LOCALIZATION OF CHEMICAL SOURCES USING STOCHASTIC DIFFERENTIAL EQUATIONS

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ABSTRACT

Localization of chemical sources and prediction of their spread is an important issue in many applications. We propose computationally efficient framework for localizing low-intensity chemical sources using stochastic differential equations. The main advantage of this technique lies in the fact that it accounts for random effects such as Brownian motion which are not accounted for in commonly used classical techniques based on Fick's law of diffusion. We model the dispersion using Fokker-Planck equation and derive corresponding inverse model. We then derive maximum likelihood estimator of source intensity, location and release time. We demonstrate the applicability of our results using numerical examples.

Index terms: Fokker-Planck, Chemical Source Localization.

1. INTRODUCTION

Signal processing techniques for detection and localization of biochemical sources have attracted significant attention in recent years because of their importance in many applications such as, environmental monitoring and homeland security. One of main concerns in all of the aforementioned applications is rapid and reliable detection and localization of possible sources. In addition, these models should provide tools for reliable decision making once a biochemical event has been detected and localized. In our previous work we proposed several inverse models [3]-[5] that can potentially be used in many of these applications.

In this paper we present a new framework for localization of chemical sources using stochastic differential models. Namely, the most challenging part of dispersion modelling lies in the statistical nature of particle (liquid, gas) motion. To properly account for random effects one has to apply computationally intensive Brownian motion inverse algorithms such as Feynman-Kac. The proposed framework accounts for stochastic nature of dispersion through the well-know Fokker-Planck equation which models the probability distribution of particle velocities. The main advantage of this approach over classical diffusion theory lies in the fact that it accounts for stochastic nature of dispersion (e.g., Brownian motion) which is of great importance if the source intensity is small which may be the case in scenarios such as biochemical attacks, drug delivery, pollutant leakage, etc. On the other hand it is computationally much more efficient than Monte Carlo simulator proposed in our most recent work [5] since it provides analytical expressions for probability density function of particle density at arbitrary locations and time points and does not require computationally intensive Monte Carlo simulations. Using the proposed model we derive the corresponding statistically efficient estimators (maximum likelihood) in the presence of noise since the chemical sensors measuring the concentration of interest may be inaccurate.

This paper is organized as follows. In Section 2 we detail the physical dispersion model and illustrate the main differences compared to classical diffusion theory. In Section 3 we derive the probability density function corresponding to our forward model and derive maximum likelihood estimator in the presence of noise. In Section 4 we demonstrate the applicability of our results using numerical examples.

2. PHYSICAL MODEL

Let us assume that at arbitrary time t_0 we introduce n_0 (or equivalently concentration c_0) particles in an open domain environment at location $\boldsymbol{r}_0$. When the number of particles is large macroscopic approach corresponding to the Fick's law of diffusion is adequate for modeling the transport phenomena. However, to model the motion of the particles when their number is small a microscopic approach corresponding to stochastic differential equations (SDE) is required.

The SDE process for the transport of particle in an open environment is given by

$$\mathrm{d}X_t = \boldsymbol{\mu}(X_t, t)\mathrm{d}t + \boldsymbol{\sigma}(X_t, t)\mathrm{d}W_t \tag{1}$$

where X_t is the location and W_t is a standard Wiener process. The function $\boldsymbol{\mu}()$ is referred to as the drift coefficient while $\boldsymbol{\sigma}()$ is called the diffusion coefficient such that in a small time interval of length $\mathrm{d}t$ the stochastic process X_t changes its value by an amount that is normally distributed with expectation $\boldsymbol{\mu}(X_t, t)\mathrm{d}t$ and variance $\boldsymbol{\sigma}^2(X_t, t)\mathrm{d}t$ and is independent of the past behavior of the process.

