Creating true gas concentration maps in presence of multiple heterogeneous gas sources

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***Abstract*—Gas distribution mapping is a crucial task in emission monitoring and search and rescue applications. A common assumption made by state-of-the art mapping algorithms is that only one type of gaseous substance is present in the environment. For real world applications, this assumption can become very restrictive. In this paper we present an algorithm that creates gas concentration maps in a scenario where multiple heterogeneous gas sources are present. First, using an array of metal oxide (MOX) sensors and a pattern recognition algorithm, the chemical compound is identified. Then, for each chemical compound a gas concentration map using the readings of a Photo Ionization Detector (PID) is created. The proposed approach has been validated in experiments with the sensors mounted on a mobile robot which performed a predefined trajectory in a room where two gas sources emitting respectively ethanol and 2-propanol have been placed.**

I. Introduction

A gas distribution model can be defined as the truthful representation of the observed gas distribution from a set of spatially and temporally distributed measurement of relevant variables, foremost gas concentration but also wind, pressure and temperature [1].

State-of-the art algorithms for gas distribution mapping assume that only a single chemical compound is released at a given time. In order for the gas distribution algorithm to be used in real world applications, this assumption has to be removed. Another shortcoming in previous works on gas distribution modelling is that the experimental validations are usually performed with non calibrated sensors, such as metal oxide (MOX) sensors. This means that the produced map do not represent true concentrations.

In this paper we present the *Multi Compound (MC) Kernel DM+V algorithm*. It addresses the problem of creating gas distribution models for scenarios where more than one gaseous analyte is present in the environment. The MC Kernel DM+V is an extension of the Kernel DM+V algorithm proposed in [1]. By using response patterns to identify the different gaseous compounds and true concentrations readings to generate the gas distribution maps, the MC Kernel DM+V creates independent distribution models, one for each compound identified in the exploration area.

This paper is structured as follows: related work is discussed in Section II, where we focus on the Kernel DM+V algorithm. In Section III we derive the equations of the MC Kernel DM+V algorithm. The experimental set-up is presented in Section IV, followed by results and discussion in Section V. We conclude this paper in Section VI, where we state our final remarks and suggestions for future work.

II. Related Work

Gas distribution modelling methods can be categorized as *model-based* and *model-free* [2]. *Model-based* methods derive the gas distribution maps using analytical equations and inferring the parameters of the equations from sensor measurements. The most common *model-based* approaches are Gaussian plume models [3]–[5], Gaussian puff models [6], Lagrangian particle models [7] and Computational Fluid Dynamics (CFD). A key limitation of *model-based* approaches, such as CFD, is that in order to remain tractable they require precise knowledge about the boundary conditions, which in most cases are unknown.

Model-free approaches on the other hand, do no make strong assumptions about the underlying functional form of the gas distribution. Instead, they treat sensor measurements as random variables and derive a statistical representation of the observed gas dispersion from the measurements. Early attempts on *Model-free* gas distribution mapping can be found in [8] and [9], where distribution maps are generated by interpolating the concentration readings from an array of chemical sensors. Lilienthal and Duckett presented in 2004 the Kernel DM algorithm [10]. The authors used two dimensional Gaussian functions to perform a spatial integration of sensor measurements collected with a mobile robot. The gas distribution model generated with this algorithm is given by a grid map in which, each cell represents the estimation of the gas distribution mean at a particular location. The key contribution of this algorithm is that, the extrapolation of the measurements allows to separate the underlying structure of the gas distribution from the transient fluctuations of the measurements.

The methods discussed above represent the gas distribution as a time constant structure and do not provide an estimation about the fluctuations in the concentration. The spatial structure of the distribution variance can provide useful information about the gas distribution. For example, areas of large concentration fluctuations can be correlated to the proximity of a gas source [2]. In addition, the estimation of the

concentration fluctuations (i.e. predictive variance) provides several advantages, such as a method to learn the meta-parameters of the distribution modelling algorithm.

