Approaches to Time-Dependent Gas Distribution Modelling

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Abstract—**Mobile robot olfaction solutions for gas distribution modelling offer a number of advantages, among them autonomous monitoring in different environments, mobility to select sampling locations, and ability to cooperate with other systems. However, most data-driven, statistical gas distribution modelling approaches assume that the gas distribution is generated by a time-invariant random process. Such time-invariant approaches cannot model well developing plumes or fundamental changes in the gas distribution. In this paper, we discuss approaches that explicitly consider the measurement time, either by sub-sampling according to a given time-scale or by introducing a recency weight that relates measurement and prediction time. We evaluate the performance of these time-dependent approaches in simulation and in real-world experiments using mobile robots. The results demonstrate that in dynamic scenarios improved gas distribution models can be obtained with time-dependent approaches.**

I. INTRODUCTION

Environmental concerns, especially in urban areas with their critical impact on the quality of human life, have become one of the top priorities in the past decade. Water and air pollution, greenhouse gas emission, and climate change are recognised by the scientific community as major challenges. To assess environmental quality and make effective decisions, a thorough knowledge of the environment is required. This knowledge is acquired using sensors. Planning where, what, how, and when to measure is a challenging problem. In [1], a mobile sensor collects gas measurement while collecting garbage. In [2], a robotic platform controls where to collect samples to monitor pollution in a lake. Moreover, using autonomous mobile sampling is beneficial in incident management scenarios where direct exposure of humans to pollutants is dangerous [3], [4].

Among different sources of pollutants, hazardous gas emission plays an important role in environmental problems. In management of such incidents, it is essential to have a good estimate of gas dispersion to highlight areas with unusual gas accumulation, estimate gas source location, and detect anomalies [3]. Sensor planning of mobile sensors can benefit from gas distribution modelling to collect the most informative samples [5].

Statistical gas distribution modelling (GDM) aims at deriving a truthful representation of the environment from a set of spatially temporally sparse measurement. Modelling spatial distribution of gas is very challenging mainly because of the chaotic nature of gas dispersal. In addition to diffusion and advection, gas dispersion is affected by turbulence at different scales, which make the distribution intermittent (patchy). The advective flow moves these patches. In controlled environments with laminar flow, patches of gas particles are distributed along the center line of the wind in a plume. In environments where wind and temperature are not controlled, advective flow and turbulence have stronger effect on gas dispersion which makes prediction of movement of gas patches more complex. This paper addresses time-dependent statistical modelling in dynamic environments.

Our main contribution for this paper is introducing two time-dependent gas distribution modelling approaches. First, we introduce a temporal sub-sampling strategy (Section V). In a dynamic environment, it is reasonable to assume that the most recent measurements are more reliable to estimate gas distribution at present. Second, we present a GDM approach which considers temporal importance for each measurement to create gas distribution model (Section VI). We apply this temporal weight concept to extend the state-of-the-art GDM approach, Kernel DM+V, to a time-dependent one, TD Kernel DM+V. In this method, a time-scale parameter relates the age of measurements to their validity to build the gas distribution model. The time-scale represents a compromise between two conflicting requirements to obtain accurate gas distribution models: (1) using as many measurements as possible and (2) using only very recent measurements. The parameters of the recency function define time-scale. The time-scale parameter in TD Kernel DM+V is learned from available measurements.

One particular motivation of this work comes from EC project Diadem [3]. Diadem addresses Distributed Information Acquisition and Decision-making for Environmental Management, particularly in cases that involve chemical incidents which cause emission of hazardous chemical gases. The use-case scenario in the project is an area of approximately $50km^2$ at the Rotterdam port in the Netherlands, a densely inhabited industrial area where several refineries and oil factories are located. To monitor the environment and to plan where to collect further measurements, gas distribution modelling is used. Gas measurements are continuously collected using a sparse stationary stationary sensor networks and a few mobile sensors to estimate a relative gas distribution map. This map will be used to identify areas with high gas accumulation, potential gas source location, and directing field investigators for collection of additional measurements. One particularly relevant conclusion in this project was that looking at the sequence of gas distribution maps can provide insightful information for the experts about the potential gas source and help them to predict further development in the gas emission. Looking at the challenges in real-world scenarios, we focused on developing better temporal and spatial sampling methods and creating time-dependent models.

