Inverse modelling for source term reconstruction

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Introduction

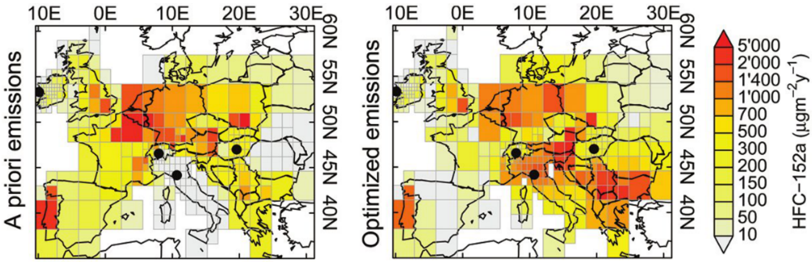
- Goals and example applications
- Inverse modeling ingredients
  - Atmospheric transport modeling
- Methodology and state-of-art
- Real world example - analysis of measurements from IMS
- Conclusion

Inverse modelling - Goals

- The ultimate goal of the inverse modelling is to provide a source-term estimate based on analysis of measurements and their systematic comparison with results of atmospheric dispersion modelling (optimization of model parameters)
- This has many applications of different purposes and various complexity

Applications: Emissions of greenhouse gasses

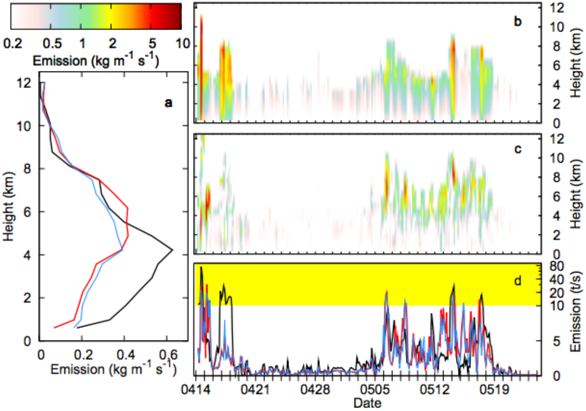
- Backtracking of emissions of trace species (e.g. halogenated hydrocarbons like CFCs) using atmospheric transport modeling to countries of their likely origin and estimation of release magnitudes
- Comparison of emissions reported from European countries with observations — multiple sources with unknown time profiles



From: Keller, Christoph A., et al. "European emissions of halogenated greenhouse gases inferred from atmospheric measurements." Environmental science & technology 46.1 (2011): 217-225.

Applications: Emissions of ash from volcanoes

- Estimation of ash emission from volcanoes for purposes of aviation using satellite observations — known source location, unknown time and height profile



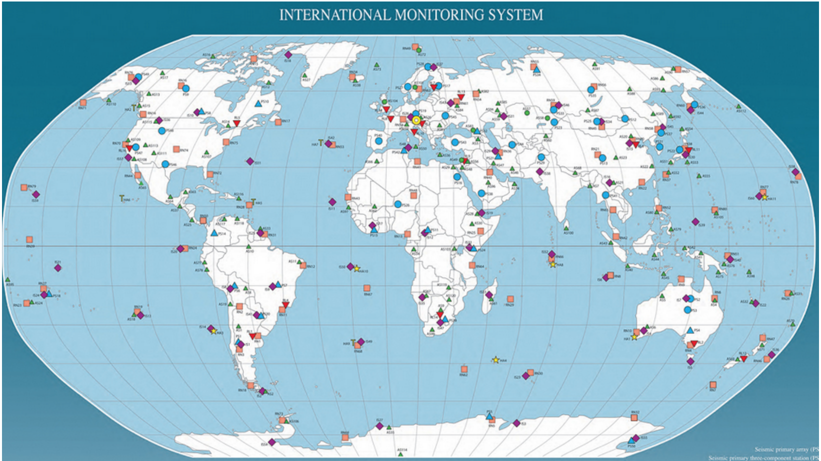
From: Stohl, A., et al. "Determination of time-and height-resolved volcanic ash emissions and their use for quantitative ash dispersion modeling: the 2010 Eyjafjallajökull eruption." Atmospheric Chemistry and Physics 11.9 (2011)

Applications: Nuclear applications — nuclear accidents

- Estimation of emissions from Fukushima accident using nuclide-specific observations — known source location, unknown time and height profile
  E.g.: Stohl, A., et al. "Xenon-133 and caesium-137 releases into the atmosphere from the Fukushima Dai-ichi nuclear power plant: determination of the source term, atmospheric dispersion, and deposition." Atmospheric Chemistry and Physics 12.5 (2012): 2313-2343.
- Estimation of emissions from Fukushima accident using bulk gamma dose rate observations (more common, higher time resolution, no nuclide information) — known source location, unknown time and height profile, source composition, isotope ratios
  Saunier, Olivier, et al. "An inverse modeling method to assess the source term of the Fukushima Nuclear Power Plant accident using gamma dose rate observations." Atmospheric Chemistry and Physics 13.22 (2013): 11403-11421.