To the author's best knowledge, only two methods that compute the predictive variance have been proposed so far. Stachniss and co-authors [11] proposed an approach that reformulates the task of gas distribution modelling as a regression problem. The authors used Gaussian Process Mixture (GPM) models to deal with the specific properties of typical gas distribution. The proposed method allows to represent the rather smooth "background signal" and the areas of high concentration using different components of the GPM. The alternative approach to learn predictive variance maps is the Kernel DM+V algorithm [1], which is presented in the following subsection.

A. The Kernel DM+V algorithm

The Kernel DM+V aims to learn a predictive model $p(c, \mathbf{x}|\mathbf{x}_{1:n}, \mathbf{c}_{1:n})$ for a measurement c at a query location $\mathbf{x}$ given a set of measurements $\mathbf{c}_{1:n}$ taken at locations $\mathbf{x}_{1:n}$.

Kernel DM+V uses a uni-variate Gaussian weighting function $\mathcal{N}$ to represent the importance of a given measurement c_i obtained at location $\mathbf{x}_i$ to model the gas distribution at a grid cell k. Thus, a weight map Ω and a weighted measurement map C are computed as follows:

$$\Omega^{(k)} = \sum_{i=1}^{n} \mathcal{N}(|\mathbf{x}_i - \mathbf{x}^{(k)}|, \sigma) \tag{1a}$$

$$C^{(k)} = \sum_{i=1}^{n} \mathcal{N}(|\mathbf{x}_i - \mathbf{x}^{(k)}|, \sigma) \cdot c_i \tag{1b}$$

were $\mathbf{x}^{(k)}$ represents the center of a given cell k, and σ denotes the kernel's width. A confidence map $\alpha^{(k)}$, that depends on the number and proximity of measurements used to compute the concentrations at each cell, is computed as follows:

$$\alpha^{(k)} = 1 - e^{-(\Omega^{(k)})^2/\sigma_\Omega^2} \tag{2}$$

$\alpha^{(k)}$ depends on three parameters, namely the kernel width σ, the size of the grid cells g_s and the scaling factor σ_Ω^2. $\alpha^{(k)}$ is used to compute the mean concentration estimate $c^{(k)}$, which is given by

$$c^{(k)} = \alpha^{(k)} \cdot \frac{C^{(k)}}{\Omega^{(k)}} + \{1 - \alpha^{(k)}\} \cdot c_0, \tag{3}$$

where c_0 is an initial estimate of the mean concentration for locations where there is not sufficient information from nearby readings, which is indicated by a low value of $\alpha^{(k)}$.

The variance distribution map $v^{(k)}$ is computed from *variance contributions* integrated in a temporary map $V^{(k)}$ as follows:

$$\begin{aligned} V^{(k)} &= \sum_{i=1}^{n} \mathcal{N}(|x_i - x^{(k)}|, \sigma) \cdot (c_i - c^{k(i)})^2, \\ v^{(k)} &= \alpha^{(k)} \cdot \frac{V^{(k)}}{\Omega^{(k)}} + \{1 - \alpha^{(k)}\} \cdot v_0. \end{aligned} \tag{4}$$

The term $k(i)$ represents the cell closest to the measurement point x_i and $c^{k(i)}$ is the mean prediction of the model for cell k. c_0 and v_0 represent the initial estimates of the distribution mean and variance respectively.

III. The Multi Compound (MC) Kernel DM+V algorithm

The MC Kernel DM+V algorithm uses true gas concentration measurements c_i (e.g. from a PID) to generate the distribution models and response patterns $\mathbf{r}_i$ (e.g. from an e-nose) to classify among gases. In addition to the mean distribution and variance maps, MC Kernel DM+V returns a classification map for each of the detected compounds. These classification maps can be interpreted as the probability of detecting a compound l at a given query location in the explored area.

In the MC Kernel DM+V algorithm, a classifier uses the response patterns $\mathbf{r}_i$ (measured at locations $\mathbf{x}_i$) to compute a vector $\mathbf{P}_i = [p_1^{(i)}, \cdots, p_l^{(i)}]^T : \sum_{l=1}^{L} p_j^{(i)} = 1$, each $p_j^{(i)}$ denotes the posterior probability of a given measurement $\mathbf{r}_i$ of belonging to class l.