To evaluate the proposed methods, we performed experiments both in simulation and real-world with mobile robot and stationary sensors (Section IV). Section VII presents evaluation results. The performance of TD Kernel DM+V in the simulation experiments demonstrates that TD Kernel DM+V improves the prediction quality of the obtained gas distribution models in dynamic situations. This represents an important step toward statistical modelling of evolving gas distributions, which is especially interesting for outdoor applications and real-world scenarios.

II. PROBLEM STATEMENT

Given a set of collected observations $D = \{(x_i, r_i, t_i)\}_{i=1}^{N}$, temporal spatial statistical distribution modelling method aims at providing a truthful representation of the observed phenomena to predict the value of r_* at the unseen location x_* and time t_* as

$$\hat{r} = p(r_*|x_*, t_*, (x_i, r_i, t_i), 1 \le i \le N). \tag{1}$$

In time-invariant distribution modelling approaches, it is assumed that changes in the environment are time constant and the average behaviour of the observed phenomena is modelled by modifying Equation 1 to

$$\hat{r} = p(r_*|x_*, (x_i, r_i), 1 \le i \le N). \tag{2}$$

III. RELATED WORK

Several publications have addressed GDM. Most of these works utilise only the spatial information to estimate gas distribution as it is formulated in Equation 2. In [7], the predictive mean was estimated by using simultaneous measurements with equidistant sensors in a small controlled environment. While a network of sensors has advantages in terms of coverage and sampling time, using a mobile sensor avoids calibration issues and allows adaptive sampling of the environment. Pyk et al. applied interpolation approaches on consecutive equidistant measurements [8]. In [9], Lilienthal et al. used an extrapolation approach, Kernel DM, to build GDM using a mobile sensor. Later, Kernel DM+V and Gaussian Process Mixture Model (GPMM) were introduced that estimate both predictive mean and variance [10], [11]. Kernel DM+V discretises the environment into grid cells. To estimate gas distribution, Kernel DM+V assigns weights to measurements based on their spatial distance from each cell center. The predictive variance enables learning meta-parameters and provides evidence of potential gas source location. Experiments were performed in uncontrolled and outdoor environment using mobile sensors. To incorporate wind information in GDM, Reggente et al. [12] extended Kernel DM+V to Kernel DM+V/W which changes spatial weight of measurements by modifying the Kernel shape based on the wind direction and intensity. In this approach, however, it is assumed that the wind field is uniform.

A crucial assumption in these methods is that the gas distribution is generated by a time-invariant random process. This means that these GDM approaches can capture fluctuations around a constant mean. This assumption allows us to average over measurements independent of their collection time. However, if the fluctuations are more than what a stationary random process can describe, the models created under the time-invariant assumption can not provide an accurate representation of the current gas distribution. In such cases, it is reasonable to use time-dependent models that handle changes in underlying random process. However, the temporal aspect of gas distribution modelling has been addressed only in a few recent publications.

The idea of recency weight to build time-dependent GDM was first introduced by Asadi et al. in [6]. In [6], Asadi et al. present recency weight, as an exponential function, to incorporate the temporal extrapolation weight to basic Kernel DM+V. The temporal weight was defined with a heuristic time-scale factor. In this paper, we extend the work in [6]. We discuss two different solutions to incorporate time-dependency in GDM and present results both in simulated and real-world experiments. The time-scale factor in the simulation experiments is learned together with spatial meta-parameters when generating the gas distribution model.

The most related works in time-dependent GDM are [13] and [14]. In [13], Monroy proposed a time-dependent GDM approach applying Gaussian Markov Random Field. Similar to TD Kernel DM+V, this method estimates gas distribution over a grid by taking into account temporal weight in addition to the Gaussian spatial weight of measurements. In [13], the proposed method is compared with Kernel DM+V in a controlled indoor environment and its corresponding simulated environment. Both qualitative and quantitative results of this comparison indicate better performance of the time-dependent method. Note that in addition to time-dependency, the method proposed in [13], considers obstacles in creating a statistical model. Therefore, the improvements in the result can be from both enhancements. The work in [13] does not provide information on how the meta-parameters are chosen. In [14], Marjovi et al. present a time-dependent gas distribution mapping method. Similar to Kernel DM+V, this method estimates gas distribution over a grid. The estimated mean is calculated as the weighted sum of the measurements. Measurements are weighted using a combination of their Euclidean spatial distance and their temporal difference to the current time when the gas distribution map is created. In this approach, meta-parameters are defined heuristically and the decline in the importance of measurements is linear.

