Parameter Estimation of a Continuous Chemical Plume Source

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\textbf{Abstract}—The problem is estimation of the strength (emission rate) and the location of a chemical source from which a contaminant is released continuously into the atmosphere. The concentration of the contaminant is measured at regular intervals by a network of spatially distributed chemical sensors. The transport of the contaminant is modeled by turbulent diffusion and fluctuating plume concentration. The source parameter estimation is solved in the sequential Bayesian framework, with the posterior expectation approximated using Monte Carlo integration. In order to deal with the vague prior, importance sampling is implemented using the progressive correction technique. The paper presents numerical analysis of statistical performance of the proposed algorithms for different sensor configurations.

\textbf{Keywords:} CBRN data fusion, chemical plume, turbulent diffusion, source localisation, Monte Carlo estimation, Bayesian inference, progressive correction.

\section{I. INTRODUCTION}

In the current era of asymmetric warfare there is a real danger of potential chemical, biological and radiological (CBR) attacks by terrorists against defence forces and civilians. Chemical attacks are of particular interest due to the availability of chemical warfare agents leftover from the past conflicts, abandoned stockpiles from rogue regimes or from the toxic industrial chemicals.

This paper deals with the problem of estimating the strength (emission rate) and the location of a chemical source from which a diffusing substance (a contaminant) is released continuously into the atmosphere. The assumption is that the concentration of the contaminant is measured with a certain sampling interval by a network of spatially distributed chemical sensors. The model of the measurement likelihood is based on diffusion and intermittency (due to the turbulent fluid flow) models which have been verified against an experimental data set [10], [11], [12]. Second, the paper proposes a sequential Bayesian solution based on Monte Carlo integration where the importance sampling step is performed using the progressive correction. A non-sequential version of this algorithm has been successfully used for localisation of gamma-radiation point sources, [13]. In the paper we study how the sensor density affects the accuracy of source position and strength estimates.

The paper is organised as follow. The problem description is presented in Section II. A brief description of the analytic model of turbulence and intermittency, together with its computer implementation, is given in Section III. The Bayesian approach to source parameter estimation using Monte Carlo integration and progressive correction is discussed in Section IV. Numerical results are presented in Section V. Section VI draws conclusions and briefly outlines future work.

\section{II. PROBLEM FORMULATION}

The source of the chemical agent is assumed to be a continuous point source, meaning that it is a dimensionless point in space with the beginning and the end of the release at $-\infty$ and $+\infty$ in time, respectively. Predicting the dispersion of chemicals in air requires modeling of turbulent transport. In
general this is a difficult task, hence we apply an approximate analytic model which takes into account the variation with height of wind speed and diffusivity [14]. This model and the model of concentration fluctuations are described in the next section.

Suppose \( S \) chemical sensors are placed in arbitrary but known positions in the area where a chemical agent has been released. The concentration measurements from the \( S \) sensors are sent to the fusion centre for processing with the sampling interval of \( \tau \) seconds. A graphical illustration of the problem is shown in Fig.1 in two-dimensions. Let the continuous point source be characterised by its location \((x_0, y_0, z_0)\) in the three-dimensional local Cartesian coordinate system \((x, y, z)\) and its release (emission) rate \( Q_0 \) (g/s). Throughout the paper we will assume that the source is on the ground \((z_0 = 0)\), and hence the source parameter vector (which we need to estimate) can be written as:

\[
x = \begin{bmatrix} x_0 & y_0 & Q_0 \end{bmatrix}^T.
\]  

where \( T \) denotes the matrix transpose. Let \((x_i, y_i, z_i), i = 1, 2, \ldots, S\) be the known position of the \(ith\) chemical sensor. A set of concentration measurements from all \( S \) sensors at time \( t_k = t_0 + k\tau\), with \( k = 1, 2, \ldots \) is denoted by \( z_k = \{z_{i,k}\}_{i=1}^S\).

In the following, index \( k \) will be the discrete time (or snapshot) index and \( i \) will be the sensor (spatial) index. A cumulative set of all temporal and spatial measurements available up to time \( t_k \) is denoted as \( z_{1:k} = \{z_m\}_{m=1}^k = \{z_1, z_2, \ldots, z_k\}\).

