indices, s_{MD} and s_{GM}, to indicate their likelihoods of being clean air. Based on the indices, these two models determine if the considered measurements are clean air accordingly with two corresponding pre-defined thresholds λ_{MD} and λ_{GM} respectively. Measurements detected as not clean air are used to train the OCNN model ad its parameters of the decision function for prediction. Finally, the resulting OCNN together with the MOCM and the OCGM form the proposed ensemble one-class classification system to perform gas detection. In the rest of this section, we will describe each one-class model in details.

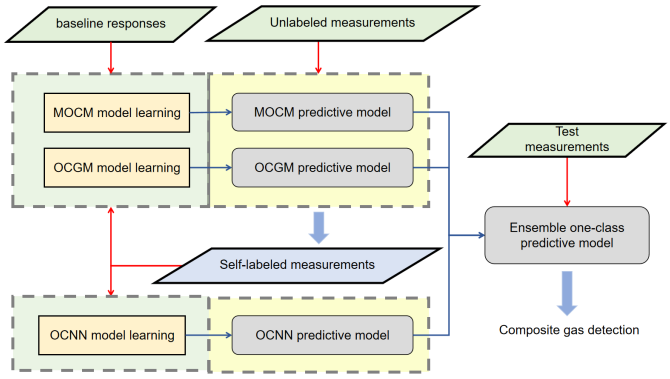

Fig. 1. The schematic diagram of the gas detection system using an ensemble of one-class classifiers.

A. Mahalanobis-based one-class model

The Mahalanobis distance d_{MD} can be used as a indicator of class separability [1]. Here we use d_{MD} as a metric to quantify the similarity between a measurement and the baseline response distribution. To do so, first, the similarity level within the baseline responses is estimated with d_{MD}. Given a group of baseline responses $\mathbf{B}$, i.e., clean air measurements, we compute the Mahalanobis distance between $\mathbf{B}$ and the estimated mean vector of the baseline responses $\mathbf{c}$, denoted as $d_{MD}(\mathbf{c}, \mathbf{B})$. Since the value of $d_{MD}(\mathbf{c}, \mathbf{B})$ reflects the similarity level between the baseline responses [8], we consider it as a reference (denoted by γ) to evaluate the similarity between a test measurement $\mathbf{r}$ and the set of baseline responses. Based on the reference γ and the Mahalanobis distance, the score s_{MD} of $\mathbf{r}$ is defined as follows:

$$\begin{cases} s_{MD} = \gamma/(d_{MD}(\mathbf{r}, \mathbf{B}) - \gamma), & \text{if} \quad d_{MD}(\mathbf{r}, \mathbf{X}) >= 2\gamma \\ s_{MD} = 1, & \text{otherwise} \end{cases} \tag{1}$$

Note that s_{MD} is always in the range of 0 to 1 by definition. The decision function of the MOCM model considers the test measurement as clean air if $s_{MD} >= \lambda_{MD}$, where the threshold λ_{MD} can be set empirically as $\lambda_{MD} = 0.995 \cdot \gamma$.

B. One-class Gaussian model

A typical one-class Gaussian classifier is a density-based model that assumes that the data of the target class form a multivariate Gaussian distribution [9]. For a given $n-$dimensional measurement $\mathbf{r}$, its probability of belonging to the target class can be estimated with the probability density function (PDF) of the Gaussian distribution. This Gaussian model assumes the data are unimodal, but it is not suitable here due to the cross-sensitivity of the MOX sensors. Instead, we model the baseline responses as a linear combination of several equally weighted single Gaussians [9]. The score s_{GM} of a test measurement is defined as follows:

$$s_{GM} = \frac{1}{n}\sum_{j=1}^{n}(1 - \frac{1}{n}\int_{0}^{\mathbf{r}^j} P(r)\mathrm{d}r) \tag{2a}$$

$$P(\mathbf{r}^j) = \frac{1}{\sqrt{2\pi(\alpha)^2}} \mathrm{e}^{-\frac{(\mathbf{r}^j - \mu^j)^2}{2(\alpha)^2}} \tag{2b}$$

where μ^j is the mean of jth sensor responses of $\mathbf{B}$, and $P(\mathbf{r}^j)$ is the PDF of the distribution estimated by the jth sensor response. α is a free parameter that determines the boundaries of the Gaussian model for each sensor. Intuitively, baseline responses used as training data are expected to have absolute high values of s_{GM}. This expectation is used as a guideline to set α, which is fit so that $s_{GM} > 0.995$ holds for all baseline responses in $\mathbf{B}$. Similar to the MOCM model, a decision function is predefined with a threshold, i.e., λ_{GM}. Given the learned OCGM model and the set of baseline responses, we let $\lambda_{GM} = 0.995 \cdot s_{GD}(\max(\mathbf{B}))$, where max(B) is the measurement with highest averaged sensor readings in $\mathbf{B}$.