This paper focuses on exploring the temporal aspect of GDM and presents two solutions: (1) temporal sub-sampling and (2) extending Kernel DM+V to capture both spatial and temporal dispersion of gas.

IV. EXPERIMENTS

To analyse the impact of time-scale in GDM, we ran two experiments in a simulated wind tunnel. To evaluate our models in real-world experiments, we use two datasets: a mobile sensor moving in a corridor with uncontrolled flow and a stationary network in a small controlled environment.

A. Simulation Experiments

Simulated experiments provide high resolution ground truth and instantaneous measurement. Thus, these experiments allow thorough analysis of gas distribution modelling.

To evaluate different time-dependent modelling approaches, we used a gas dispersion simulation engine developed by [15]. This gas dispersal simulation package integrates OpenFOAM fluid flow simulation and the filament-based gas propagation model proposed in [16]. The wind tunnel environment was selected to match available data from experiments performed in the wind-tunnel of the DISAL lab, EPFL, Lausanne [17]. Two simulation experiments were performed in wind tunnel ($16 \times 4m^2$), with an inlet of approximately $1m/s$ on the left and ethanol gas source at ($1m$,$2m$), to simulate the gas dispersion under effect of predominantly laminar (*No-Obstacle* and turbulent flow (*With-Obstacle*). Turbulence is particularly created in one experiment by placing an obstacle in the tunnel. Measurements in both experiments have been collected at random locations.

B. Real-world Experiments

The first real-world experiment, *SmallNet*, was performed in a controlled indoor environment where a network of 10 stationary metal oxide sensors collect gas measurements. These measurements are collected in an experiment carried out by Wada et al. [18] in a $4.85 \times 3.42 \times 2.10m^3$ closed room. In SmallNet, an airflow of approximately $0.15m/s$ was generated by arrays of fans mounted on the floor and walls. An Ethanol gas source with a constant flow rate ($0.2l/min$) was placed at the floor close to the center.

The second real-world experiment, *Corridor*, was performed in an uncontrolled indoor environment [19]. In the Corridor experiment, the robot collected gas measurements in a random walk trajectory in a corridor over a long period of time. The investigation area was $14 \times 2m^2$ with an ethanol gas source on the floor close to the center. The mobile robot was equipped with set of metal oxide gas sensors.

V. TEMPORAL SUB-SAMPLING

In most of the existing GDM works, the behaviour of the gas distribution can be represented by a stationary random process. However, in the study of an evolving plume, changes in the frequency of sampling can have impact on the quality of gas distribution modelling. It is reasonable to assume that sample selection from more recent measurements capture more accurate information about the current behaviour of gas distribution instead of an average description. To analyse the impact of temporal sub-sampling on the quality of gas distribution models, we used basic Kernel DM+V introduced by Lilienthal et al. [11] and developed a multiple time-scale approach to create gas distribution models. First, we sort the samples according to their recording time. Then, we sub-sample the available measurements to select 50% of them for creating gas distribution model. To sub-sample the available measurements, we applied two different time-scales to sub-sample:

- D_{T_1} that selects all samples r_i from the second half of the sampling time ($\{t_{\lfloor N/2 \rfloor} \leq t_i \leq t_N\}$), and
- D_{T_2} that selects samples r_i evenly from the entire period of sampling ($\{t_1 \leq t_i \leq t_N | i = 2k+1, 0 \leq k < \lfloor N/2 \rfloor\}$).

A. Evaluation and Result

To compare two models, we use negative log predictive density (NLPD) [20]. Smaller values of NLPD imply that the likelihood of the predicted measurements is higher. Tab. I presents an NLPD comparison of using Kernel DM+V applying two different time-scales for the temporal sampling. The comparison is based on datasets from two different experiments: Corridor and SmallNet. In both experiments models were created using 80% of the samples that were recorded first, were used as a training set, and evaluated on 20% of the data that were recorded afterwards. To sub-sample the training set, we applied the two approaches we proposed earlier in this section: D_{T_1} and D_{T_2}. The width of the spatial kernel and the cell size were learned using 5-fold cross-validation, optimising NLPD.

The preliminary results presented in Tab. I indicate that sample selection from more recent measurements improves the performance of Kernel DM+V.

TABLE I. COMPARISON OF MODELS CREATED WITH KERNEL DM+V USING DIFFERENT SUB-SAMPLING TIME-SCALES.

