Sensitivity of a Bayesian source-term estimation model to spatiotemporal sensor resolution

Derek D. Jensen, Donald D. Lucas, Katherine A. Lundquist, Lee G. Glascoe

Lawrence Livermore National Laboratory

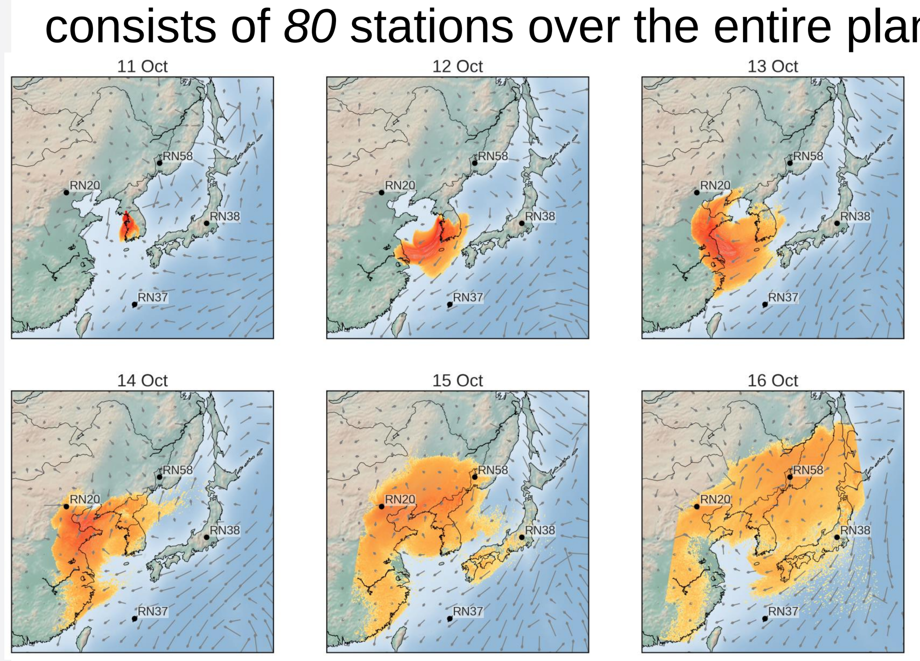
University of California National Laboratories

DATA SCIENCE INSTITUTE

Source term estimation (STE) attempts to calculate the most-likely source characteristics of an atmospheric release given concentration observations. The confidence in the STE depends on the time and space scales of the observations, sensor locations, and release parameters. Previously, we developed a probabilistic STE algorithm that was validated using high-resolution spatiotemporal observational data[1]. Here, the STE algorithm receives significant improvements, which extend applicability of the STE to coarser-resolution datasets. The skill of the improved algorithm is quantified over a broad range of sensor configurations and release scenarios

Operational Networks are Sparse

The Radionuclide Network of the International Monitoring System (IMS) consists of *80* stations over the entire planet.

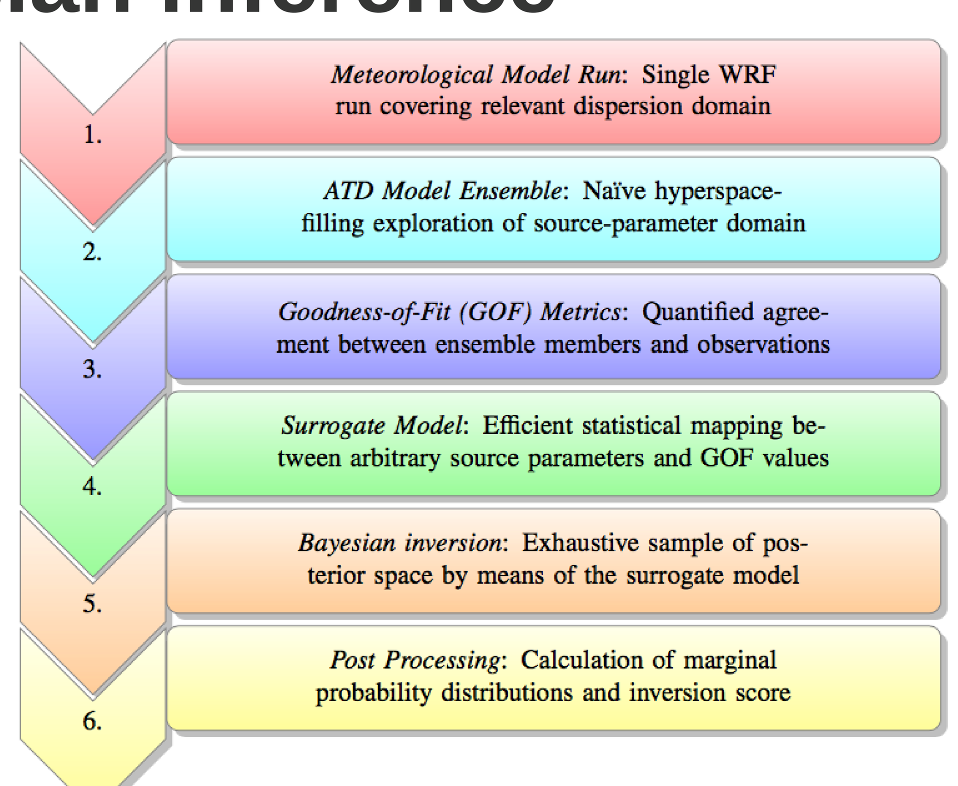


	RN20	RN37	RN38	RN58
11 Oct	0	0	0	0
12 Oct	0	0	0	0
13 Oct	0	0	0	0
14 Oct	1	0	0	0
15 Oct	1	0	1	1
16 Oct	1	0	1	1