The classification maps $d_l^{(k)}$ are then computed by spatially interpolating the posteriors vector $\mathbf{P}_i$ predicted for each measurement point. The spatial extrapolation is calculated using equations 1 to 3 and using $1/l$ as a prior estimate for those regions in α with a low confidence value.

The predictive mean distribution maps are computed using equations 5a to 5c. The posterior probabilities $\mathbf{P}_i$ are included in the computation of $C_l^{(k)}$ by introducing the term ψ_l^i, which is a weighting function that models the importance of the measurement i for the mean distribution map of the compound l, given the posterior $p_l^{(i)}$. C_{l0} is the initial mean estimate for each class and it is computed according to equation 5b.

$$C_l^{(k)} = \frac{\sum_{i=1}^{n} \left[\mathcal{N}(|\mathbf{x_i} - \mathbf{x_k}|, \sigma) \cdot \psi_l^i \cdot c_i\right]}{\sum_{i=1}^{n} \left[\mathcal{N}(|\mathbf{x_i} - \mathbf{x_k}|, \sigma) \cdot \psi_l^i\right]} \tag{5a}$$

$$C_{l0} = \frac{\sum_{i=1}^{n} \left[\psi_l^i \cdot c_i\right]}{\sum_{i=1}^{n} \psi_l^i} \tag{5b}$$

$$c_l^{(k)} = \alpha^{(k)} \cdot C_l^{(k)} + (1 - \alpha^{(k)}) \cdot C_{l0} \tag{5c}$$

Similarly, an extension to include $\mathbf{P}_i$ to the computation of the predictive variance map is presented in equations 6a to 6c.

$$V_l^{(k)} = \frac{\sum_{i=1}^{n} \left[\mathcal{N}(|\mathbf{x_i} - \mathbf{x_k}|, \sigma) \cdot \psi_l^i \cdot (c_i - c_l^{(k(i))})^2\right]}{\sum_{i=1}^{n} \left[\mathcal{N}(|\mathbf{x_i} - \mathbf{x_k}|, \sigma) \cdot \psi_l^i\right]} \tag{6a}$$

$$V_{l0} = \frac{\sum_{i=1}^{n} \left[\psi_l^i \cdot (c_i - c_l^{(k(i))})\right]}{\sum_{i=1}^{n} \psi_l^i} \tag{6b}$$

$$v_l^{(k)} = \alpha^{(k)} \cdot V_l^{(k)} + (1 - \alpha^{(k)}) \cdot V_{l0} \tag{6c}$$

IV. Experimental Set-up

A. Robotic platform

The robotic platform shown in Figure 1 was used in the experiments. A Pioneer P3-DX (MobileRobots) was equipped with an e-nose of six commercially available *MICS e2v* MOX sensors and a ppbRAE 3000 Photo Ionization Detector (PID). The e-nose provides the input to a pattern recognition algorithm that performs gas identification, while the PID provides calibrated gas concentration readings once the chemical compound is known.

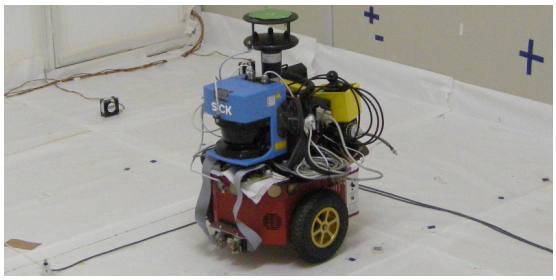


Fig. 1. The P3-DX robotic platform.