Experiment	Sub-sampling	NLPD	$\sigma(m)$	$c(m)$
Corridor	D_{T_1}	-0.98	0.36	0.12
	D_{T_2}	-0.56	0.21	0.10
SmallNet	D_{T_1}	-1.97	0.41	0.11
	D_{T_2}	-1.78	0.41	0.11

VI. TD KERNEL DM+V

The TD Kernel DM+V approach adds the temporal importance of measurements to the spatial extrapolation of the basic Kernel DM+V algorithm, through a time-dependent recency weight. This recency weight is defined by a time-scale factor. Having a set of samples as triple (r_i, x_i, t_i), we want to create a model to estimate a snapshot of the gas distribution at time t^* (See Eq. 1). To build the time-dependent model, we introduced a time-dependent extension of Kernel DM+V called as TD Kernel DM+V. In TD Kernel DM+V, the spatial kernel is the same as in the basic Kernel DM+V algorithm, except for a temporal term φ, which is defined as follows:

$$\varphi(t_*, t_i) = \exp^{(-\beta(t_* - t_i))} \tag{3}$$

where t_i is the time stamp of measurement r_i with $t_1 \leq t_i \leq t_*$ (i.e. we do not include future measurements into the prediction for t_*). $t_* - t_i$ denotes the temporal distance of the i^{th} measurement from the prediction time. β is a scaling factor for the recency of the measurements compared to time t_*. The temporal-spatial weight function can be formulated as

$$\omega_i^{(k)} = \mathcal{N}(|x_i - x^{(k)}|, \sigma)\varphi(t_*, t_i) \tag{4}$$

where $\mathcal{N}(|x_i - x^{(k)}|, \sigma)$ is the spatial weight function from the basic Kernel DM+V. $|x_i - x^{(k)}|$ is the spatial distance of measurement i from the cell center k, and σ is the kernel width. The time-scale, kernel width and cell size are learned by optimising the NLPD value of the predictive model using cross-validation on a training set.

VII. EXPERIMENTS AND RESULT

We investigated the performance of the proposed time-dependent gas distribution models in both simulation and real-world.

1) Evaluation in Real-world Experiments: The model was created in both Corridor and SmallNet experiments using 80% of the samples that were recorded first, and evaluated on 20% of the samples that were recorded afterwards. A model was created for the target time t_* at which the last measurement in the test set was collected. In both SmallNet and Corridor experiments, the kernel width, cell size, and temporal weight are learned using 5-fold cross-validation, optimising NLPD over the training set. The results presented in Table II show that TD Kernel DM+V performs better than original Kernel DM+V in our experiments. The corresponding predictive mean and predictive variance maps created using original Kernel DM+V (up) and TD Kernel DM+V (bottom) on data from Corridor and SmallNet are illustrated in Figure 1 and Figure 2, respectively. In these figures, red indicates larger values and blue represents smaller values in the model.

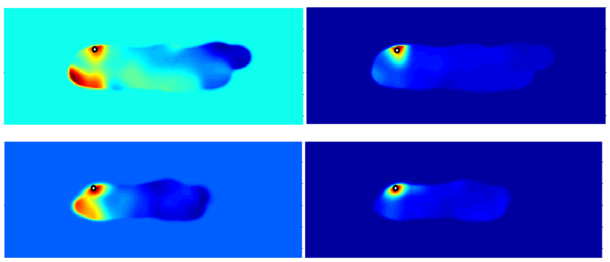

Fig. 1. Predictive mean (left) and variance (right) maps created for the Corridor experiment. Top: Original Kernel DM+V (σ=0.40m, c=0.10m). Bottom: TD Kernel DM+V (σ=0.41m, c=0.10m, β=7.2 $\times$ $10^{-3}s^{-1}$).

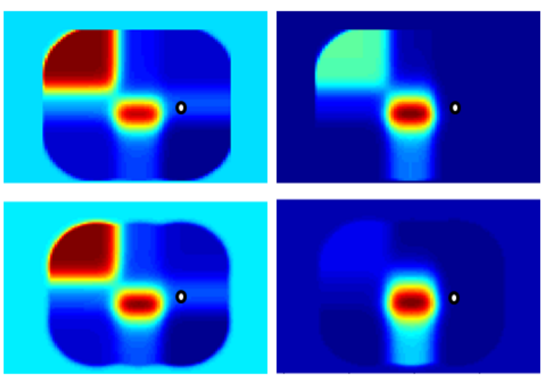

Fig. 2. Predictive mean (left) and variance (right) maps created for the SmallNet experiment. Top: Original Kernel DM+V (σ=0.41m, c=0.10m). Bottom: TD Kernel DM+V (σ=0.42m, c=0.10m, β=7.8 $\times$ $10^{-4}s^{-1}$).