(left) 24-hr averaged concentration contours of a hypothetical atmospheric release on11 Oct. 2006. (right) IMS Boolean hit/miss observations for such a release

1. Can we estimate the source parameters from sparse observational networks like the IMS?
2. How does our confidence in the source term vary with spatial and temporal sensor resolution?

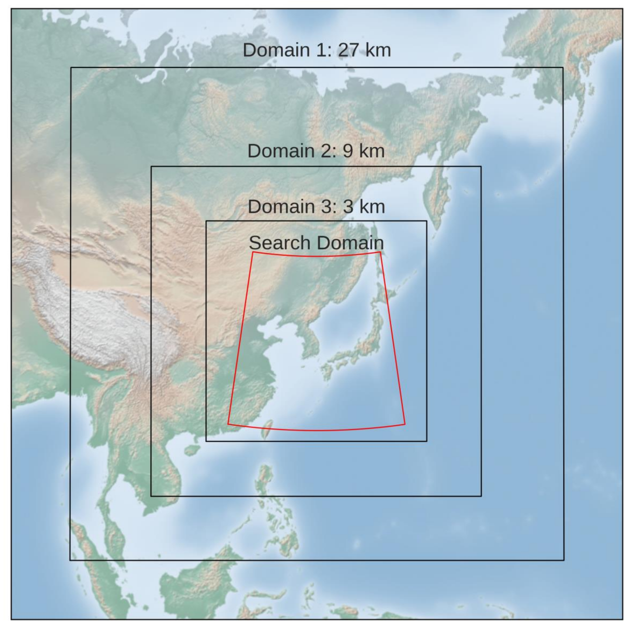
STE Combines HPC, ML and Bayesian inference



Schematic of the STE algorithm

1 – 3: FLEXPART-WRF and GOF

- Single-run WRF output drives 20,000 member FLEXPART ensemble
- The STE searches for release locations everywhere within the search domain
- The goodness-of-fit between observations and a given ensemble member is computed with Spearman's rank correlation, r_r, and a modified f_1 score that allows for regression[2].



Input Parameters ($\boldsymbol{\theta}$)	Min. Value	Max. Value
Source Latitude	23.871°	49.776°
Source Longitude	114.7°	143.331°
Source Release Start Time [UTC]	09 Oct 2006 00:00	14 Oct 2006 00:00
Source Duration [hr]	2	24
Source Amount [kg]	10	1000

		Actual	
		1	0
Predicted	1	True Positive	False Positive
	0	False Negative	True Negative

(Left) Domain limits of the five-dimensional hyperspace defining the STE search space. (Top) The WRF, FLEXPART and Search Domains. (Right) Binary classification confusion matrix.

$$\text{Precision} = \frac{TP}{TP+FP} = \frac{\sum_{\phi(\hat{y}_i)\geq t_E} \alpha(\hat{y}_i, y_i) * \phi(\hat{y}_i)}{\sum_{\phi(\hat{y}_i)\geq t_E} \phi(\hat{y}_i)} \quad \text{Recall} = \frac{TP}{TP+FN} = \frac{\sum_{\phi(y_i)\geq t_E} \alpha(\hat{y}_i, y_i) * \phi(y_i)}{\sum_{\phi(y_i)\geq t_E} \phi(\hat{y}_i)}$$

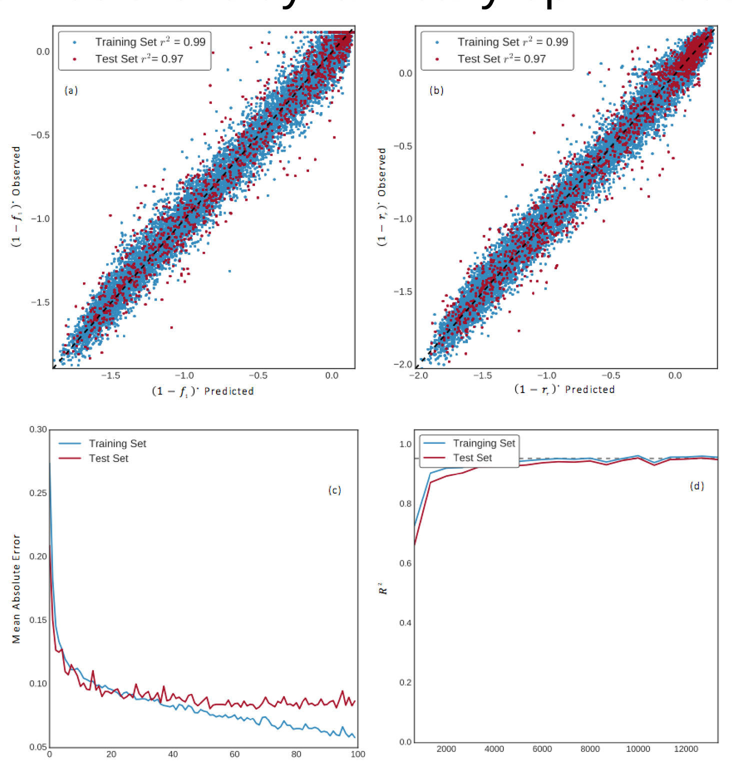
$$f_1 = 2\frac{\text{precision} * \text{recall}}{\text{precision} + \text{recall}} \qquad r_r = 1 - \frac{6\sum_{i=1}^{n} D_i^2}{n(n^2-1)} \qquad \boldsymbol{J} = [1 - r_r, 1 - f_1]^T$$

