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A baseline for source reconstruction using the inverse atmospheric modelling tool FREAR

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Forensic Radionuclide Event Analysis and Reconstruction - the "FREAR" code

- Initially developed with the purpose of CTBT verification
- Required input:

(1) source-receptor sensitivities (*M*)

(2) observed airborne activity concentrations (*y*)

(Can deal with both detections and instrumental non-detections; it takes into account the possibility for misses and false alarms)

- FREAR can solve the inverse modelling problem using two independent methods: a cost function optimization method and a Bayesian MCMC method
- Users can select the most appropriate source parameterization for a given problem (such as multiple release segments or a release from a fixed location), and can add their custom source parameterization if needed
- The Bayesian inference approach provides an estimate on the uncertainties in a natural way. Furthermore, an ensemble of atmospheric transport modelling can be used to better estimate model uncertainty
- Code written in R, available on GitLab under GPLv3

FREAR challenges and outlook

Some challenges:

- How to include different sources of observations (such as gamma dose rate measurements and deposition measurements)?
- FREAR performed well when applied to previous case studies; will it perform well when applied to the next case?

- Inclusion of deposition measurements \rightarrow talk Stijn Van Leuven
- Apply FREAR over a set of test cases \rightarrow this talk

Purpose: to establish a baseline for source reconstruction to facilitate testing of data, methods and settings

Constructing a set of cases

- ¹³³Xe observations at four monitoring stations for the period 1 September 2014
 – 30 December 2014 (120 d)
- Detections are linked with emissions from a (former) medical isotope production facility Chalk River Laboratories (CRL)
- Can we reconstruct the (known) source location of CRL?
- Two sets of case studies:
 - i. 8 cases with 15 d of observations
 - ii. 24 cases with 5 d of observations





ATDM and FREAR setup

ECMWF input: 3-hourly at 0.5° x 0.5° for full NH

Flexpart output: daily at 0.5° x 0.5°, 0 – 100 m, full NH

5-day cases: 10 daily release segments

15-day cases: 20 daily release segments

FREAR

Х

Bayesian inference

- infer source term
- infer source location
- y = M x

Cost function

- optimize source term
- for each grid box
- y = M x



maximum-in-time PSR using Pearson / Spearman correlation

- for each grid box
- correlation between y and M

Accumulated-in-time FOR

- for each grid box
- area where M[y>0] > 0 for any time

Three verification metrics for source localisation



Results: example of different inverse modelling methods and verification metrics

Residual cost after optimisation

Bayesian source location probability

0.5 2e-01

1e-01

5e-02

2e-02

1e-02

5e-03

2e-03

1e-03

5e-04

2e-04

1e-04 5e-05

2e-05

1e-05

Ω



Fraction of overlapping SRS of detections



maximum-in-time PSR (Spearman)

maximum-in-time PSR (Pearson)



| Method | Distance [km] | CDS | FDE |
|----------|------------------|-------|-------|
| bayes | 199 | 0.000 | 0.998 |
| cost | 226 | 0.884 | 0.949 |
| corr (P) | 2274 | 0.979 | 0.355 |
| corr (S) | 1494 | 0.942 | 0.091 |
| FOR | 1685 | 0.928 | 0.252 |

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Results: comparing different methods for 5 days and 15 days of observations (1/2)



Comparing methods:

• *bayes* and *cost* are able to locate the source much better than other methods

Comparing 5 d vs 15 d observations:

 bayes and cost show a significant improvement (from 800 km to 270 km)

Results: comparing different methods for 5 days and 15 days of observations (2/2)



Comparing methods:

- bayes: poor CDS score, other methods comparable
- *bayes* and *cost*: exclude large fraction of search domain

Comparing 5 d vs 15 d observations:

- bayes and cost show a deterioration in CDS score and an improvement in the fraction of domain excluded
- other methods show an improvement in the CDS score and a deterioration in the fraction of domain excluded

bayes at times overconfident as a very large fraction of the domain is excluded and the true source location has zero probability

Increasing uncertainty in the Bayesian inference: introducing multipliers (1/2)

| Default | Multipliers | |
|--|---|--|
| normal likelihood | ~ | |
| elaborate model for non-detections, false alarms, misses | ~ | |
| uncertainty sigma is replaced by a heavy-tail distribution | ~ | |
| one relative uncertainty for all observations (s = 1) | ~ | |
| | $y_i = m_i M_{ij} x_j + \varepsilon_i$ $m_i \in [0.1, 10]$ multipliers inferred | |

Increasing uncertainty in the Bayesian inference: introducing multipliers (2/2)

Default (s = 1)







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Increasing uncertainty in the Bayesian inference: uncertainties inferred (1/2)

| Default | Multipliers | Uncertainty inferred | |
|--|---|--|--|
| normal likelihood | ~ | ~ | |
| elaborate model for non-detections, false alarms, misses | ~ | simple model for dealing with non- detections | |
| uncertainty sigma is replaced by a heavy-tail distribution | ~ | sigma is used | |
| one relative uncertainty for all observations (s = 1) | ~ | one relative uncertainty for each station, inferred $\sigma \in [0.3, 10]$ | |
| | $y_i = m_i M_{ij} x_j + \varepsilon_i$ $m_i \in [0.1, 10]$ multipliers inferred | | |

Increasing uncertainty in the Bayesian inference: uncertainties inferred (2/2)

Default (s = 1)

Uncertainties inferred





Using multipliers



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Increasing uncertainty in the Bayesian inference: very high input uncertainty (1/2)

| Default | Multipliers | Uncertainty inferred | Default with high s |
|--|---|--|---------------------|
| normal likelihood | ~ | ~ | ~ |
| elaborate model for non-detections, false alarms, misses | ~ | simple model for dealing with non- detections | ~ |
| uncertainty sigma is replaced by a heavy-tail distribution | ~ | sigma is used | ~ |
| one relative uncertainty for all observations (s = 1) | ~ | one relative uncertainty for each station, inferred $\sigma \in [0.3, 10]$ | s = 10 |
| | $y_i = m_i M_{ij} x_j + \varepsilon_i$ $m_i \in [0.1, 10]$ multipliers inferred | | |

Increasing uncertainty in the Bayesian inference: very high input uncertainty (2/2)

Default (s = 1)

Uncertainties inferred









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Default (s = 10)



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All methods succeed in increasing the uncertainty in the selected case, but when applied to all cases...



Summary and conclusions

Two sets of case studies have been defined for inverse modelling using ¹³³Xe observations associated to a (former) medical isotope production facility Chalk River Laboratories:

• 8 cases using 15 days of observations and 24 cases using 5 days of observations

These sets allow for:

- a comparison of data (observation selection, NWP input, ATM input, ...)
- a comparison of methods (inverse modelling methods, source parameterizations, ...)
- the testing of new or modified inverse modelling algorithms

Findings:

- Bayesian inference and cost function optimization are able to exclude a large fraction of the location search domain, contrary to simpler methods
- Bayesian inference underestimates uncertainties since the true source location sometimes falls outside the possible source region (note: other methods do not optimize for source location)
- By considering several test cases, the best method can be selected

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