ADAPTIVE BAYESIAN ALGORITHMS FOR THE ESTIMATION OF SOURCE TERM IN A COMPLEX ATMOSPHERIC RELEASE

A. Ickowicz[2] , F. Septier[1,2], P. Armand[3], Y. Delignon[1,2]

[1]Institut Mines-Télécom / Télécom Lille1, France
[2]LAGIS UMR CNRS 8219, Lille - France
[3]CEA / DAM /DIF, Arpajon - France

Abstract: In this paper, we present an adaptive algorithm for the estimation of source parameters when a release of pollutant in the atmosphere is observed by a sensor network in complex flow field. Due to the error-based observations, inverse statistical methods have to be used to perform an estimation of the parameters (position of the source, time and mass of the release) of interest. However, given the complexity of the dispersion model, even with a Gaussian assumption on the sensor-based errors, direct inversion cannot be done. In order to have quick results, classical MCMC, while accurate, is too slow. We then demonstrate the accuracy of using adaptive techniques such as the AMIS (Population Monte-Carlo based). We finally compare the results with the classical MCMC estimation in term of accuracy and velocity of implementation.

Key words: *Source term estimation, bayesian inference, Monte-Carlo techniques, adaptive algorithms.*

INTRODUCTION

Nowadays, the threat of pollution due to the release, either accidentally or deliberately, of Chemical, Biological, Radiological or Nuclear (CBRN) agents is high. As a consequence, rapid detection and early response to a release of a CBRN agent could dramatically reduce the extent of human exposure. The capability to detect and estimate the pollutant source term parameters is therefore a problem of great importance.

In this paper, we address the problem of estimating the source parameters from noisy measurements. For realistic modelling of the pollutant dispersion, a Lagrangian particle model is generally used in order to take into account inhomogeneities in the flow and turbulence fields (Reynolds, A.M., 1996). Given the complexity of such dispersion model, even with a Gaussian assumption on the concentration measurement errors by the sensors, direct inversion cannot thus be done. As a consequence, this challenging problem is becoming an important subject of study.

Existing techniques include both stochastic and deterministic approach. A first approach is backward modelling, also known as Lagrangian backtracking. Fundamentally, there is an intrinsic time-symmetry in atmospheric transport, which is the basis of backtracking for inverting concentration measurements of atmospheric tracer (Issartel, J.-P. and J. Baverel, 2002), (Hourdin, F., O. Talagrand and A. Idelkadi, 2006). Other non-stochastic techniques mostly present the optimization of a cost function. Among approaches that deal with noisy observations, the most popular is the Bayesian Monte Carlo method, that has been introduced in (Patwardhan, A. and M.J. Small, 1992) and used since then (Dilks, D.W., R.P. Canale P.G. Meier, 1992) and (Bergin, M.S. and J.B. Milford, 2000). In (Yee, E., 2008), the authors propose to use a Markov chain Monte Carlo (MCMC) algorithm with reversible jump to perform an estimation of a variable dimension parameter. This classical algorithm produces good results but suffers from a weak convergence rate and strong dependencies on the starting values.

In order to contribute on this problem, we propose in the present work adaptive Monte-Carlo based methods. More specifically, the proposed method, called *adaptive multiple importance sampling* (AMIS) (Cornuet, J.M., J.M. Martin, A. Mira and C.P. Robert, 2012) is derived from the Population Monte Carlo methods (Cappé, O., A. Guillin, J.M. Marin and C.P. Robert, 2004) which are based on Importance Sampling (Glynn, P.W. and D.L. Iglehart, 1989), a well-established method used to simulate a difficult target distribution. The advantage over MCMC is that the scheme is unbiased at any iteration and thus can be stopped at any time, while iterations improve the performances of the importance function. The adaptive step in the AMIS makes us believe in the accuracy of this algorithm regarding the classical MCMC methods. We also present an adaptive MCMC-based algorithm, called Adaptive Metropolis-within-Gibbs, which will be compared to the proposed AMIS.