In the sequential Bayesian framework, the goal is to estimate at each discrete-time step \( k \), the posterior pdf \( p(x|z_{1:k})\). The posterior expectation will then be the minimum mean square error (MMSE) estimator of the parameter vector \( x \).

III. TURBULENT DIFFUSION AND INTERMITTENCY

A. Modeling

Predicting the dispersion of air contaminants requires modeling of turbulent transport. While the full description of turbulence is beyond either theory or simulation, there are a few analytic approximations. Gaussian puff models are a typical choice, being a computationally simple approximation. Gaussian puff model, however, assumes the wind speed and diffusivity to be uniform, and as a result the plume height and decrease of ground level concentration are underestimated.

In our work we use a more realistic analytic approximation, where the concentration \( C_i \) that occurs at the \(ith\) sensor at a particular time instance is a random number due to the stochastic nature of the atmospheric turbulence. Concentration \( C_i \) is thus represented as a sum of the mean and the fluctuating components:

\[
C_i = \bar{C}_i + \tilde{C}_i.
\]

For the model of mean concentration we use an analytic solution of the turbulent diffusion equation; the fluctuating part is modeled by a probability density function (pdf).

Suppose the three-dimensional Cartesian coordinate system in use is such that the \( x-y \) plane is the horizontal plane with the positive \( x \)-axis along the wind direction, and the \( z \)-axis is pointing up. The wind velocity vector is then \( \mathbf{v} = (u_x, 0, 0) \).

It is known that for the power-law mean wind velocity profile in the atmospheric boundary layer (ABL), expressed by

\[
u_x(z) = v_0 \left( \frac{z}{\lambda_0} \right)^\beta,
\]

the corresponding mean concentration at a location \((x, y, z)\) can be represented as

\[
\overline{C}(x, y, z) = \overline{C}_y(x, y) \overline{C}_z(x, z),
\]

with analytical expressions for \( \overline{C}_y \) and \( \overline{C}_z \) derived from the advection-diffusion equation of turbulent dispersion [15], [16], [17]. Here \( \overline{C}_y(x, y) \) is the concentration profile in the \( y \) direction (crosswind), and \( \overline{C}_z(x, z) \) is the vertical concentration profile. Parameter \( v_0 \) in (3) is the reference wind speed at a reference height \( \lambda_0 \) (note that for \( z > \lambda_0 \), the wind speed \( u_x > v_0 \)). Parameter \( \beta \), which takes values in the range \([0, 1]\), depends on the meteorological conditions and the smoothness of the surface. All parameters \( \lambda_0, v_0, \beta \) can be estimated by fitting the meteorological field data, but they can be also related to the main parameters of turbulent flow in ABL (see [18]).

\[
v_0 = av_s, \quad a = \frac{\ln Re}{\sqrt{3}} + \frac{5}{2}, \quad \beta = 3 \frac{1}{2 \ln Re},
\]

where \( v_s \) is the friction velocity, \( Re \) is the Reynolds number of the flow.

Under our assumption that the source is on the ground \((z_0 = 0)\), adopting the velocity profile (3) and the linear profile for turbulent diffusivity in the surface layer, \( \overline{C}_y(x, y) \) has a Gaussian shape (see [15], [18], [19], [17], [16]):

\[
\overline{C}_y(x, y) = \frac{1}{\sqrt{2\pi}\sigma_y} \exp\left(-\eta^2/2\right),
\]

where \( \eta = (y - y_0)/\sigma_y \). Parameter \( \sigma_y(x) \) is a plume crosswind spread that increases with the downwind distance (see (11) below), and the vertical concentration obeys the stretched-exponential profile (see [15], [19], [17], [16]):

\[
\overline{C}_z(x, z) = C_0 \exp\left(-\zeta^\alpha\right).
\]