Applications: Nuclear applications — verification of CTBT

- Verification of the CTBT (Comprehensive Nuclear-Test-Ban Treaty) by the means of CTBTO Int. Monitoring System (IMS) (Operationally estimated **possible source regions** using correlations of samples with source sensitivities)
- Unknown source location, unknown time and height profile of source, background sources cluttering useful signal



Inverse modelling — basic ingredients

- Set of observation (and their error statistics)
- Results of atmospheric transport modeling (and corresponding error statistics)
- Prior information about the source: source type (e.g. point source), location, magnitude of release, effective release height (and corresponding error statistics)
- A metric quantifying compatibility between measured data and source hypothesis (cost function, likelihood, KL-divergence etc.)

Atmospheric transport modelling (ATM)

- Let $\mathbf{x}^T = [x_1, \ldots, x_I]$ be a vector of sources characterized by their spatial-temporal characteristics (a point for point-sources/3D grid cell for volume sources and a release time interval) and $\mathbf{y}^T = [y_1, \ldots, y_J]$, be a set of observations—sampling points given their location and sampling time (interval). A general atmospheric chemistry transport model can be understood as a non-linear operator $\mathcal{M}(\cdot)$ transforming sources to measurements

$$\mathbf{y} = \mathcal{M}(\mathbf{x}) + \epsilon.$$

- ϵ is an overall error caused by measurements errors, dispersion model imperfection, errors in its inputs including meteorological fields etc.

ATM: Source-receptor sensitivity

- Important concept in air quality modeling describing the sensitivity of a receptor to a source
- Source-receptor sensitivity of j-th sample and i-th source is defined

$$m_{ij} = \frac{\partial y_j}{\partial x_i}$$

- For a linear model $\mathcal{M}$, i.e. passive tracers and substances which do not undergo nonlinear chemical transformation (advection and dispersion is a linear process) and substances with a prescribed decay or growth rate (e.g. radioactive decay):

$$m_{ij} = \frac{y_j}{x_i}$$

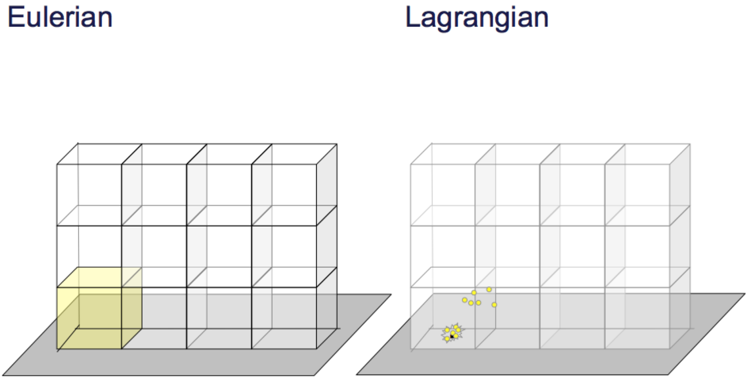
ATM: Source-receptor sensitivity

- Given a source-receptor matrix $\mathbf{M} \in \mathbb{R}^{I \times J}$, the resulting receptor values can be obtained simply by matrix-vector multiplication, avoiding evaluation of the whole model $\Rightarrow$ from mathematical point of view the problem is fully described by $\mathbf{M}$, $\mathbf{y}$ and (optionally) their error statistics and a prior

$$\mathbf{M}\mathbf{x} = \mathbf{y}$$

- Unfortunately, the system is often ill-conditioned and cannot be solved for $\mathbf{x}$
- How to obtain $\mathbf{M}$?