In a first part, we present the dispersion model on which we decided to start the construction of our estimation method, and the observation model. Then, we present the Bayesian solution we propose to tackle this challenging problem. We finally present the main ideas of the proposed adaptive algorithm before comparing it to the classical and an adaptive extension of the MCMC method used in (Yee, E., 2008) in a complex scenario located in a quarter of Paris.

THE CONVECTION-DIFFUSION MODEL

Assuming that we are interested in the concentration of hazardous material evolving during a certain time in a certain place of interest, it would be very useful to work with an accurate convection-diffusion model. So far, their exists a great number of models, based on various hypothesis, including varying boundaries constraints, for example. Anyway, based on (Wilson, J.D. and B.L. Sawford, 1996), a general expression can be extract though. C being the concentration of hazardous material, u the (homogeneous) wind velocity vector, K the eddy-diffusion coefficient, and Q the strength of the source, we have:

$$\frac{\partial C}{\partial t} + u\nabla C - \nabla(K\nabla C) = Q \qquad (1)$$

$$\text{s.t. } \nabla_n C = 0 \text{ at } \partial\Omega$$

Moreover, $Q = q_s\,\delta(x - x_0)[H(t - t_{on}) - H(t - t_{off})]$, with H the Heaviside unit step function. This concentration formulation is based on the stochastic evolution of a pollutant release in the atmosphere. The initial modelling for one particle is formulated with a system of stochastic differential equations such that :

$$dX_t = U_t dt$$

$$dU_t = a(X_t, U_t, t)dt + \left(C_0 \varepsilon(X_t, t)\right)^{1/2} dW_t \qquad (2)$$

where X and U correspond to the position and velocity respectively of a marked fluid particle. $a(.)$ represents the drift coefficient vector, $\varepsilon(.)$ the volatility and C_0 the Kolmogorov universal constant. This Lagrangian Stochastic model will be used for the simulation of the marked fluid particles needed to obtain the mean concentration of pollutant.

PROBLEM FORMULATION

Given a set of measurements $Z_{t_j}^i$ obtained at several times t_j and at several positions $i \in \{1, \ldots, N_c\}$ defined by the N_c sensors located in the surveillance area, the objective consists in estimating the source term characteristics Θ which include the source position (x_s, y_s, z_s), the mass and the time of the release, i.e. q_s and t_s respectively. The measurements are generally defined as :

$$Z_{t_j}^i = g(\Theta, t_j, i) + \upsilon_{t_j}^i \qquad (3)$$

where $\upsilon_{t_j}^i$ denotes a normal random variable that takes into account potential noise in the sensor as well as the uncertainty on the dispersion model. The function $g(\Theta, t_j, i)$ corresponding to the measured concentration at the i-th sensor at time t_j for some source characteristics Θ is defined as :

$$g(\Theta, t_j, i) = \int_{t_j}^{t_j+T} \int_{\Omega} C(x, t; \Theta) h(x, t \mid x_i, t_j) dx dt \qquad (4)$$

where C is the previously defined concentration function, and h the filter function associated to the i-th sensor for a measurement at time t_j. Since in this study we consider a Lagrangian stochastic model, this concentration function does not have an analytical expression with respect to the parameters of interest Θ and thus is approximated by generating N_p marked fluid particles from the dispersion model.

Consequently, the estimation of the source term charateristics from the measurements is a challenging problem with no analytical solution with such complex dispersion model. In order to have a solution, one can resort to indirect inference through the use of Bayesian Monte-Carlo techniques.

BAYESIAN SOLUTION

In a Bayesian context, the aim is to compute the posterior distribution in order to be able to give an estimate of the parameters of interest. Using Bayes' rule, this posterior distribution can be expressed

$$p(\Theta \mid Z) \propto p(Z \mid \Theta) p(\Theta) \quad (5)$$

which corresponds to the product of the likelihood and the prior distribution of Θ. By assuming that the measurement noises, defined in Eq. (3), are independent and identically distributed, the likelihood distribution used in this paper is

$$p(Z \mid \Theta) \propto \prod_{i=1}^{N_c} \prod_{j=1}^{N_T} \exp\left(-\frac{1}{2\sigma_{obs}^2} \left(Z_{t_j}^i - g(\Theta, t_j, i) \right)^2 \right) \quad (6)$$