2) Evaluation in Simulated Experiments: We performed two simulation experiments in a wind tunnel to simulate gas dispersion under predominantly laminar and turbulent flow. In these experiments, it takes approximately 13-14 seconds for the plume to reach the right end of the wind tunnel. During this time, the plume evolves. Measurements in both experiments have been collected at random fixed locations over the first 16 seconds. Temporal factor β, kernel width, and cell size of the predictive model are learned by cross-validation over the training set, optimising the NLPD value. The model is then used to estimate the gas distribution for the 20^{th} second. The corresponding predictive mean and predictive variance maps created using original Kernel DM+V (up) and TD Kernel DM+V (bottom) in the experiment No-Obstacle and With-Obstacle are illustrated in Fig. 3, and Fig. 4 respectively. In these figures, red indicates larger values and blue represents smaller values in the model.

The predictive mean maps created by using TD Kernel DM+V tend to capture more recent characteristics of the plume compared to the ones created by using the basic Kernel DM+V algorithm. The NLPD comparison presented in Tab. II shows for both experiments a substantial improvement when using TD Kernel DM+V.

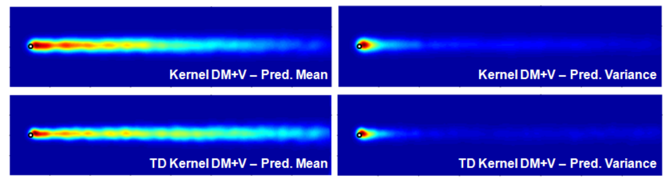

Fig. 3. Predictive mean (left) and variance (right) maps created for the experiments with No-Obstacle. Top: Original Kernel DM+V (σ=0.21m, c=0.05m). Bottom: TD Kernel DM+V (σ=0.21m, c=0.05m, β=21.8 $\times$ $10^{-2}s^{-1}$). The gas source location is shown with a white filled circle.

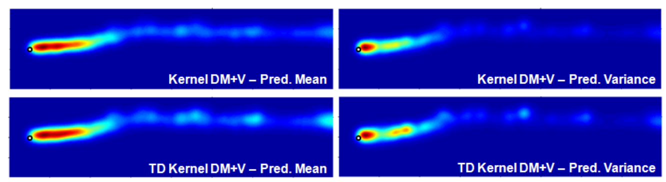

Fig. 4. Predictive mean (left) and variance (right) maps created for the experiment With-Obstacle. Top: Original Kernel DM+V (σ=0.16m, c=0.07m). Bottom: TD Kernel DM+V (σ=0.16m, c=0.07m, β=23.5 $\times$ $10^{-2}s^{-1}$). The gas source location is shown with a white filled circle.

VIII. Temporal Weight in Prediction Over Time

The results in previous section indicated that the introduction of temporal weight improves the performance of GDM. However, in the study of an evolving plume, one important question to answer is that for how far in future, TD Kernel DM+V can capture the temporal dynamic of gas dispersion. In the simulated experiments presented in Section VII-2, the prediction of the model was computed for a single given time (t_*=20). In another experiment, we compared the prediction quality for different prediction times. In this experiment, the training set has been collected during the first 16 seconds of the experiment. Here, we use a sampling frequency of 1 Hertz to make the experiment more similar to the sampling rate of a real sensor. The validation set is collected in the time interval t_{val}=$\{17, 18\}$. Using the training and validation set, a time-scale was learned (with fixed kernel width and cell size), and the predictive model was then computed and evaluated for t_*=$\{20, 21, ..., 25\}$. The recency weights (assigned to the training samples) change for a different prediction time even though the learned time-scale that was learned on the same data remains the same. For t_*=20, for example, the training samples at t=16 are more recent than for t=25.

Fig. 5 shows changes in NLPD values obtained for the two simulation datasets. As expected, the NLPD values over the test set tend to get worse as the predictive model time

TABLE II. PERFORMANCE COMPARISON OF ORIGINAL KERNEL DM+V AND TD KERNEL DM+V IN TERMS OF NLPD.