Here \( \zeta = f_z B z/\sigma_z, \sigma_z(x) \) is a vertical plume spread (defined below):

\[
B = \frac{\Gamma(2/\alpha)}{\Gamma(1/\alpha)} f_z = \frac{\Gamma(3/\alpha)}{\Gamma(1/\alpha)} \frac{1}{B^2},
\]
\( \Gamma(\cdot) \) is the gamma function and

\[
C_0 = G \frac{Q_0}{v_0 \sigma_y \sigma_z} \left( \frac{\lambda_0}{\sigma_z} \right)^\beta. \tag{9}
\]

\( Q_0 \) was introduced in Sec.II as the emission rate of the source,

\[
G = \frac{\alpha B}{\Gamma(1/\alpha)} \frac{f_1^{1+\beta}}{f_u}, \quad f_u = \Gamma \left( \frac{1 + \beta}{\alpha} \right) \left[ \Gamma \left( \frac{1}{\alpha} \right) B^\beta \right]. \tag{10}
\]

There are two conventional models of turbulent diffusion for which the value of the parameter \( \alpha \) in (7) can be derived analytically: the model of conjugate diffusivity profile (\( \alpha = 1 + 2 \beta \)) and the model of linear diffusivity profile (\( \alpha = 1 + \beta \)), for details see [17], [15]. For neutral stability conditions \( \beta \ll 1 \) and the two profiles are almost identical.

For the plume spread we assume [16]

\[
\sigma_z(x) = H \lambda_0 \left( \frac{x_0 - x}{\lambda_0} \right)^{1/\alpha}, \quad \sigma_y(x) = D \sigma_z(x), \tag{11}
\]

with \( D = \sigma_v / \sigma_w \approx 1.74 \) [15] \( \sigma_v, \sigma_w \) are the standard deviations of velocity fluctuations in the vertical and horizontal directions near the surface) and

\[
H = \frac{1}{q} [1 + (1 + \beta) \kappa q/a]^{1/\gamma}, \quad q = \left[ \frac{\Gamma(2/\alpha)}{\Gamma(1/\alpha)} \right]^{1/\gamma}, \tag{12}
\]

where the parameter \( \alpha \) is determined in (5) and \( \kappa = 0.4 \) is Von-Karman constant.

It should be emphasized that the model (6),(7) explicitly takes into account the flow shear (parameter \( \beta \)), the underlying surface influence (no-flux boundary condition \( \partial_z C = 0 \) at \( z = 0 \)) and the strong turbulence anisotropy in the surface layer (parameter \( D \)). As such this model is an evident generalization of the well known Gaussian plume models. Note however that even in the limiting case \( \beta = 0 \) (the wind speed independent of the height), the adopted model (7) turns into exponential, thus is different from the Gaussian plume model.

The fluctuating part of the concentration, \( \tilde{C}_i \) in (2), is modeled by the probability density function of \( C \) with the mean \( \overline{C} \) as a parameter (for details see [11], [12]):

\[
\rho(C|\overline{C}) = (1 - \omega) \delta(C) + \omega^2 \left( \frac{\gamma - 1}{\overline{C} (\gamma - 2)} \right) \left( 1 + \frac{\omega}{(\gamma - 2) \overline{C}} \right)^{-\gamma}. \tag{13}
\]

Here the value \( \gamma = 23/6 \) was chosen to make it compliant with the theory of tracer dispersion in Kolmogorov turbulence [11]. The parameter \( \omega \), which models the tracer intermittency in the turbulent flow, can be in the range \( [0, 1] \), with \( \omega = 1 \) corresponding to the non-intermittent case. For \( \omega \neq 0 \), the pdf \( \rho \) of (13) has a delta impulse at zero, meaning that the measured concentration in the presence of intermittency can be zero on some occasions. It can be easily shown that the pdf of (13) integrates to unity.

Neglecting the influence of additive measurement noise in the chemical sensors, equation (13) will represents the measurement likelihood function, where the mean concentration \( \overline{C} \) is a function of the parameter vector \( x \).

\section*{B. Implementation}

To generate realistic concentration data, a synthetic environment was implemented in MATLAB®. The mean concentration \( \overline{C} \) at location \((x, y, z)\) is a deterministic quantity and is computed directly using the analytic form given by eqs.(4)-(12).