ATM: Eulerian vs. Lagrangian models



Immediate dilution in the grid cell

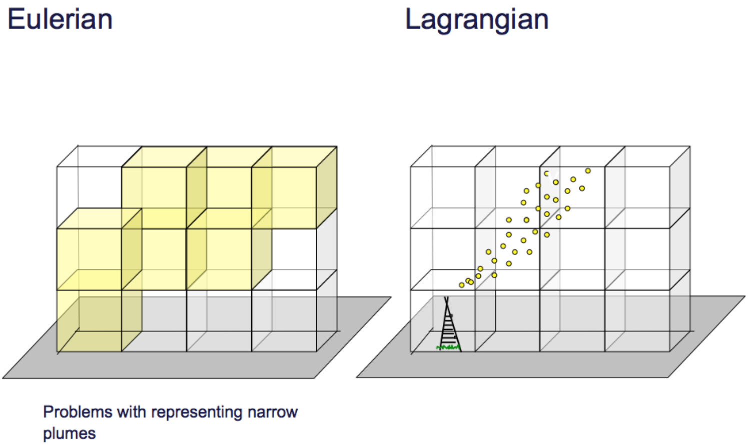
Point source sub-model then needed

LPDM can deal naturally with point sources

The grid is only applied to output fields

From D. Arnold, FLEXPART training course 2013

ATM: Eulerian vs. Lagrangian models

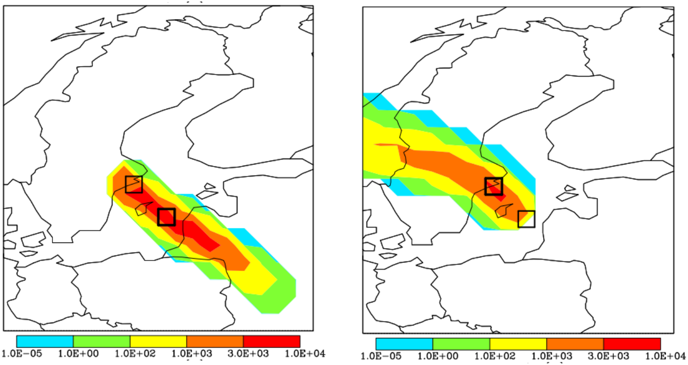


From D. Arnold, FLEXPART training course 2013

ATM: Lagrangian transport modelling

- PROs:
  - Can be computationally very efficient (depending on size of plume): only the fraction covered with particles is simulated
  - Turbulent processes are included in a more natural way unlike Eulerian models
  - There is no numerical diffusion due to a computational grid
  - Many first order processes can be easily included with a prescribed rate: radioactive decay, dry deposition, washout, etc.
  - One particle can carry more than one species
  - Better for treatment of point sources and receptors
- CONs:
  - It is quite difficult and computationally expensive to include non-linear chemical reactions (also in Eulerian, $\Delta t \sim$ reaction speed)
  - To do the chemistry in LPDM we have to do an intermediate gridding to get concentrations and then redistribute particles again, so we loose advantages of Lagrangian approach. Normally, we do the gridding only at the end.

ATM: Forward vs. backward calculation



From: Seibert, P., and A. Frank. "Source-receptor matrix calculation with a Lagrangian particle dispersion model in backward mode." Atmospheric Chemistry and Physics 4.1 (2004): 51-63.

ATM: Forward vs. backward calculation

- Forward is beneficial when we have more samples than potential source
- Backward is beneficial when we have more potential sources than samples
- Lagrangian ATM:
  - Forward run: particles released from sources
  - Backward run: models is "self-adjoint"—particles released from receptors with negative time sign
- Eulerian ATM:
  - Forward run: solving forward model with different right hand sides as many times as the size of control vector $\mathbf{x}$
  - Backward run: solving adjoint equations with different right hand sides as many times as the size of measurement vector $\mathbf{y}$

Parametrization of a source

- Source can be viewed as a mapping $s(x, y, z, t) : \mathbb{R}^4 \rightarrow \mathbb{R}^S$, where x, y, z are spatial coordinates, t is time and S is a number of species emitted
- Each time slot/spatial grid cell is a random quantity
- E.g.: a source at know location with unknown emission height/time can be parametrized as a source with possible emissions from different heights at different times: $\mathbf{x}^T = [x_{z=1,t=1}, \ldots, x_{z=Z,t=1}, \ldots, x_{z=1,t=T}, \ldots, x_{z=Z,t=T}]$, i.e. **we need SRS of measurements to all possible emission heights and times** where z and t are suitable discretized
- Large number of unknowns $\Rightarrow$ usually leads to an ill-conditioned problem which must be heavily **regularized**

ATM FLEXPART

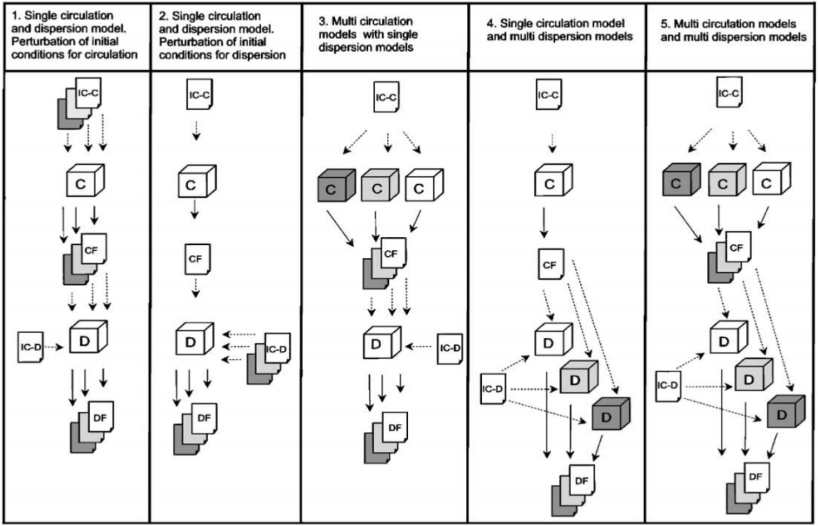
- A notable representative of the family of Lagrangian models
- Lagrangian particle dispersion model developed maintained mainly at NILU Norway (http://flexpart.eu/)
  Stohl, A., Markus Hittenberger, and Gerhard Wotawa. "Validation of the Lagrangian particle dispersion model FLEXPART against large-scale tracer experiment data." Atmospheric Environment 32.24 (1998): 4245-4264.
- $>$ 35 users from $>$ 15 countries
- Released under the GNU General Public License V3.0
- Evaluates dosimetric quantities in post-processing
- Two main alternative meteorological inputs:
  - ECMWF data http://www.ecmwf.int/
  - US National Weather Service - GFS data, available for download from http://nomads.ncdc.noaa.gov/

ATM: How to estimate model error?

