Analysis of elevated I-131 samples observed in 2011 over Europe

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1. Introduction

We are concerned with analysis of elevated I-131 samples observed between September and November 2011 across Europe. Later on these samples were connected with I-131 emissions from the Hungarian Institute of Isotopes in Budapest. Using the data from multiple European countries we attempt to estimate (i) the source term given the source location is known and (ii) the source location itself.

We compare first results provided by two methods. Firstly, we use a standard source inversion approach based on minimization of a quadratic objective function. Secondly, we use a more advanced method based on Variational Bayes approximation. Here, all uncertainties are formulated as a prior probabilistic model which is capable of introducing some additional assumptions on the solution like sparsity or smoothness. Since the inference of the model is intractable, we follow Variational Bayes approximation yielding an iterative algorithm for estimation of all model parameters. Thus, the source term and elements of covariance matrices are estimated from the data automatically.

2. Theoretical background

General foundations for both methods are provided by Bayes' theorem. Let $p(x)$ and $p(y)$ be probability density functions (pdfs) of vectors x (source term) and y (measurements), respectively:

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)} = \frac{p(y|x)p(x)}{\int p(y|x)p(x)dx} \propto p(y|x)p(x).$$

The goal is to obtain posterior distribution $p(x|y)$. Optimum estimate of $\hat{x}$ is then, e.g., a maximum or mean of this posterior.

2.1 Cost function optimization

If both likelihood function $p(y|x)$ and prior $p(x)$ are Gaussian pdfs

$$p(y|x) = \mathcal{N}(Mx, R) = \frac{1}{(2\pi)^{isx/2}\sqrt{|R|}} \exp\left(-\frac{1}{2}(y - Mx)^T R^{-1}(y - Mx)\right),$$

$$p(x) = \mathcal{N}(x_a, B) = \frac{1}{(2\pi)^{itx/2}\sqrt{|B|}} \exp\left(-\frac{1}{2}(x - x_a)^T B^{-1}(x - x_a)\right),$$

then maximizing $p(x|y)$ is equivalent to

$$\hat{x} = \arg\min\left(0.5(y - Mx)^T R^{-1}(y - Mx) + 0.5(x - x_a)^T B^{-1}(x - x_a) + const\right). \quad (1)$$

Here, R and B represent error covariances of observations and source prior which must be known (selected) in advance. i.e. it is a subjective method. For simplicity, both these matrices are usually assumed to be diagonal, i.e. all measurements and source term elements are assumed to be independent. Observation error contains not only measurement error itself but it should contain also a model error caused by wrong conceptualization of a physical phenomena in the model.

The first term on r.h.s of (1) measures deviations of model from observations and the second term acts as a regularization and measures deviation of source hypothesis from prior x_a. Optimal source $\hat{x}$ is found via minimizing cost function

$$J(x) = \underbrace{(y - Mx)^T R^{-1}(y - Mx)}_{\text{model-obs mismatch}} + \underbrace{(x - x_a)^T B^{-1}(x - x_a)}_{\text{regularisation}}$$

This can be done analytically by $\frac{\partial J}{\partial x_i} \stackrel{!}{=} 0,\ i = 1, \ldots, \dim(x)$ which leads to a system of linear equations for $\hat{x}$ (after subtracting x_a):

$$(M^T R^{-1} M + B^{-1})(\hat{x} - x_a) = M^T R^{-1}(y - Mx_a). \quad (2)$$

Posterior error covariance matrix of $\hat{x}$ is then

$$\Sigma_x = (M^T R^{-1} M + B^{-1})^{-1}. \quad (3)$$

We have not made any assumptions on constraining the solution so far. Usually we are interested in emission which are non-negative. This is achieved by repetitive solution of (2) with increased regularization on prior which prevents problematic elements of the solution to diverge from (non-negative) prior values.

2.2 Prior model for unknown covariance

The second fully Bayesian method drops the assumption on diagonal error covariance matrices. Consider the following structure of matrix B:

$$B = L^T \Upsilon L, \quad L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ l_1 & 1 & 0 & 0 \\ 0 & \ddots & 1 & 0 \\ 0 & 0 & l_{n-1} & 1 \end{pmatrix}, \quad \Upsilon = \begin{pmatrix} v_1 & 0 & 0 & 0 \\ 0 & v_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & v_n \end{pmatrix}.$$

where the vectors of unknowns are $\mathbf{l} = [l_1, \ldots, l_{n-1}], \boldsymbol{v} = [v_1, \ldots, v_n]$. The Bayesian formalism requires to define prior distribution on all unknowns. We choose

$$p(v_i) = \mathcal{G}(a_0, b_0) \qquad p(l_i) = \mathcal{N}(-1, \sigma_0) \quad (4)$$