The measured concentration time series is generated by drawing random samples from the probability density function given in (13). The random number generator is implemented using the inverse transform method [20] based on the following steps:

1. Draw a sample \( u \) from the standard uniform distribution: \( u \sim U[0, 1] \).
2. Compute the value of \( C \) that satisfies \( F(C) = u \) where \( F(\cdot) \) is the cumulative distribution function (cdf) of the distribution of interest.
3. The value of \( C \) computed in the previous step is a random sample drawn from the desired probability distribution.

The cdf \( F(\cdot) \) needed for inverse transform sampling is obtained by integrating the pdf in (13), and is given by:

\[
F(C) = 1 - \omega \left[ 1 + \left( \frac{2}{\gamma - 2} \right) \frac{C^\gamma}{\overline{C} \Gamma(1/\gamma)} \right]^{1-\gamma}. \tag{14}
\]

The use of this cdf in the inverse transform sampling procedure generates the value of concentration:

\[
C = \begin{cases} \left( \frac{2}{\gamma - 2} \right)^{1-\gamma} \overline{C}^{-\gamma} - 1, & u \geq 1 - \omega, \\ 0, & u < 1 - \omega. \end{cases} \tag{15}
\]

The simulated mean concentration profile in the \( y-z \) plane due to a continuous point source located at the coordinate origin \((x_0 = y_0 = z_0 = 0)\) and a constant wind vector in the positive \( x \) direction, is shown in Figure 2(a). The values used in simulations are:

- \( Q_0 = 40 \) g/s;
- \( \beta = 1 \);
- \( v_0 = 5 \) m/s;
- \( \lambda_0 = 10 \) m.

A corresponding random concentration realisation across the same plane is shown in Figure 2(b) for \( \omega = 0.9 \). A slice of the concentration corresponding to both Figures 2(a) and (b) at \( z = 0.15 \) is shown in (c). Similarly, the mean concentration and a random concentration realisation across the \( x-z \) plane are shown in Figures 3(a) and (b), respectively.

Figure 4 shows a time series of the normalised concentration \( (C/\overline{C}) \), generated at a single point within the plume.

\section{IV. Source Parameter Estimation}

The Bayesian approach for parameter estimation assumes that a prior distribution \( \pi_0 \) is available for the source parameters. In the case of chemical source backtracking problem, such prior distribution information may come, for example, from intelligence reports or observations of symptoms in personnel exposed to the chemical. Therefore, prior to receiving any measurements from the sensors, we assume that \( x \sim \pi_0 \).
The MMSE estimator, as the optimal Bayesian estimator, at time $k$ is the posterior expectation:

$$\hat{x}_k = E(x|z_{1:k}) = \int xp(x|z_{1:k})dx,$$

(16)

where

$$p(x|z_{1:k}) \propto \pi_0(x) \prod_{m=1}^{k} p(z_m|x)$$

(17)

and $p(z_m|x)$ is the likelihood function of the measurement set at time $m$, $z_m = \{z_{1m}, z_{2m}, \ldots, z_{Sm}\}$, given $x$. According to Sec.III-A, this likelihood can be written as:

$$p(z_m|x) = \prod_{i=1}^{S} p(z_{im}|x) = \prod_{i=1}^{S} ((1 - \omega)\delta(z_{im}) + \frac{\omega^2 (\gamma - 1)}{C (\gamma - 2)} \left(1 + \frac{\omega}{\gamma - 2} \frac{z_{im}}{C}\right)^{-\gamma})$$

(18)

The posterior pdf $p(x|z_{1:k})$ and, therefore, the posterior expectation cannot be found exactly for this problem. Of many numerical methods that can be used to approximate integrals of the form of (16), Monte Carlo methods have

1 Here we assume the temporal independence of concentration measurements. In reality the temporal correlation of concentration $C_t$ ttail off in the matter of seconds [11]. If we adopt the sampling interval $\tau$ to be sufficiently long, the temporal correlation of measurements becomes negligible.
gained much interest because of their excellent performance and ease of implementation [20]. We use importance sampling, one such Monte Carlo technique, to approximate the posterior expectation.