- Model error often much more significant (higher) than the measurement error
- Critical particularly near the “edge of a plume”
- How to estimate it?
  - Assume model error proportional to measured value - a very poor man’s approach
  - Estimate “local error statistics” of a measurement using samples of model results around receptors - poor man’s approach (uncertainty in wind field, not in turbulence properties)
  - Difference between forward and backward runs
  - Ensemble approach — model error is estimated using an ensemble of INDEPENDENT and REPRESENTATIVE model runs. This assumption is not fulfilled in real world applications (models similar with common “parents”) and an ensemble should be inspected in terms of member covariance before use, see Potempski and Galmarini (2009)
  - Estimation of model error using hyper-parametrized models

ATM: How to estimate model error?

Different ensemble types:



From Galmarini et al. (2004)

Inverse modelling for source reconstruction — Methodology

1. Optimization approaches: $||\mathbf{y} - \mathbf{M}\mathbf{x}||^2 \rightarrow$ min by the means of solution of (ill-conditioned) system of linear equations
2. Fully Bayesian solution: Let $p(\mathbf{x})$ and $p(\mathbf{y})$ be probability density functions (pdfs) of vectors $\mathbf{x}$ and $\mathbf{y}$, respectively:

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

   - The goal is to obtain posterior distribution $p(\mathbf{x}|\mathbf{y})$
   - How? Different approaches for with different assumptions suitable for different scenarios and of a different complexity
     - Analytical approaches (conjugate distributions)
     - Approximate sampling-based approaches

- Sometimes, these two approaches are equivalent, as we will see...

Inverse modelling — Variational approach

- If both likelihood function $p(\mathbf{y}|\mathbf{x})$ and prior $p(\mathbf{x})$ are assumed to be Gaussian: $p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{M}\mathbf{x}, \mathbf{R})$, $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}_a, \mathbf{B})$, then Maximum A-Posteriori (MAP) estimate can be obtained as the mode of the posterior

$$\hat{\mathbf{x}} = \arg\max_{\mathbf{x}}(p(\mathbf{y}|\mathbf{x})p(\mathbf{x}))$$

- This is equivalent to

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

- $\mathbf{R}$ and $\mathbf{B}$ represent error covariances of observations and source prior (usually assumed to be diagonal)
- 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

$$\mathbf{R} = \mathbf{R}_{\mathrm{mod}} + \mathbf{R}_{\mathrm{mea}}$$

Inverse modelling — Variational approach

$$J_1(\mathbf{x}) = \underbrace{(\mathbf{y} - \mathbf{M}\mathbf{x})^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{M}\mathbf{x})}_{\text{model-obs mismatch}} + \underbrace{(\mathbf{x} - \mathbf{x}_a)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_a)}_{\text{regularisation w.r.t prior}} \rightarrow 0$$

- The first term on r.h.s measures deviations of model from observations and the second term acts as a regularization and measures deviation of source hypothesis from prior $\mathbf{x}_a$ (analogy to Tikhonov regul.)
- Minimization can be done analytically by $\frac{\partial J}{\partial x_i} \stackrel{!}{=} 0, \; i = 1, \ldots, I$
- We solve the following system for $\mathbf{x}$:

$$(\mathbf{M}^T \mathbf{R}^{-1} \mathbf{M} + \mathbf{B}^{-1})(\mathbf{x} - \mathbf{x}_a) = \mathbf{M}^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{M}\mathbf{x}_a)$$

- A-posteriori error

$$\mathbf{P} = (\mathbf{M}^T \mathbf{R}^{-1} \mathbf{M} + \mathbf{B}^{-1})^{-1}$$

Variational approach — Regularization

- We can impose also additional types of regularization (cost function does not need to be quadratic then):
  - **quadratic cost $\Rightarrow$ analytical minimization:** Stohl, A., et al. "Xenon-133 and caesium-137 releases into the atmosphere from the Fukushima Dai-ichi nuclear power plant: determination of the source term, atmospheric dispersion, and deposition." Atmospheric Chemistry and Physics 12.5 (2012): 2313-2343.
  - **numerical minimization:** Saunier, Olivier, et al. "An inverse modeling method to assess the source term of the Fukushima Nuclear Power Plant accident using gamma dose rate observations." Atmospheric Chemistry and Physics 13.22 (2013): 11403-11421.