The formal solution of the estimate is difficult to evaluate:

$$p(x|y, M, \boldsymbol{v}, \mathbf{l}) = \int p(y|x, M)p(x|\mathbf{l}, \boldsymbol{v})p(\mathbf{l}, \boldsymbol{v})d\mathbf{l}, \boldsymbol{v}. \quad (5)$$

Analytical solution of (5) is not available and a suitable approximation has to be found. Following the Variational Bayes approximation ([1]), the posterior estimate can be obtained by solving the following equations:

$$\tilde{p}(x|y, M) \propto \exp\left(\int \tilde{p}(\boldsymbol{v}|y)\tilde{p}(\mathbf{l}|y) \log p(x, y, \mathbf{l}, \boldsymbol{v}|M) d\boldsymbol{v}\, d\mathbf{l}\right),$$

$$\tilde{p}(\mathbf{l}|y, M) \propto \exp\left(\int \tilde{p}(x|y)\tilde{p}(\boldsymbol{v}|y) \log p(x, y, \mathbf{l}, \boldsymbol{v}|M) dx\, d\boldsymbol{v}\right),$$

$$\tilde{p}(\boldsymbol{v}|y, M) \propto \exp\left(\int \tilde{p}(x|y)\tilde{p}(\mathbf{l}|y) \log p(x, y, \mathbf{l}, \boldsymbol{v}|M) dx\, d\mathbf{l}\right),$$

which can be solved iteratively. The iterative algorithm requires to evaluate moments of all unkonws, namely:

$$\mathrm{E}(x) = \hat{x}, \quad \mathrm{E}(x^T x) = \hat{x}^T \hat{x} + \Sigma_x,$$

Since the source term can not be negative, we seek only for positive solutions of the problem. Hence, we may restrict the support of prior $p(x)$ to positive domain only using truncated normal distribution

$$p(x_j) = t\mathcal{N}(0, \sigma_{x_j}^{-1}, \langle 0, \infty \rangle),$$

which moments are non-trivial but available as

$$\widehat{x} = \mu - \sqrt{\sigma}\frac{\sqrt{2}[\exp(-\beta^2) - \exp(-\alpha^2)]}{\sqrt{\pi}(erf(\beta) - erf(\alpha))}. \quad (6)$$

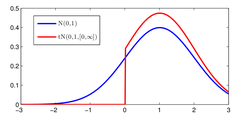

Figure 1: Example of the normal distribution $\mathcal{N}(1, 1)$, blue line, and the truncated normal distribution $t\mathcal{N}(1, 1, < 0, \infty >)$, red line.

Václav Šmídl and Anthony Quinn.
The variational Bayes method in signal processing.
Springer Science & Business Media, 2006.

3. Experiment settings

- Computational grid 30×30 with $\Delta_x = \Delta_y = 1deg$
- 26 I-131 concentration samples from Ring of Five network included into inversion
- Sampling interval of measurements were rather long — from 3 to 7 days
- For each sample a backward FLEXPART 9.2 approx. 50 days back was done, each with just 100k particles
- Model forced with GFS forecasts with horizontal resolution 0.5 deg and 26 vertical levels, 3 hours temporal resolution
- Ground layer 0–300m agl
- No iodine in gaseous form assumed, just an aerosol
- Resolution of the source set to 1 day

4. Measurements

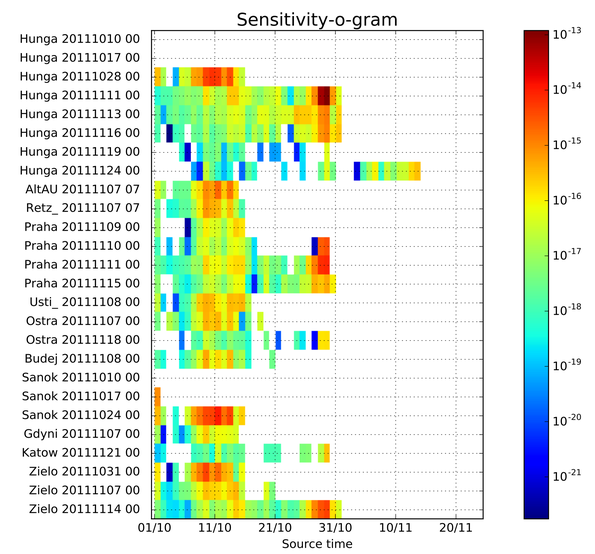

Figure 2: Sensitivity-o-gram — source-receptor sensitivities of 26 for which we did backward runs of FLEXPART.