C. One-class nearest neighbor classifier

After the MOCM and the OCGM are learned with baseline responses, gas detection can be performed to recognize the measurements that significantly deviate from clean air. These different measurements, corresponding to chemical analytes, are used to learn a One-Class Nearest Neighbor (OCNN) model, which can further improve the performance of recognizing baseline responses. The OCNN developed in this work is based on a two-layer-neighborhood one-class model proposed in [10]. Fig. 2 depicts the consideration of two-layer-neighborhood.

We consider that the measurements detected as chemicals simply belong to one class "non-air". In this way, they can be used to learn the OCNN model as follows:

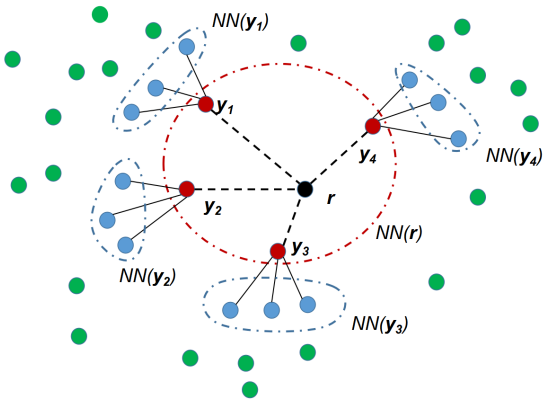

Fig. 2. An example of considering two layers of neighborhoods for a given measurement $\mathbf{r}$. The data points in red correspond to the first layer neighbors, and the data points in blue correspond to the second layer neighbors. The data points in green are outside the two layers of neighborhoods of $\mathbf{r}$. In this example, the first layer was selected with neighborhood size $J = 4$ and the second layer was selected with neighborhood size $K = 3$. $NN(y)$ is the set of K nearest neighbors of the data point $\mathbf{y}$.

1) The detected non-air measurements are taken as the representative data of the target class for the OCNN model.
2) A test measurement is assigned with a score s_{NN} using the following algorithm:

   Input: the data of the target class $\mathbf{X}$, the test sample $\mathbf{r}$
   Output: the OCNN score of the test sample s_{NN}

   Compute the distances between $\mathbf{r}$ and its J nearest neighbors in $\mathbf{X}$, and find the median value M_r
   for all nearest neighbors $\mathbf{y} \in NN(\mathbf{r})$ **do**
      Compute the distances between $\mathbf{y}$ and its K nearest neighbors $NN(\mathbf{y})$ in $\mathbf{X}$, and find the median M_y
      if $M_r < M_y$ **then**
         $s_{NN} \leftarrow (s_{NN} + 1)/J$.
      end if
   end for
   return s_{NN}
3) Use the OCNN model to process the data in $\mathbf{B}$, and find the mean μ_{NN} and variance σ_{NN} of the outputted s_{NN} scores. The test measurement is identified as baseline response if its s_{NN} falls inside the interval $[\mu_{NN} - 3\sigma_{NN}, \mu_{NN} + 3\sigma_{NN}]$.

Once the OCNN is learned, the ensemble classification system is formed up. For a test measurement, it will be recognized as a baseline response if it satisfies $s_{GM} > \lambda_{GM}$ and $s_{MD} > \lambda_{MD}$, or s_{NN} falls in the interval of $[\mu_{NN} - 3\sigma_{NN}, \mu_{NN} + 3\sigma_{NN}]$.

III. Experiments and Results

We conducted six experiments in a basement with a narrow corridor connecting two rooms. A ground robot equipped with three MOX sensors was driven into plumes of ethanol (95% pure) and 1-propanol (99.5% pure)/acetone (100% pure) at different locations. The MOX sensors used in our experiments are sensitive to these chemical analytes [11]. The gaseous chemicals were released from a beaker filled with liquid of the chemicals, and bubbler was used to facilitate evaporation. Before the experiments were started, the sensor arrays were heated up for 10 to 30 minutes. During the sampling processes, the robot was commanded to pause at several locations that were near the gas sources (within 1 m) as well as distant from any gas source (more than 2 m away). The data sets of the above experiments are used and reported in [12].