Variational approach — Regularization

- Regularization on smoothness of $\hat{\mathbf{x}}$: additional term $\epsilon(\mathbf{D}\mathbf{x})^T(\mathbf{D}\mathbf{x})$, where $\mathbf{D}$ is a numerical approximation of *Laplacian operator* and ϵ its weight.
- Optimal source $\hat{\mathbf{x}}$ is found via minimizing cost function

$$J(\mathbf{x}) = \underbrace{(\mathbf{y}-\mathbf{M}\mathbf{x})^T\mathbf{R}^{-1}(\mathbf{y}-\mathbf{M}\mathbf{x})}_{\text{model-obs mismatch}} + \underbrace{(\mathbf{x}-\mathbf{x}_a)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_a)}_{\text{reg. w.r.t prior}} + \epsilon\underbrace{(\mathbf{x}-\mathbf{x}_a)^T\mathbf{D}^T\mathbf{D}(\mathbf{x}-\mathbf{x}_a)}_{\text{reg. w.r.t smoothness}}$$

- Barrier functions suitable for multiple species with unknown ratios bounded by conditions

$$\frac{1}{b_i} \leq \frac{x_1}{x_i} \leq a_i$$

$$r(x_i) = \exp\left(\frac{x_1}{x_i} - a_i\right) + \exp\left(\frac{x_i}{x_1} - b_i\right)$$

$$J(x) = J_1(x) + \sum_{i=2}^{I} r(x_i)$$

Cost function is no longer quadratic, must be minimized numerically, e.g. by a gradient descent method

Inverse modelling — Bayesian approach

- Sampling (brute force) approach
- Hierarchical models — hyper-parameters of anything
- Variational Bayes
- Marginalized models ... and many more

Examples:

- **MLE on hyperparameters**: Winiarek, Victor, et al. "Estimation of the caesium-137 source term from the Fukushima Daiichi nuclear power plant using a consistent joint assimilation of air concentration and deposition observations." Atmospheric Environment 82 (2014): 268-279.
- **MCMC**: A. Ganesan, M. Rigby, A. Zammit-Mangion, A. Manning, R. Prinn, P. Fraser, C. Harth, K.-R. Kim, P. Krummel, S. Li & others, Characterization of uncertainties in atmospheric trace gas inversions using hierarchical Bayesian methods, Atmospheric Chemistry and Physics 14, 3855-3864 (2014)
- **sequential MC**: Šmídl, Václav, and Radek Hofman. "Efficient Sequential Monte Carlo Sampling for Continuous Monitoring of a Radiation Situation." Technometrics (2013), doi 10.1080/00401706.2013.860917

Conclusion

- The spectrum of methods spans from simple regression to advanced Bayesian methods
- The problem can be reduced to linear algebra operations — what we need is just a SRS matrix, corresponding vector of observations (optionally their error statistics and a prior)
- Different datasets are available, e.g., in a database hosted at NILU: http://actris.nilu.no/

Real life application:

Analysis of the April 2013 radioxenon detections based on formal inverse modeling

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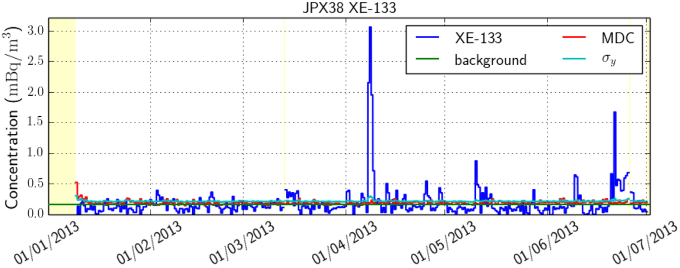
23 Sep 2014, ATM workshop 2014, Stockholm, Sweden

Objectives

- Our goal is to analyze 3 significant ^{133}Xe detections made 7–9 April 2013 at Takasaki station (JPX38, CTBTO IMS)
- We attempt to estimate time- and height-dependent source shapes using a cost function based inverse modeling technique
- Scenarios with both known and unknown source location are studied
- Demonstration of fusion with waveform events of period of 30 Jan – 26 Feb 2013

Samples included into inversion

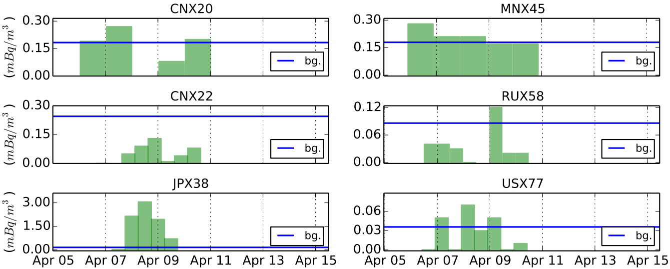
- *Triggering samples* — 3 significant JPX38 detections:
  - 08 April 2013 06:54 UTC collection stop
  - 08 April 2013 18:53 UTC collection stop
  - 09 April 2013 06:54 UTC collection stop

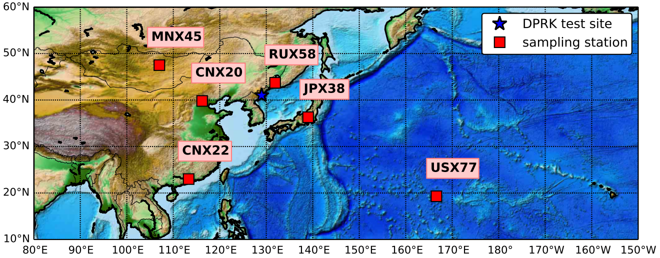


- *Other relevant samples* (incl. nondetections to confine the source) — samples spatially and temporally adjacent:
  - Spatially we include additional samples from 5 adjacent stations (RUX58, MNX45, CNX20, CNX22 and USX77)
  - Temporally ±1 sampling period for JPX38 and ±2 otherwise

Samples included into inversion – Summary

- 36 detections and nondetections enter *source inversion* algorithm where systematically compared with *atmospheric transport modeling* to give us some inference about the source (location, strength...)