B. Experimental scenario

Data collection was conducted in the $5\ m \times 5\ m \times 2\ m$ closed room shown in Figure 1. Although no artificial airflow was induced, a weak circulating airflow field ($0.01-0.03\ m/s$) was formed in the room by natural convection. Ethanol and 2-propanol vapours were used as detection targets, and were released from two tubes at a constant flow rate ($0.2\ l/min$). The robot was programmed to follow a spiral trajectory, stopping for $30\ s$ at regularly spaced way points for data collection. Four repetitions were conducted with a single source inside the room (one for each analyte), and two repetitions were conducted with both analytes at the same time, with separations of $0.5\ m$ and $1.5\ m$ between them.

C. Parameter selection

We used a Multi Variate Relevance Vector Machine (MVRVM) [12] in order to discriminate between ethanol, propanol, and fresh air, labelled as $\mathbf{L} = [1, 0, 0]$, $\mathbf{L} = [0, 1, 0]$, and $\mathbf{L} = [0, 0, 1]$ respectively. MVRVM is an extension to the Relevance Vector Machine (RVM) classifier, a sparse Gaussian process originally proposed by Tipping [13]. The MVRVM already proved to be successful for gas discrimination in [14].

Considering that the response $\mathbf{r}$ of the e-nose is given by a $30\ s$ six dimensional time series, we opted for a kernel from the family of autoregressive kernels for time series proposed by Cuturi in [15]. These kernels are parametrized by an order o and a constant α. We trained the MVRVM classifier using a dataset $\mathbf{D} = \{\mathbf{r}, \mathbf{L}\}$ composed by the way point measurements obtained in the single source experiments. The optimal combination (o_b, α_b) was selected from the vectors $\boldsymbol{\alpha} = [0.1, 0.2, \cdots, 0.9]$ and $\mathbf{o} = [2, 4, \cdots, 30]$ using cross validation. Half of the data points were used for training and the remaining half for testing ($\mathbf{D}_{test}$). The classifier's performance was evaluated using the following loss function:

$$f_{loss}(\mathbf{D}_{test}) = \sum_{i=1}^{n_{test}} \sum_{j=1}^{l} \frac{L_i[j] \cdot \log(\mathbf{p}_i[j])}{\sum_{k=1}^{n_{test}} L_k[j]}, \qquad (7)$$

where n_{test} is the number of elements in the testing set, l is the number of classes and $\mathbf{p}_i$ is the posterior probability vector. For the dataset $\mathbf{D}$ the pair (o_b, α_b) that minimizes f_{loss} was found to be $(16, 0.75)$.

While it is possible to learn the mapping parameters g_s and σ from the data using the Negative Log Predictive Density (NLPD) [1], we selected g_s and σ in a systematic way. The rationale behind this decision is that, in the case of multiple source experiments, there is no ground truth to evaluate (g_s, σ). Thus, g_s and σ were set to $0.05\ m$ and $0.35\ m$ respectively.

The weighting function ψ_l^i is shown in in Figure 2. It depends on the posteriors p_l^i and p_{air}^i. Weight values closer to 1 will be given to those samples where the label is predicted as l or as *air* with high confidence. On the other hand, ψ_l^i will tend to zero when the classification confidence is low.

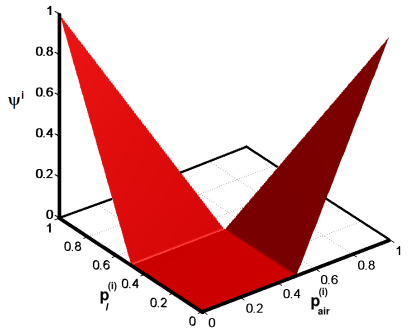
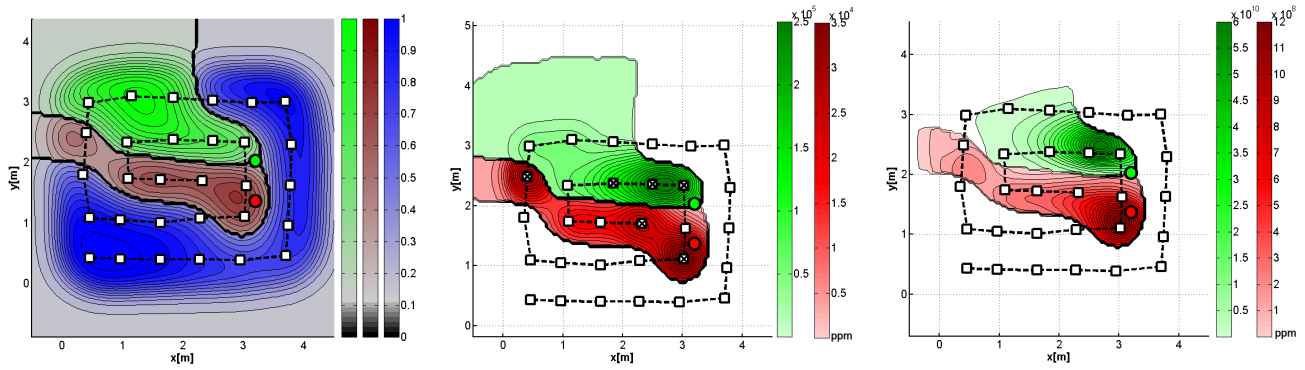