Experiment		Kernel DM+V			TD Kernel DM+V			
		NLPD	$\sigma(m)$	$c(m)$	NLPD	$\sigma(m)$	$c(m)$	$\beta(s^{-1})$
Real-world	Corridor	-0.79	0.40	0.10	-1.75	0.41	0.10	7.8×10^{-4}
	SmallNet	-1.71	0.41	0.10	-2.15	0.42	0.10	6.7×10^{-3}
Simulation	No-Obstacle	-6.43	0.20	0.05	-14.43	0.16	0.07	21.8×10^{-2}
	With-Obstacle	-5.80	0.20	0.05	-11.97	0.21	0.05	23.5×10^{-2}

increases. This trend is much stronger for the experiment With-Obstacle. One possible reason is that in this experiment a stationary situation is not fully reached after the 16^{th} second. Accordingly, the predictive model computed from the first 16 seconds, represents the measurement values poorly.

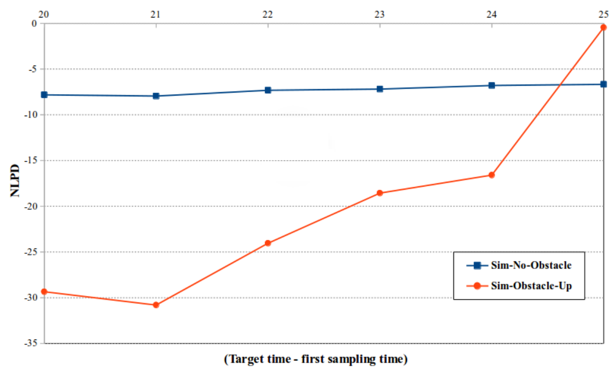

Fig. 5. Comparisons of models built with TD Kernel DM+V for different predictive model times. The blue line with square markers presents the results for No-Obstacle experiment with optimised meta-parameters ($c = 0.10m$, $\sigma = 0.20m$, $\beta = 11.1 \times 10^{-2} s^{-1}$). The red line with circle markers presents the results for experiments With-Obstacle with optimised meta-parameters ($c = 0.10m$, $\sigma = 0.20m$, $\beta = 13.7 \times 10^{-2} s^{-1}$).

In a stationary situation, the learned time-scale is expected to be very high (corresponding to a low value of the parameter β) and TD Kernel DM+V degenerates to the basic, time-invariant algorithm Kernel DM+V. In Tab. II, the time-scale factor is larger for the SmallNet and Corridor experiments and has its lowest value in the simulation experiment with obstacle.

IX. CONCLUSIONS AND FUTURE WORK

In experiments where a time-invariant random process cannot describe the changes of the observed gas distribution, time-dependent methods can improve the quality of estimated gas distribution. In this paper, two time-dependent GDM solutions were presented: (1) temporal sub-sampling, and (2) introduction of time-scale factor to capture both spatial and temporal dispersion of gas.

We first presented a sub-sampling strategy which selects samples based on their recency. A comparison of models created using samples from two different time-scales indicated that the models created from more recent measurements represent the current gas distribution.

The results in real-world experiments indicated that selection of the time-scale in sub-sampling can improve the performance of GDM. Introducing an adaptive temporal sub-sampling method which finds the best time-scale is the next step to be addressed; this is especially important when we want to apply GDM in outdoor environment where the changes in gas dispersion are stronger and more frequent. One potential solution for sub-sampling is to select sampling intervals where there is more evolution in the gas distribution. To identify these intervals, one idea is to divide the sampling time into intervals and create gas distribution models for each interval by using TD Kernel DM+V. A comparison of created models in subsequent intervals can provide a measure for choosing a time-scale for sub-sampling.

TD Kernel DM+V introduces a recency weight function that relates the age of a measurement to its importance for building the gas distribution model. The recency function is defined with a time-scale parameter that represents a compromise between: using as many measurements as possible and using only very recent measurements. The evaluation in simulation and real-world experiments with mobile gas sensors demonstrates that TD Kernel DM+V improves the obtained gas distribution models in dynamic situations and shows the limits of the approach in situations where the gas distribution changes in ways that cannot be inferred by a statistical method alone. The value of the time-scale depends on the fluctuation present in the experiment. The learned time-scale factor has to be selected so that the model can capture the fluctuations in the environment. We learn the meta-parameters by optimising NLPD.

ACKNOWLEDGMENT

This work was partly supported by the EC (contract number FP7-224318-DIADEM).

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