In using importance sampling to approximate the integral of (16), the integral is approximated by the following weighted sum:

\[ \hat{x}_k \approx \sum_{n=1}^{N} w_n^p x_n^p, \]  

(19)

where \( x_n^p, n = 1, 2, \ldots, N \) is the \( n \)th sample drawn from an importance density \( q \), and \( w_n^p \) is the corresponding importance weight computed as

\[ w_n^p = C p(x_1|z_{1:k})/q(x_n^p). \]

Here \( C \) is a normalising constant chosen such that \( \sum_{n=1}^{N} w_n^p = 1 \). Although \( p(x_1|z_{1:k}) \) is not known exactly, because the normalisation factor of (16) cannot be computed, this difficulty can be avoided by rewriting the expression for the weights as

\[ w_n^p = C p(x_{1:k}|x_n^p)\pi_0(x_n^p)/q(x_n^p) \]  

(20)

and allowing the normalising constant to be absorbed into \( C \).

The prior distribution at time \( k \), \( p(x|z_{1:k-1}) \), (which for \( k = 1 \) is simply \( \pi_0 \)) would be the simplest importance density for this problem, as the computation of the importance weights will then simplify to

\[ w_n^p = C p(x_{1:k}|x_n^p) \]  

(21)

However, because the prior will often be much more diffused than the likelihood (especially at the initial stages, for small \( k \)), straightforward use of the prior as the importance density will result in very few or even no samples being drawn from useful parts of the parameter space. A multistage approach referred to as progressive correction [21] in which samples are drawn from a series of distributions that progressively approach the true posterior distribution was used to estimate the source parameters. Importance sampling with progressive correction has been used successfully in [13] to localise multiple radiological sources and [22] to localise sensor nodes in an ad hoc sensor network. The complete procedure for progressive correction at time \( k \) is summarised in Table I. A detailed description of the implementation of importance sampling using the progressive correction technique (for single time-step processing) is given in [13]. The main feature of the technique is that the likelihood function is raised to the power \( \Gamma_p \) at stage \( p = 1, \ldots, P \). Function \( \Gamma_p \) is a monotonically increasing function of \( p \), and reaches its maximum at \( \Gamma_P = 1 \). This means that at early stages (small \( p \)) the weights are computed using a broadened likelihood function. Only at the last stage \( p = P \), the true likelihood is used.

### V. Numerical Results

In this section we present some numerical results obtained by applying the progressive correction algorithm to data generated using the synthetic environment described in Sec.III-B.

### Table I

THE PROCEDURE FOR IMPORTANCE SAMPLING WITH PROGRESSIVE CORRECTION AT TIME \( k \); \( P \) IS THE NUMBER OF STAGES; THE INPUT AND OUTPUT PARTICLE SET, \( \{x_n^{p-1}\}_{n=1}^{N} \) AND \( \{x_n^p\}_{n=1}^{N} \) RESPECTIVELY, HAVE UNIFORM WEIGHTS.

| Inputs: \( \{x_n^{p-1}\}_{n=1}^{N}; z_k \) |
| Select coefficients \( \gamma_p \in (0, 1) \), s.t. \( \sum_{p=1}^{P} \gamma_p = 1 \) |
| for \( n = 1, \ldots, N \) do |
| \( x_n^p = x_n^{p-1} \) \( \triangleright \) Initial stage, \( p = 0 \) |
| end for |
| for \( p = 1, \ldots, P \) do |
| for \( n = 1, \ldots, N \) do |
| Compute weights \( w_n^{p,p} = C_p [p(z_k|x_n^{p,p})]\gamma_p \) \( \triangleright \) Regularisation |
| end for |
| Draw \( \epsilon_n^{p,p} \sim g \) (kernel density) |
| \( x_n^{0,p} = x_n^{p,p-1} + \epsilon_n^{p,p} \) |
| end for |
| for \( n = 1, \ldots, N \) do |
| \( x_n^p = x_n^{p,p} \) |
| end for |
| Output: \( \{x_n^p\}_{n=1}^{N} \) |

### A. Single run results

First we illustrate the performance of the algorithm to estimate the parameters of a strong continuous point source, of magnitude \( Q_0 = 10^4 \) g/s, located at coordinates \( x_0 = 7000 \)m, \( y_0 = 20 \)m, \( z_0 = 0 \). The concentration measurements were collected from a grid of \( 4 \times 4 \) chemical sensors located downwind of the source. Other than the source parameters, all other parameter values were identical to those given in Section III-B, except that \( \beta = 1/7 \). The progressive correction algorithm used \( N = 400 \) random samples (particles) which were initialised such that the \( x \) and \( y \) values were normally distributed around the centroid of the sensor grid and the source magnitudes were Gamma distributed with shape parameter 1.0 and scale parameter \( 10^6 \).