Assuming three-dimensional environment $\boldsymbol{r} = (x_1, x_2, x_3)$, the probability density function of one particle occupying space around $\boldsymbol{r}$ at time t is given by solution to the Fokker-Planck

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equation [6]

$$\frac{\partial f(\boldsymbol{r},t)}{\partial t} = \left[-\sum_{i=1}^{3} \frac{\partial}{\partial x_i} D_i^1(\boldsymbol{r}) + \sum_{i=1}^{3}\sum_{j=1}^{3} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}^2(\boldsymbol{r}) \right] f(\boldsymbol{r},t) \quad (2)$$

where partial derivatives apply the multiplication of D and $f(\boldsymbol{r},t)$, D^1 is the drift vector and D^2 is the diffusion tensor given by

$$\begin{aligned} D_i^1 &= \boldsymbol{\mu} \\ D_{ij}^2 &= \frac{1}{2}\sum_l \boldsymbol{\sigma}_{il}\boldsymbol{\sigma}_{lj}^T \end{aligned} \quad (3)$$

In this paper we assume an infinite two-dimensional (2D) space (extension to three-dimensional space is straightforward) i.e., the domain of interest is much larger than the diffusion velocity. We also assume the space to be homogeneous, isotropic and without the drift . Note that the above formulation can easily deal with both drift and reflection from boundaries since these can be included as boundary conditions for (2) and the corresponding equation can then be solved numerically. However our main goal in this paper is to demonstrate the applicability of localizing chemical sources using Fokker-Planck equation and corresponding difference compared with classical approach. For the simplified environment the solution to (2) is given by

$$f(\boldsymbol{r},t) = \frac{1}{4\pi D(t-t_0)} e^{-\|\boldsymbol{r}-\boldsymbol{r}_0\|^2/4D(t-t_0)} \quad (4)$$

where D is the coefficient of diffusivity.

Note that the above solution represents **the probability density function** of one particle occupying space around $\boldsymbol{r}$ at time t assuming it was released from location $\boldsymbol{r}_0$ at time t_0. For a large number of particles starting from the same point (source location) the iso-concentric lines are given by concentric circles, see Figure 1. This is an expected results since for large number of the particle the classical approach based on the well known Fick's law of diffusion

$$\frac{\partial c}{\partial t} = \mathrm{div}\,(\mathcal{K}\nabla c) \quad (5)$$

where $\mathcal{K}$ is 3×3 diffusivity matrix is applicable and c is the concentration.

However, for a small number of particles the overall dispersion does not quite behave as a circle which can be seen from Figure 2. As a result estimation of the initial properties (intensity, location, time) can be inaccurate which may deteriorate our possibility for correct decision making which is the main motivation for the proposed approach.

3. STATISTICAL MODEL

To model the measurement we assume a spatially distributed sensor array consisting of m sensors located at $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots \boldsymbol{r}_m$.

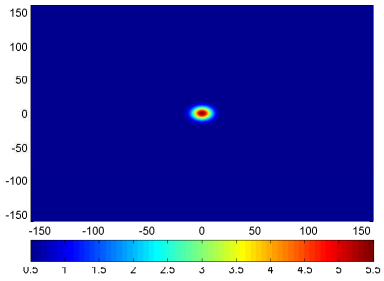

Fig. 1. Concentration distribution of 1000 particles after 20 time steps – classical model.

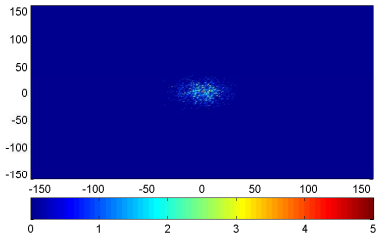

Fig. 2. Concentration distribution of 1000 particles after 20 time steps – Stochastic model.

Further, we assume that each sensor takes measurements at times $t_1, \ldots t_k$. To obtain the measurement model we first assert that chemical sensors count number of particles in certain areas (volumes) around their locations $\boldsymbol{r}_i$. Let y_{ij} be the number of particles measured by sensor located at $\boldsymbol{r}_i$ and time t_j.

Next we compute the corresponding probability mass function (PMF) of the number of particles in an arbitrary area ($\Delta_i = \Delta(\boldsymbol{r}_i)$) which corresponds to the sensor measurements i.e., we compute probability that there are n_i particles within

$$\Delta_i = (x_i - \Delta \le x_i \le x_i + \Delta, y_i - \Delta \le y_i \le y_i + \Delta) \quad (6)$$

at time t_j which is given by

$$\mathrm{P}_j(y_{ij} = n) = \binom{n_0}{n} P_{j,\Delta_i}^n (1 - P_{j,\Delta_i})^{n_0 - n} \quad n = 1, \ldots, n_0 \quad (7)$$

where P_{j,Δ_i} is the probability of a particle to occupy an area Δ_i and n_0 is the initial number of particles.