Atmospheric transport modeling

- Source-receptor sensitivities (SRS) calculated using backward runs of FLEXPART 9.0
- 36 samples = runs, each with 1 mio particles, ≤15 days back
- SRS calculations performed with high accuracy:
  - ECMWF input data 0.25° horizontal resolution, 91 vertical levels, 3 h temporal resolution
  - FLEXPART output on lon-lat grid with $\Delta x = 0.25°$ and $\Delta y = 0.2°$ every 3 hours
  - Convection enabled in FLEXPART
- We assume 5 vertical layers in order to account for complex terrain at the DPRK test site which varies between 500 and 2200 m asl: 0–100 / 100–500 / 500–1000 / 1000–1500 / 1500–2000 m (metres above model ground), model ground is 880 – 1500 m asl
- We assume point releases only (from a single grid cell – implicit a-priori knowledge)

Inversion methodology

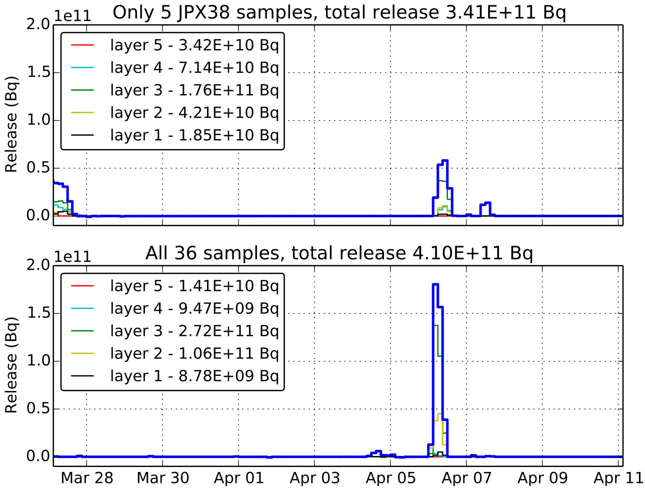
- Estimation of temp. shape of a release in 5 vertical layers over $\approx$ 15-day time window: **121** *possible 3-hour release intervals* $\times$ **5** *vertical layers* = **605** *unknowns*
- Problem is ill-conditioned – data do not constraint enough all elements of the source vector $\mathbf{x}$ $\Rightarrow$ we need **regularization**
- Solution is found via minimizing the cost function

$$J(\mathbf{x}) = \underbrace{(\mathbf{y}-\mathbf{M}\mathbf{x})^T\mathbf{R}^{-1}(\mathbf{y}-\mathbf{M}\mathbf{x})}_{\text{model-obs mismatch}} + \underbrace{(\mathbf{x}-\mathbf{x}_a)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_a) + \epsilon(\mathbf{D}\mathbf{x})^T(\mathbf{D}\mathbf{x})}_{\text{regularisation}}$$

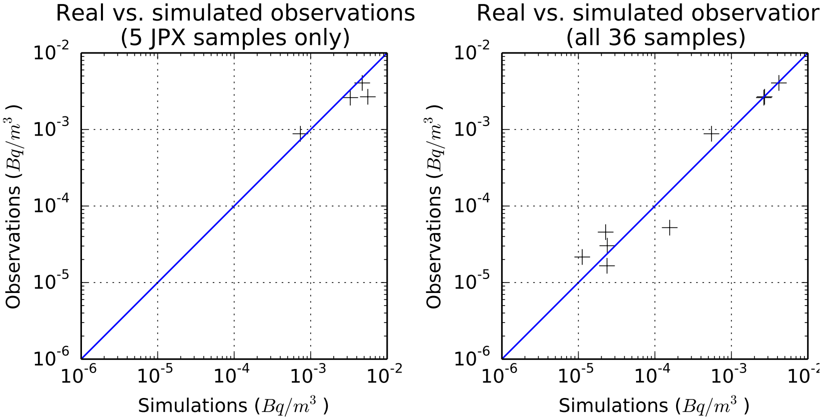
- Model error estimated using "pseudo-ensemble" of model runs (SRS shifted in time and space) and added to obs. error
- First-guess solution $\mathbf{x}_a = 1 \cdot 10^3$ Bq (≈ 0); $\sigma_x = 3 \cdot 10^{11}$ Bq per element of solution vector, thus total can be larger
- Negative parts of solution were suppressed via iterative process reducing first-guess error for appropriate solution parts

Case 1: Cont. release at DPRK test site – temp. shape

- Simultaneous estimation of the source strength as a function of release time and height
- Addition of non-detections suppressed releases at the beginning of assumed interval