Figure 5(a) shows the mean concentration of the plume, the \( 4 \times 4 \) grid of sensors (pink dots), the source location (green star), and the initial particle distribution (white dots). The different-sized circles around the sensor locations are used as a crude indication of the relative magnitudes of sensor measurements. Due to the random nature of the concentration measurements, see eq.(13), it is possible that more distant sensors measure higher concentration than those closer to the source (see for example Figure 5(a)). The distribution of the particles after applying the progressive correction to the first snapshot of sensor measurements, \( z_1 \), is shown in Figure 5(b). Further convergence of particles to the true source occurs as the progressive correction is recursively applied to the successive snapshots of measurements; Figure 5(c) shows the final result using 10 sets of measurements, \( z_{1:10} \). The final estimated source parameter values on this occasion are: \( \hat{x}_0 = 702.33 \)m, \( \hat{y}_0 = 20.22 \)m, and \( \hat{Q}_0 = 2.3 \times 10^5 \) g/s. While
the location estimate is very precise, the estimate of the release rate is not.

B. Monte Carlo run results

In this subsection, we present the results of Monte Carlo runs carried out using grids of different numbers of sensors. The root mean square (RMS) estimation errors of source position and emission rate, obtained using $3 \times 3$, $4 \times 4$, $5 \times 5$, $6 \times 6$ and $9 \times 9$ grids of sensors and by averaging over 100 Monte Carlo runs are shown in Figure 6. The locations of the sensors at the four corners of the grid were identical in each configuration. Thus the area populated by sensors was kept constant in each sensor configuration, only their density was varied.

As expected, both estimation RMS errors (the positional and the emission rate errors) decrease with the increase of the sensor density and with the use of more measurement snapshots from sensors. The estimation error drops most significantly during the first two to three measurement steps and more slowly thereafter. While it appears that excellent source position estimates can be achieved, the emission rate estimation errors are fairly high.

Next we carried out Monte Carlo simulations using the $5 \times 5$ grid of sensors and with a varying value of the emission rate: $Q_0 = 10^5$, $10^4$, $10^3$, $10^2$ g/s. The results for the RMS positional error (in meters), obtained by averaging over 100 runs, are shown in Fig.7. It is remarkable to observe that even for a weaker source, the positional error is decreasing with time, albeit very slowly. Thus, in the adopted setup, to localize a source of strength $Q_0 = 10^3$ g/s (red line in Fig.7) with positional RMS error of about 10m, it is required to collect the data over at least 35 sampling intervals. On the contrary, a source of strength $Q_0 = 10^4$ g/s (green line in Fig.7) could be localized with the same precision after only 3 sampling times. The results in Fig.7 indicate that the chemical source localization system performance is a tradeoff between the density of sensors and the response time of the system: for a given source strength and the maximum tolerable response interval, we can determine the required density of sensors.

VI. CONCLUSIONS

Using a realistic turbulent diffusion and intermittency model of chemical plume dispersion, the paper explored the problem of continuous point source parameter estimation in the Bayesian framework. The numerical results indicate an excellent performance (accuracy, robustness) of the importance sampling scheme based on progressive correction. The localization error of less than 10 m is achievable for a relatively strong source even using only a sparse sensor array within a few sampling intervals. Future work is envisaged in a few directions: (a) a study of the robustness of the estimation algorithm in the presence of imperfectly known environmental parameters (of particular interest is to investigate if the parameter $\beta$ can be included in the source parameter vector); (b) refinement of the intermittency model to include a meandering
wind; (c) consideration of an instantaneous and decaying chemical point sources.

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