ESTIMATING SOURCE TERM PARAMETERS THROUGH PROBABILISTIC BAYESIAN INFERENCE: AN APPROACH BASED ON AN AMIS ALGORITHM

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The context of this work is to contribute to the response to Chemical, Biological, Radiological and Nuclear (CBRN) threats.

The identification of a possible CBRN source is important in order to evaluate the consequences of such an event and support the first-response teams.

The goal of the source term estimation (STE) is to detect the source and assess the parameters of the CBRN release:

- With sufficient accuracy
- With a quantification of the uncertainty
- Within a reasonable amount of time
There are several approaches for the same objective in the field of STE

1) **Adjoint transport modelling and retro-transport**
   - Pudykiewicz (1998)
   - Issartel and Baverel (2003)

2) **Data assimilation and deterministic Bayesian inference**
   - Issartel (2005)
   - Winiarek *et al.* (2012)

3) **Genetic algorithms**
   - Haupt (2005)
   - Rodriguez *et al.* (2011)

4) **Bayesian inference coupled with stochastic sampling**
   - Delle Monache *et al.* (2008)
   - Chow *et al.* (2008)
   - Keats *et al.* (2007)
   - Yee (2008)

Mainly focused on Markov Chain Monte Carlo (MCMC) methods
The Bayesian framework allows:

- Taking into account errors from the model and from the observations
- Dealing with the presence and absence of prior information
- Estimating the uncertainty of the results

In our case, we consider the observations $Y$ given by $N_C$ sensors

$$Y = (y_{1,t1}, y_{1,t2}, \ldots, y_{1,tT}, y_{2,t1}, \ldots, y_{Nc,tT})$$

The parameters of the source are the position $\theta = (x_s, y_s)$ and the release rate vector $q$
which is discretized into $T_s$ time steps (instantaneous or continuous release)

The data model can be written as follows:

$$Y = C_{\theta}q + b$$

Observations

Source-receptor matrix

Noise vector

Independent and identically distributed

Gaussian-distributed $N(0, \sigma^2_{\text{obs}})$
About the source-receptor matrix, at a given position $\theta$…

- The vector $q$ is a discretization in time of the emitted quantity during the continuous release.

- Each element of the matrix $C_\theta$ is the concentration obtained from a unitary release for a source at $\theta$.

- Each column $i$ can be seen as the result of an instantaneous release $q_i$.
The goal of our Bayesian approach is to approximate the posterior distribution of the parameters, namely \( p(q, \theta | Y) \).

We adopt a two-step method by first estimating separately \( \theta \) then \( q \).

Considering the posterior as a conditional joint distribution, we have:

\[
p(q, \theta | Y) = p(q | \theta, Y) \ p(\theta | Y)
\]

\( p(\theta | Y) \) is the posterior distribution of \( \theta \), and its computation allows to estimate the position of the source (spatial aspect).

\( p(q | \theta, Y) \) is the conditional posterior of \( q \), and its computation allows to quantify the release-rate vector (temporal aspect).

\textit{N.B. It can only be computed once we have an estimation of \( \theta \) given by the previous step.}
The Bayesian framework (4)

1\textsuperscript{st} step (spatial aspect) \( p(\theta|Y) \)

- The posterior of \( \theta \) can be expressed, following Bayes formula, as follows:

\[
p(\theta|Y) = \frac{p(Y|\theta)p(\theta)}{p(Y)} \propto p(Y|\theta)p(\theta)
\]

\textit{Likelihood of \( \theta \)} \hspace{2cm} \textit{Prior information on \( \theta \)}

(implies the computation of \( C_\theta \) through a dispersion model)

- The rest of the presentation is focused on the spatial aspect which can’t be computed directly and needs the use of numerical methods described further

2\textsuperscript{nd} step (temporal aspect) \( p(q|\theta,Y) \)

- If we assume that the prior \( p(q) \) is Gaussian, then the conditional posterior of \( q \) is also Gaussian (conjugate priors)

- With a known estimation \( \hat{\theta} \), \( p(q|\hat{\theta},Y) \) can be computed analytically
Sampling and the AMIS algorithm (1)

- The separation described previously allows us to work on a 2-dimension problem (estimating $\theta$) instead of a $T_s + 2$ problem (estimating $(\theta, q)$).