Next assuming there are m sensors ($i = 1, \ldots m$) the joint PMF is given by

$$\mathrm{P}_j(y_{1j} = n_1, \ldots, y_{mj} = n_m) = \binom{n_0}{n_1 \cdots n_m} \cdot \left(1 - \sum_{i=1}^{m} P_{j,\Delta_i}\right)^{n_0 - \sum_{i=1}^{m} n_i} \cdot \prod_{1}^{m} P_{j,\Delta_i}^{n_i} \quad (8)$$

To model sensor inaccuracies we assume that the measurement noise can be modeled using Poison distribution (note

that chemical sensors count number of particles which is a discrete random variable). In that case the resulting distribution has to be computed numerically either using Monte Carlo simulations or as the convolution of the multinomial and Poison distributions. To simplify the computational complexity in this paper we propose to compute the unknown parameters in the presence of noise using least-squares estimator. Note that our Brownian motion simulator proposed in requires additional Monte Carlo simulations for forward modeling.

In the absence of noise the log likelihood function is given by

$$l(n_0, \boldsymbol{r}_0, t_0) = \sum_{j=1}^{k} \log \binom{n_0}{y_{1j} \cdots y_{mj}} + \\ + \sum_{j=1}^{k} \sum_{i=1}^{m} y_{ij} \log P_{j,\Delta_i} \\ \sum_{j=1}^{k} \left\{ \left(n_0 - \sum_{i=1}^{m} y_{ij} \right) \log \left(1 - \sum_{i=1}^{m} P_{j,\Delta_i} \right) \right\} \quad (9)$$

In the presence of noise the corresponding PMF is given by

$$\mathrm{P}(y_{1j} = n_1, \ldots, y_{mj} = n_m) = \prod_{i=1}^{m} \sum_{\tau=0}^{n_i} \frac{\lambda^\tau e^{-\lambda}}{\tau!} \binom{n_0}{n_i - \tau} \cdot \\ \cdot P_{j,\Delta_i}^{n_i - \tau} (1 - P_{j,\Delta_i})^{n_0 - n_i + \tau} \quad (10)$$

with the corresponding log likelihood function

$$l(n_0, \boldsymbol{r}_0, t_0, \lambda) = \sum_{j=1}^{k} \sum_{i=1}^{m} \log \sum_{\tau=0}^{n_i} \frac{\lambda^\tau e^{-\lambda}}{\tau!} \binom{n_0}{n_i - \tau} \cdot \\ \cdot P_{j,\Delta_i}^{n_i - \tau} (1 - P_{j,\Delta_i})^{n_0 - n_i + \tau} \quad (11)$$

In the remainder of the paper we will assume that λ is known since in principle it can be estimated in the calibration phase when only noise is present. In that case the maximum likelihood estimator is computed by minimizing the above likelihood functions (9 and 11).

In the remainder of the paper we will assume that time of release t_0 is known i.e., we estimate only the source location and intensity. Note that in principle the initial guess of the release time can be obtained using classical approach and then it can be further refined through stochastic estimation.

4. NUMERICAL EXAMPLES

We present numerical examples to demonstrate the applicability of the proposed algorithms. Unless otherwise stated we assume source strength of $n_0 = 1000$particles and Poison noise with mean $\lambda = 0.03$ which means that most likely value for sensor noise is 2. In addition unless otherwise stated we assume that the number of sensors is given $m = 400$ and number of time samples is $k = 15$. In all the figures unless otherwise stated we illustrate the results for 10000 runs of the forward model. In all the examples we define the relative error as

$$\mathrm{err} = \frac{\|\hat{\boldsymbol{r}}_0 - \boldsymbol{r}_0\|}{\boldsymbol{r}_0} \quad (12)$$

	Classical	Stochastic
Estimating intensity	6.5%	0.64%
Estimating location		2.5%
Estimation time		1.53 %

Table 1. The estimation results of classical and stochastic estimation

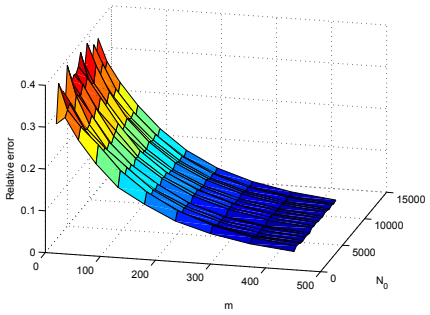

Fig. 3. Relative error as a function of source intensity and number of sensors.

where $\boldsymbol{r}_0$ is the true value and $\hat{\boldsymbol{r}}_0$ is the corresponding estimate.