Let us remark that the proposed algorithm can be used whatever the likelihood is. Concerning the prior information related to the source term characteristics, we will consider in this study that we are in the worst case scenario, meaning we have no prior information on the parameter. The corresponding law is then a classical uniform law on some compact support. Since we do not have an explicit expression of the function $g(.)$ that links the parameters of interest and the observations, the value of Θ that maximizes the posterior distribution could not be found analytically. As a consequence, some approximation methods have to be used. Existing approaches that deal with such probabilistic model are mainly based on Monte-Carlo methods. These computational algorithms rely on repeated random sampling to obtain numerical approximations of some untractable distribution of interest. However, such algorithms could be computationally intensive if ‘‘naïve’’ proposal distributions are used. In order to overcome this problem, we propose to use some recent advances in Monte-Carlo methodology by using adaptive scheme.

Proposed Adaptive Multiple Importance Sampling

The real challenge with the Importance Sampling is the choice of the proposal distribution. The closer the proposal is from the target distribution, the faster (and thus efficient) is the algorithm. The AMIS facilitates that constraint by adapting automatically the proposal at each iteration of the algorithm. For instance, parameters which define the proposal distribution are updated such that the Kullback-Leibler divergence between the target and the proposal is minimized. In this paper, a mixture of D normal distributions has been chosen. The update step thus concerns the mean vector, the covariance matrix as well as the weight associated to each component of the mixture. This method has the potential advantage to converge faster than classical MCMC algorithms (such as the one proposed in (Yee, E., 2008) for source term estimation). The proposed method is summarized in Algorithm 1.

SIMULATION RESULTS

In this section, we compare the proposed AMIS algorithm with the Metropolis-within-Gibbs (MWG) used in (Yee, E., 2008). As shown in Fig. 1, we consider an instantaneous release at time $t_s = 200s$ with mass $q_s = 50$ in the ‘‘Opera Garnier’’ quarter of Paris.

Let us remark that the complexity of each method is directly related to the number of algorithmic particles as well as the number of fluid particles used in the dispersion model. Indeed, at each time we propose a new algorithmic particle which corresponds to new values of the source term characteristics, the likelihood function defined in Eqs. (3-4) has to be evaluated and thus the dispersion model has to be run in order to approximate the function $g(\Theta, t_j, i)$.

From Fig. 2, we can see the approximation of the source characteristics posterior distribution defined in Eq. (5) obtained with AMIS and MWG. From these results, we can clearly remark that the proposed AMIS allows to have a better exploration of the solution space. Indeed, the true value of the source characteristics are close to the mode of the approximate posterior distribution from the AMIS whereas it is not the case with the MWG. Finally, as illustrated in Table 1, the AMIS outperforms the MWG by giving us better posterior probability values evaluated around the true location of the source.

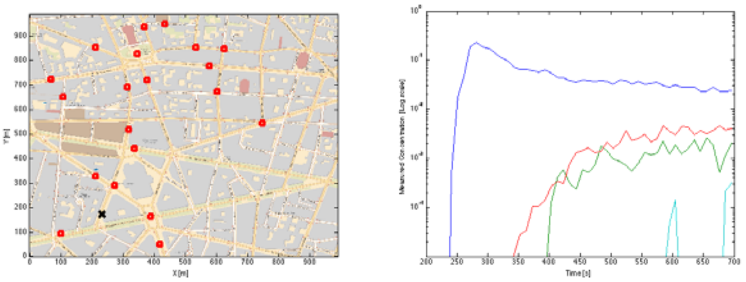

Figure 1. Scenario considered in this paper. On the left: location of the sensors (red circles) and the source (black cross) – on the right: Measured concentration of the different sensors in log scale.