Fig. 3 is an example of the incorporation of the three classifier. As shown in Fig. 3(a), from the time series of the MOX sensor responses one can observe that two gas exposures interacted with the e-nose. These two gas exposures took place when the robot paused in front of the ethanol and the propanol source respectively. Fig. 3(b) to Fig. 3(d) show the incorporation of the three one-class models. The s_{GM} and s_{MD} decreased as the e-nose began to interact with the the first gas source. According to the intersections between the threshold $\lambda_{GM}/\lambda_{GM}$ and the curve of s_{GM}/s_{MD} (see Fig. 3(b) and Fig. 3(c)), one can find that the OCGM has better detection performance than the MOCM, but the latter is more robust to the selection of $_{MD}$ in detecting gas exposure. In Fig. 3(d), once the OCNN is finished learning (marked with the blue vertical line), the outputted s_{NN} scores stayed in the interval $[\mu_{NN}+3\sigma_{NN}, \mu_{NN}-3\sigma_{NN}]$ when the sensors did not exhibit significant responses. As the sensors became exposed to the second gas source, most s_{NN} fell outside of the decision interval. After the second gas exposure, the baseline responses will be recognized by the OCNN after 2500 s as s_{NN} went back to the decision interval. Another experimental trial is shown in Fig. 4, in which three gas exposures were set to interact with the e-nose. In this case, the MOCM only contribute to the detection of the first gas exposure because the corresponding parameter $_{MD}$ was set too large. Nevertheless, the composite prediction from the OCGM and the OCNN together managed to respond to the gas exposures occurred after 1500 s.

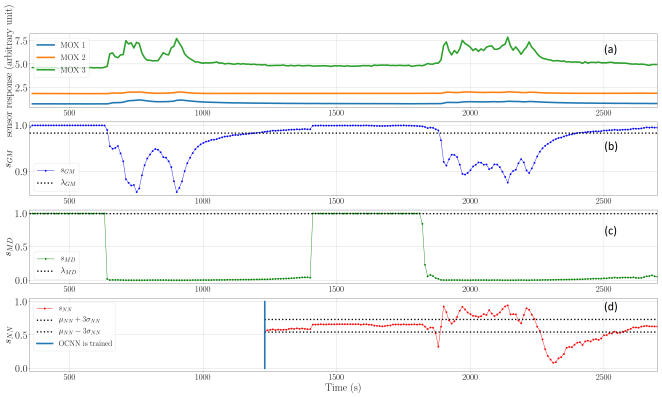

Fig. 3. A representative example of the incorporation of the ensemble one-class classifier gas detection system. In this experimental trial, the e-nose encountered two gas exposures. The details of each subplot are mentioned in the text.

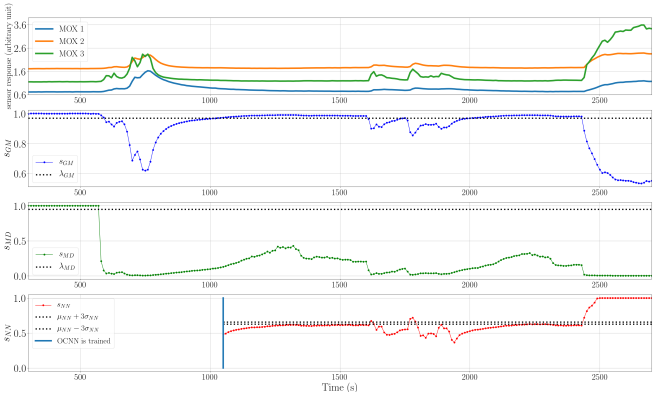

Fig. 4. Another example of the incorporation of the ensemble one-class classifier gas detection system. In this experimental trial, the e-nose encountered three gas exposures.

IV. Conclusions

In this paper, we propose an ensemble one-class classification system for gas detection using an e-nose, which reduces the reliability on prior knowledge of the target analytes. The proposed approach has a twofold learning phase. The Mahalanobis-based and the Gaussian-based one-class model are initialized with clean air only. The resulting models allow subsequent model learning for one-class nearest neighbor classifier in an unsupervised process. We validated the ensemble classifiers with the data sets collected by an open sampling system in real-world experiments. As a trade of reducing dependency on prior knowledge, it does not overcome long recovery time (recognize clean air before the responses are fully recovered), which is a limitation compared to sensor modeling approaches such as [3].

Regarding the future work, since the proposed approach includes several free parameters, i.e., λ_{GM}, λ_{MD}, and α, the sensitivity to the parameter selection should be fully tested. We will have a thorough investigation on the stability and adaptivity of the detection performance of our approach, e.g. evaluating the measures such as true alarm ration, false alarm ration, and delay of detection in experiments that more types of gases are considered and the experimental parameters such as sensor heating time, the time and distance of the interaction between the gas source and the e-nose are strictly controlled. For some real-world applications such as environmental monitoring, the potential issue of sensor drift should be addressed since the drifts in signals might have a negative impact on the performance of the classification model [6].

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