For comparison, in Table 1 we illustrate the estimation results of classical and stochastic estimation. As expected the stochastic approach outperforms classical technique since the number of particles is relatively small. Note that in this comparison we used least-squares estimator in both cases.

In Figure 3 we illustrate the relative error source intensity estimation as a function of source intensity and number of sensors using maximum likelihood estimator and with $\lambda = 0$. As expected the error decreases significantly as m increases which may potentially be useful in sensor array design.
In Figure 4 we illustrate the relative error using least-squares estimator as a function of λ. As expected the error increases as noise variance increases however even for relatively large levels of noise the estimation error is smaller than 10%.

In Figures 5-7 we illustrate the histogram of relative errors for 1000 runs for $\hat{n}_0, \hat{\boldsymbol{r}}_0$ and $\hat{t}_0$ using maximum likelihood and $\lambda = 0$. These histograms can be used for evaluation of con-

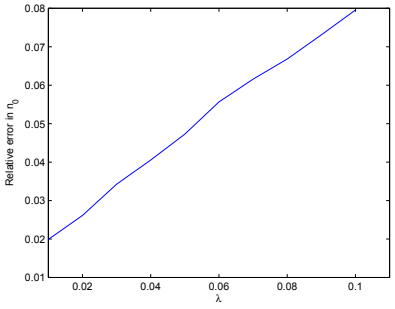

Fig. 4. Relative error as a function of λ – intensity estimation.

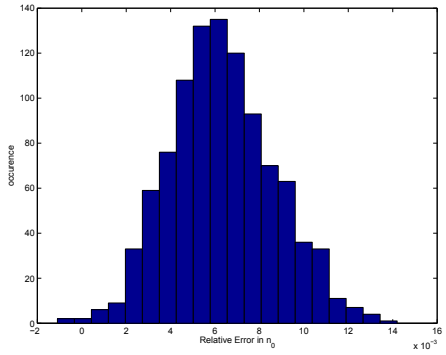

Fig. 5. Error histogram – intensity estimation.

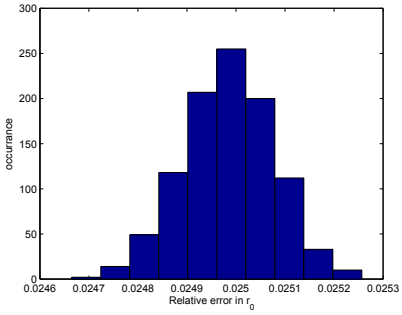

Fig. 6. Error histogram – location estimation.

fidence intervals for the proposed estimators. As it can be seen (as expected from Table 1) we are most confident in estimating the intensity of the source which is important for the prediction phase where this estimate must be used in order to find expected size of regions where the expected concentration will be above certain thresholds.

5. CONCLUSIONS

We addressed the problem of estimating low-intensity chemical sources using stochastic differential equations (SDE). To model the chemical dispersion we employed the Fokker-Planck equation. This approach can be easily extended to various scenarios such as urban environment consisting of buildings, complex tunnel structures, turbulence etc., by properly defining drift as a non-homogeneous variable. We used the maximum likelihood method to estimate the unknown parameters in the presence of the Poison noise. Numerical examples were used to illustrate the applicability of the proposed algorithms.

Future research will extend these techniques to 3D scenarios. We will also address the issue of computational complexity and compare it to the complexity of the Brownian motion estimator.

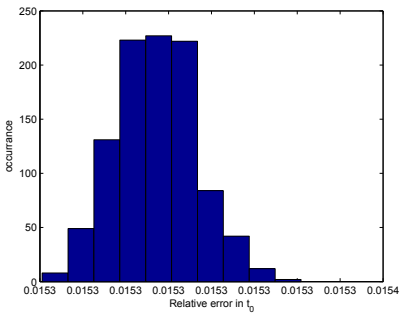

Fig. 7. Error histogram – release time estimation.

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