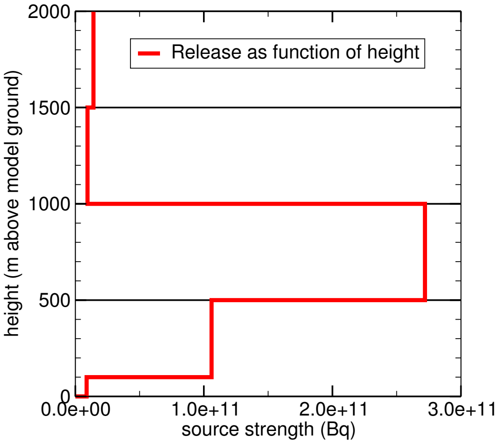


Case 1: Agreement of retrieved STs with observations



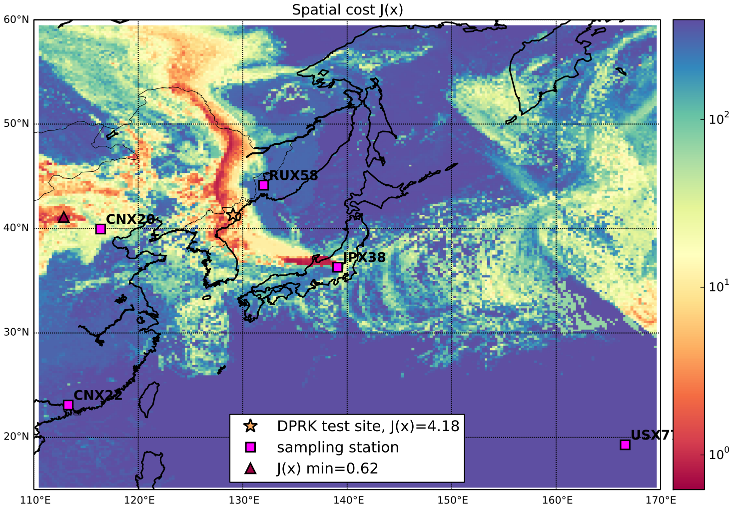
Case 1: Cont. release at DPRK test site – vertical profile

- Important to use elevated release
- Main release 100–1000 m agl (model)
- Corresponds roughly to 1000-2500 m asl – quite reasonable



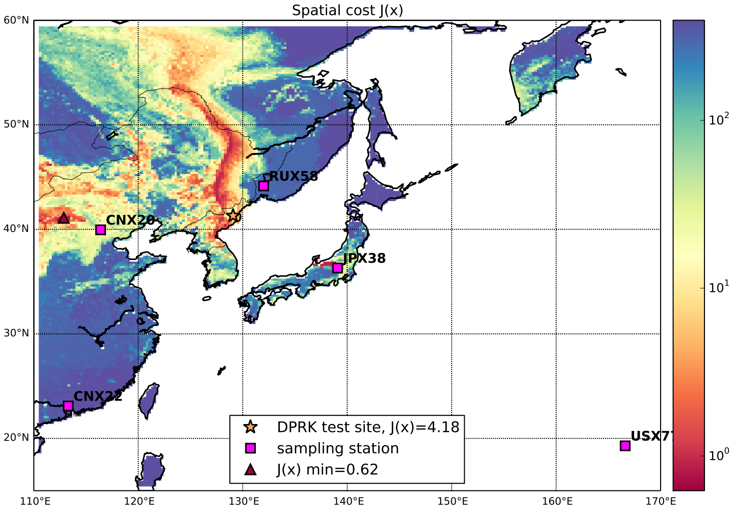
Case 2: Cost function all over the domain

- Test each grid cell as an *independent* candidate source, determine release time/shape by inversion and plot cost function per grid



Case 2: Cost function all over the domain

- Oceans masked

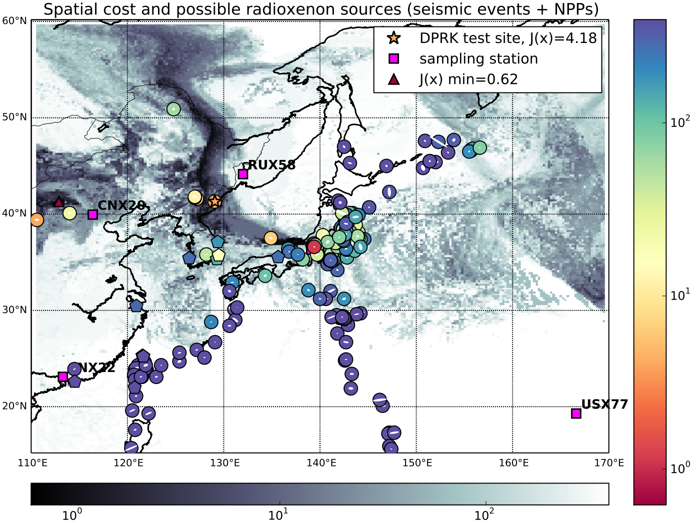


Fusion with possible sources – Method

- Select a list of relevant seismic events (time period, region)
  - Here: 193 seismic events from 30 Jan – 26 Feb 2013 in our inversion domain
- Select other possible sources of emissions (medical isotope production facilities, NPPs...)
  - Here: 10 NPPs from China, Taiwan, South Korea and Japan (the only operating nuclear power plant in Japan during the time of interest was NPP Ohi)
- Attribute cost function value to all assumed 203 events/sources based on their location (in which grid cell(s) they fall)
- Exclude events which fall into regions with high cost function
- Plot/rank remaining events by their cost function value