- How to compute an approximation of $p(\theta | Y)$?

- Posterior distributions which can’t be easily derived are usually approximated by numerical techniques such as Monte Carlo methods.

- One of the most popular algorithms of stochastic sampling is the Markov Chain Monte Carlo (MCMC) algorithm, widely used in many domains, including STE problems…

  … However, MCMC is often slow to converge, hence not quite appropriate in a first-response context.

- Our study then focuses on another branch of Monte Carlo methods, based on the principles of Importance Sampling (IS).
Sampling and the AMIS algorithm (2)

- IS consists in drawing a set of samples (called particles) from a proposal distribution \( \phi \) and compute importance weights \( w \) in order to approximate the target distribution \( \pi \)

\[
\forall i \in \{1, \ldots, N\}, \ w_i = \frac{\pi(x_i)}{\phi(x_i)}
\]

\[
\pi(x) = \frac{1}{N} \sum_{j=1}^{N} w(x_j) \delta_{x_j}(x)
\]

- Iterative schemes of IS have been designed among them the Population Monte Carlo (PMC) algorithm allows to tune adaptively the proposal at each iteration.

- The Adaptive Multiple Importance Sampling (AMIS) algorithm enhances the PMC by adding a recycling process of the importance weights over all the previous iterations in order to accelerate the convergence.
Sampling and the AMIS algorithm (3)

- **AMIS algorithm**

  1. Draw $N$ particles from the proposal $\phi_t$ (sampling step)
  2. For the $N$ particles, compute the importance weights $w_t$ (involves the computation of $C_\theta$ and therefore the use of a dispersion model)
  3. Update all the previously computed weights $w_{1:t-1}$ of the previous particles
  4. Update the parameters of $\phi_t$ (with a Kullback-Leibler divergence minimization criterion)

- In our case, the chosen proposal is a mixture of $D$ multivariate Gaussian distributions

\[
\phi(\theta|\alpha, \Xi) = \sum_{d=1}^{D} \alpha^d \phi_d(\theta|\Xi_d)
\]

where $\Xi_d = (\mu_d, \Sigma_d)$ are the parameters of the $d$-th component of the mixture

and $\alpha_d$ is an importance relative to the cluster sampled after the $d$-th component
Simulations and results (1)

- A synthetic case is carried out with a grid of 25 sensors on a square domain
- D = 4 (number of mixture components in the proposal)
- Source is located at (10, 20)
- Dispersion model is a simple Gaussian puff model

View of the source and the sensors making detections and making no detection
Simulations and results (2)

MCMC (Metropolis-Hastings)

Histogram of the posterior:
- 5000 iterations
- Random initialization

AMIS

Probability density function of the posterior:
- 5 iterations
- 100 particles sampled per iteration
Simulations and results (3)

- Experimental case: trial #7 of the FUSION Field Trial 07 experiment
- Study on a subset of the 25 sensors (the whole network contains 100 sensors) closest to the source
- Dispersion model is a simple Gaussian puff model

**View of the simulation domain, the source, the sub-array of sensors and the positions of the initial particles**

**Averaged concentration measurements for the trial #7 of FFT07 experiment**
First results of the AMIS algorithm provide a satisfying estimation of the source position

\[ D = 4 \quad 10 \text{ iterations} - 100 \text{ particles per iteration} - \text{Computation time} = 502 \text{ s} \]

Estimated position (Minimum Mean Square Error) at 12.7 m of the real source

Map of the weighted particles approximating the posterior distribution

PDF of the posteriors for the position
(in green: coordinates of the real source)
AMIS is an original Bayesian stochastic approach to solve Source Term Estimation problems in non-instantaneous cases.

The first results on synthetic data are encouraging, and more results with FFT07 experimental data are yet to come to validate the method, as well as the validation of the temporal aspect (retrieving the form of the release rate).

Other improvement projects are on the table:
- Using a more accurate dispersion model to factor in urban conditions (LPDM)
- Taking into account the wind uncertainty into the estimation
- Build a parallel version for large-scale computations