5. Source term estimation

Here we assume the source location to be precisely known and estimate just the temporal profile of the source term. Reference source term was obtained from a press release published by IAEA after the event.

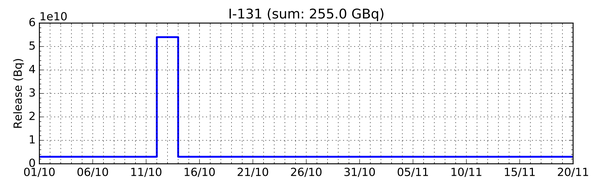

Figure 3: Reference source term published by IAEA after the event.

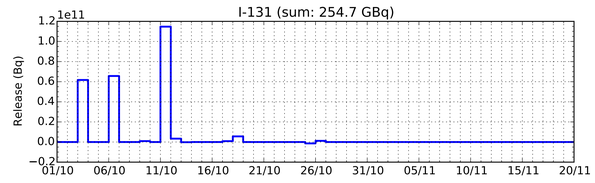

Figure 4: Source term estimated using cost function minimisation. Location of the main peak is in accordance with the reference source term. Also, the overall magnitude of release is quite close to that reported by IAEA.

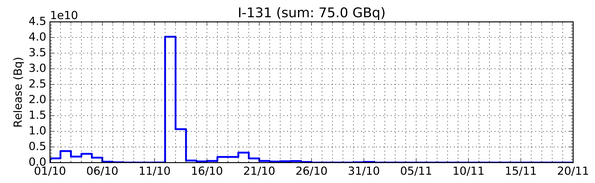

Figure 5: Source term estimated using Bayesian method. Timing of the main peak is in correspondence with the reference source term, however its magnitude is a little bit lower.

6. Source location

Source inversion was done using both methods for all grid cells in our domain (for a single grid cell at a time, no correlation among them were assumed). In total we did 31^2 inversion with each method.

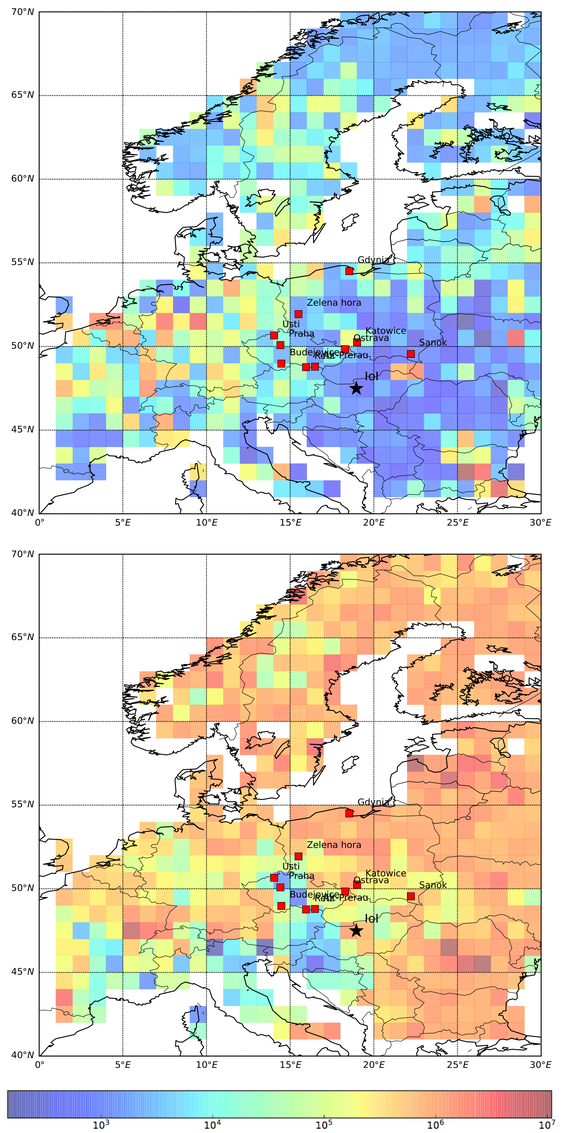

Figure 6: Results of source location. **Top:** Source location using cost function approach. **Bottom:** Source location using fully Bayesian approach. Results were transformed to be comparable. Lower value means higher change that the release originated from a particular grid cell.

The methods are quite different. Cost function approach evaluates cost function for each grid cell. It does not give any useful information in this case since it assigned low cost function values to a large number of dispersed grid cells. Bayesian approach provides for each grid cell a probability containing the source. It performed better in this case — as a possible source region it confined much smaller area not too far from the true source location.

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