Fig. 2. Weighting function ψ. The *importance* assigned to a given measurement i will depend on its posterior probability $p_l^{(i)}$ and the posterior probability $p_{air}^{(i)}$.

V. Results

The obtained classification and concentration maps can be seen in Figures 3(a) to 3(c). Due to space constraints, in this paper we present only the results from the experiment where the separation between gas sources was $0.5\ m$. The classification map is presented in the form of a maximum a posteriori plot. It can be noticed that the probability of detecting an analyte is higher at locations where neighbouring data samples are classified as l with high confidence. At the borders of the exploration area, the confidence level drops to 33%, which intuitively says that there is not enough information to make a consistent prediction due to the lack of the neighbouring measurements.

The predictive mean concentration map in Figure 3(b) was generated by combining the individual mean concentration maps for each substance masked with the classification maps. While we do not have ground truth to evaluate the accuracy of the distribution maps, it can be noticed that the mean



(a) (b) (c)

Fig. 3. Gas distribution maps for the experiment where the gas sources were separated by $0.5\ m$. The classification map is given in the form of a maximum a posteriori plot (*a*). The mean map is shown in (*b*) and the variance map is shown in (*c*). In all Figures, the black dashed lines denote the robot's exploration path. The likelihoods, concentrations and variances of ethanol, 2-propanol and fresh air are shaded in green, red and blue respectively. The actual locations of the ethanol and 2-propanol sources are denoted by green and red circles respectively. The concentration measurements are given in parts per million (ppm).

distribution maps are consistent, since high concentration values are predicted at neighbouring areas around the way points where high average concentration was measured for each analyte (denoted by black crosses). The variance map in Figure 3(c) highlights areas near the actual location of the gas sources providing in this way, valuable information that could be used for the task of gas source localization.

VI. Conclusions

In this paper we presented an approach that extends the Kernel DM+V algorithm by considering the uncertainty in the gas discrimination for the computation of multiple gas distribution models. Broadly speaking, our algorithm fuses the information coming from two different inputs, namely the gas concentration, reported by a PID and the uncertainty in the gas identification, computed from the sensor responses from an e-nose. The MC Kernel DM+V algorithm produces l different gas distribution models, one for each detected analyte. We tested the proposed algorithm with data collected with a robotic platform inside a closed room, where two different gas sources were placed together. The obtained results show consistent mean distribution maps where plume shaped structures predict high concentration areas around measurement points where high average concentrations were sensed. In addition, the variance maps implicitly predicted the gas source location by highlighting areas around the actual sources.

Future work will aim to extend the proposed algorithm to construct models where mixture of gases are considered. This would require to train classifiers to discriminate between mixtures and pure samples. Also as a future work, it is required to develop new quantitative evaluation approaches for gas distribution models of multiple analytes. The MC Kernel DM+V algorithm can be extended to learn mapping parameters from the data itself. These learned parameters have to be evaluated not only in their accuracy to predict concentration values, but also in their capabilities to predict class labels.

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