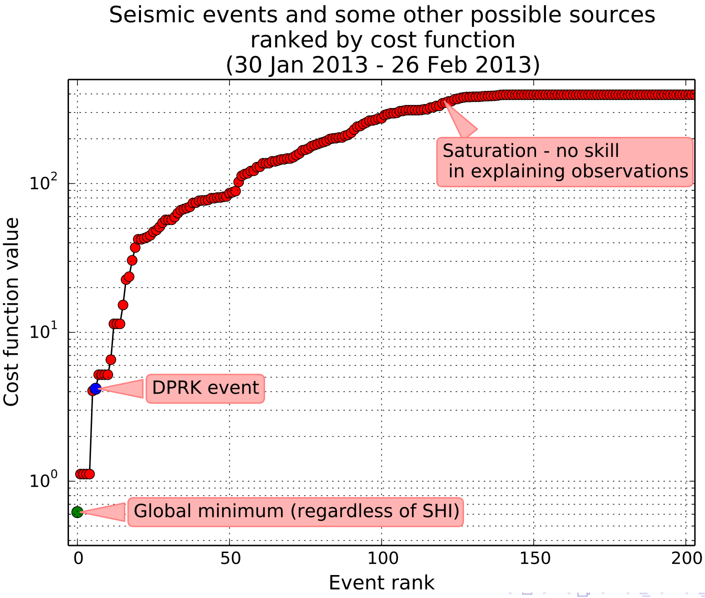
Fusion with possible sources – Result

- Cost function in the background as grayscale
- Ellipses surrounded by circle coloured with the cost at ellipse centre
- NPPs marked by pentagons coloured with the cost at NPP site



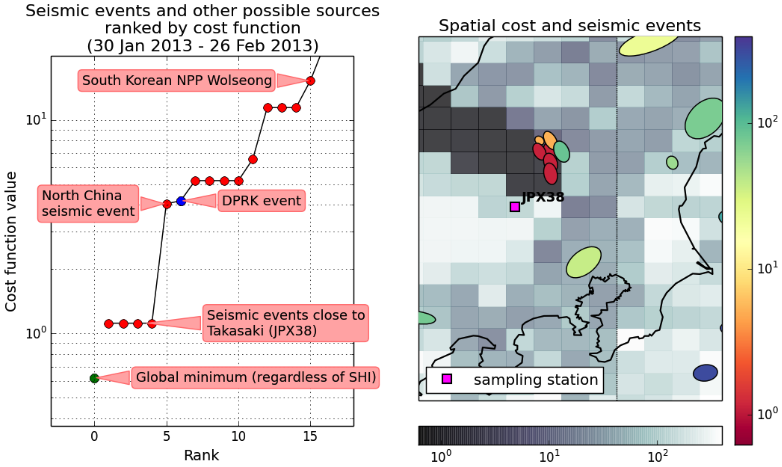
Fusion with possible sources – Result (rank plot)

- Events ordered according to their cost function value



Fusion with possible sources – Result (rank plot)

- Closer look on events with lowest cost function values



- Currently, cost function values taken from a single point (ellipse center) — this can lead to misclassification of an event (red and green ellipses), maybe some averaging (smoothing) appropriate

Conclusions of experiment

- The DPRK test 2013 / April 2013 Xe-133 detections were used as a test for inverse-modelling based source location and quantification
- The problem is heavily ill-conditioned (36 samples, mostly non-detections, 605 unknowns), regularization methods for obtaining physically reasonable solution must be employed.
- Release shape estimated using different variants of the method is consistent and appears to be a stable feature
- Magnitude of release ($\approx$ 4E11 Bq) is lower than previously suggested due to different inversion strategy and settings
  - Might be influenced by regularization, further tests needed
- DPRK test site is among the region of lower cost function though not at the global minimum

Conclusions (2) – Fusion

- Cost function from the inversion can be used as a measure of compatibility between assumed source location and observed radionuclide concentration — regions with low cost function are possible source regions
- Because of the uncertainties involved, the source does not need to be in the very minimum of the cost function
- The source was found to be associated with the 5th lowest cost function among all the assumed sources in the time window considered
- By clipping events at some value of the cost function, the number of candidate events could be reduced substantially
- Of course, many possibilities exist for refinements and extensions

Options for future improvements

- Better quantification of errors both for the input and the results
  - Use different resolution of met. data and SRS data for ATM uncertainty quantification
  - Use ensemble of SRS data from different transport models
  - Include off-diagonal terms in error covariance matrices
  - Work on quantifying background uncertainty
  - Experiment more with regularisation
- Try to include known background radioxenon sources into inversion
- Try also inversion of ^{131m}Xe data
- Do next iteration of relevant RN samples which could be useful for narrowing down further the likely source regions

Thank you!

Acknowledgements:

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