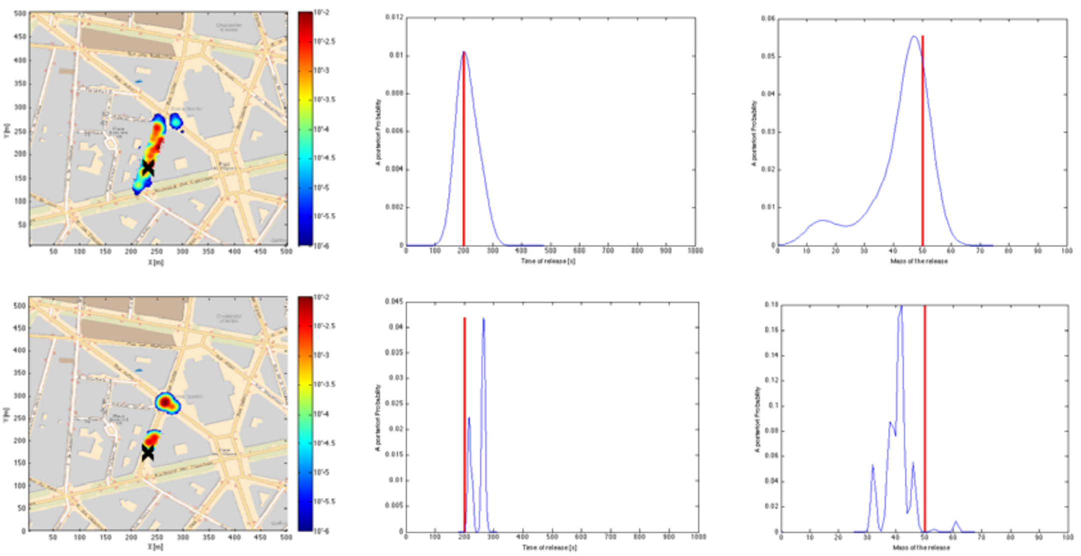

Figure 2. Results obtained with the proposed AMIS (first row) and the existing MWG (second row) with 400 algorithmic particles. From left to right: Approximation of the posterior of the source location – Approx. of the release time posterior (true value in red) – Approx. of the release mass posterior (true value in red).

Table 1. Approximation of $p\left((x_s, y_s) \in \left(x_s^{TRUE} \pm \Delta, x_s^{TRUE} \pm \Delta\right) \middle| Z\right)$ obtained with the different algorithms.

# Algorithmic Particles		*200*	*400*	*600*	*800*	*1000*	*2000*
$\Delta = 20m$	AMIS	**0.1557**	**0.1574**	**0.1597**	**0.1658**	**0.1765**	**0.2199**
	MWG	4.10^{-6}	8.10^{-6}	4.10^{-2}	0.1061	0.1289	0.1487
$\Delta = 10m$	AMIS	**0.0135**	**0.0266**	**0.336**	**0.379**	**0.0632**	**0.0916**
	MWG	9.10^{-12}	1.10^{-10}	2.10^{-3}	0.013	0.0213	0.0281
$\Delta = 5m$	AMIS	**0.0010**	**0.005**	**0.0081**	**0.0115**	**0.0156**	**0.0265**
	MWG	9.10^{-16}	6.10^{-14}	9.10^{-5}	0.0014	0.0043	0.0073

CONCLUSION

We present in this article an efficient adaptive Bayesian algorithm for source term estimation. The accuracy of the estimate obtained with the proposed approach in a complex scenario is better than with existing schemes based on MCMC, thus clearly showing the benefit of adaptive strategy for solving such challenging problems.

Algorithm 1: Proposed Adaptive Multiple Importance Sampling (AMIS)

<u>*Initialization:*</u> $t = 0$

Draw independently N_0 particles $\{\Theta_0^{(i)}\}_{i=1}^{N_0}$ from a proposal distribution $q_0(.)$

For $1 \le i \le N_0$ do

Compute $\delta_0^{(i)} = N_0 q_0(\Theta_0^{(i)})$ and the importance weights $w_0^{(i)} = p(\Theta_0^{(i)} \mid Z) / q_0(\Theta_0^{(i)})$

End For

Update the parameters of the proposal distribution $\{\alpha_0^d, \Xi_0^d\}_{d=1}^{D}$ by using a criterion such as the Kullback-Leibler divergence and the weighted set of particles $\{\Theta_0^{(i)}, w_0^{(i)}\}_{i=1}^{N_0}$

<u>*Iterations of the algorithm:*</u> $t = 1, \ldots, T$

For $t = 1, \ldots, T$ do

Draw independently N_t particles $\{\Theta_t^{(i)}\}_{i=1}^{N_t}$ from a proposal distribution $q(\Theta \mid \alpha_{t-1}, \Xi_{t-1})$

For $1 \le i \le N_t$ do

Compute $\delta_t^{(i)} = N_0 q_0(\Theta_0^{(i)}) + \sum_{l=1}^{t} N_l q(\Theta_t^{(i)}; \alpha_{l-1}, \Xi_{l-1})$ and $w_t^{(i)} = p(\Theta_t^{(i)} \mid Z)\left[\delta_t^{(i)} / \sum_{j=0}^{t} N_j\right]^{-1}$

End For

For $0 \le l \le t-1$ and $1 \le i \le N_t$ do

Update the importance weights of the particles generated at previous iterations $\delta_l^{(i)} = \delta_l^{(i)} + N_t q(\Theta_l^{(i)}; \alpha_{t-1}, \Xi_{t-1})$ and $w_l^{(i)} = p(\Theta_l^{(i)} \mid Z)\left[\delta_l^{(i)} / \sum_{j=0}^{t} N_j\right]^{-1}$

End For

Update the parameters of the proposal distribution $\{\alpha_t^d, \Xi_t^d\}_{d=1}^{D}$ by using a criterion such as the Kullback-Leibler divergence and the weighted set of particles $\left\{\{\Theta_l^{(i)}, w_l^{(i)}\}_{i=1}^{N_0}\right\}_{l=0}^{t}$

End For

REFERENCES

Bergin, M.S. and J.B. Milford, 2000: Application of Bayesian Monte Carlo analysis to a Lagrangian photo- chemical air quality model, *Atm. Environment*, **34**, 781–792.

Cappé, O., A. Guillin, J.M. Marin and C.P. Robert, 2004: Population Monte-Carlo, *J. of Computational and Graphical Statistics*, **13**, 907-929.

Cornuet, J.M., J.M. Marin, A. Mira and C.P. Robert, 2012: Adaptive multiple importance sampling, *Scandinavian Journal of Statistics*.

Dilks, D.W., R.P. Canale and R.P. Meier, 1992: P.G., Development of Bayesian Monte Carlo techniques for water quality model uncertainty. *E. Modeling*, **62**, 149–162.

Glynn, P.W. and D.L. Iglehart, 1989: Importance sampling for stochastic simulations, *Management Science*, 1367-1392.

Hourdin, F. and O. Talagrand and A. Idelkadi, 2006: Eulerian backtracking of atmospheric tracers. I and II: Adjoint derivation and parametrization of subgrid-scale transport, *Q. J. of the Royal Meteorological Society*, **132**, 567–603.

Issartel, J.-P. and J. Baverel, 2002: Adjoint backtracking for the verification of the Comprehensive Test Ban Treaty, *Atm. Chemistry and Ph. Discussions*, **2**, 2133–2150.

Patwardan, A. and M.J. Small, 1992: Bayesian methods for model uncertainty analysis with application to future sea level rise, *R. Analysis*, **12**, 513–523.

Reynolds, A.M. 1996: Review on Lagrangian Stochastic Models for Trajectories in the Turbulent Atmosphere, *Boundary-Layer Meteorology*, **78**, 191–210

Roberts, G.O. and J.S. Rosenthal, 2009: Examples of adaptive MCMC, *J. of Comp. and Graph. Stat.*, **18**, 2, 349–367, 2009

Wilson, J.D. and B.L. Sawford, 1996: Review of Lagrangian stochastic models for trajectories in the turbulent atmosphere, *Boundary-Layer Meteorology*, **87**, 191-210.

Yee,E., 2008: Theory for reconstruction of an unknown number of contaminant sources using probabilistic inference, *Boundary-layer meteorology*, **127**, 359–394.