4 – 6: Deep Learning and Bayes' Thm

A fully-connected NN is trained to map any combination of source parameters $\boldsymbol{\theta}$ to their cost $\boldsymbol{J}$. The architecture is dynamically optimized.

Hyperparameter	Possible Values
Number of Layers	10, 12
Maximum Number of Neurons	350, 400, 450

Layer (type)	Output Shape	Param
relu 1 (Dense)	(None, 84)	504
relu 2 (Dense)	(None, 163)	13855
relu 3 (Dense)	(None, 242)	39688
relu 4 (Dense)	(None, 321)	78003
relu 5 (Dense)	(None, 400)	128800
relu 6 (Dense)	(None, 400)	160400
relu 7 (Dense)	(None, 322)	129122
relu 8 (Dense)	(None, 244)	78812
relu 9 (Dense)	(None, 166)	40670
relu 10 (Dense)	(None, 88)	14696
relu 11 (Dense)	(None, 10)	890
linear 12 (Dense)	(None, 2)	22



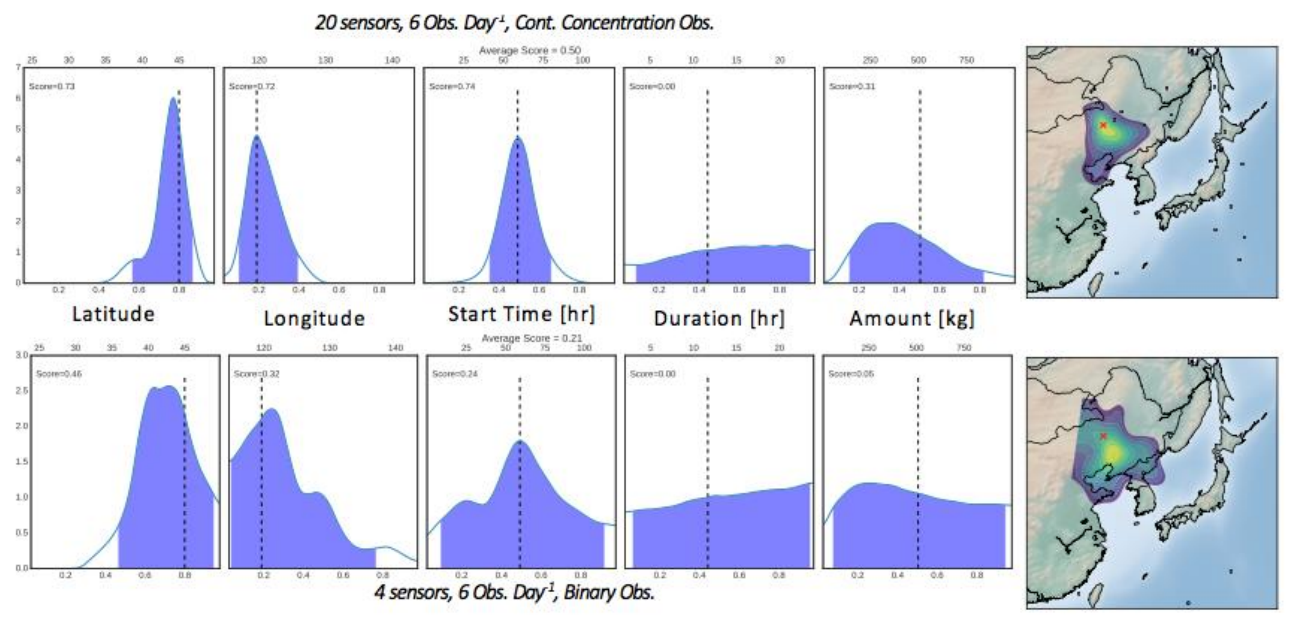
(Top Left) Hyperparameters sampled during NN tuning phase. (Bottom Left) Architecture for 12 layers and 450 max neurons. (Right) One-to-one plots, convergence plot and learning curve

The posterior space is exhaustively sampled with the NN and Latin hypercube sampling.

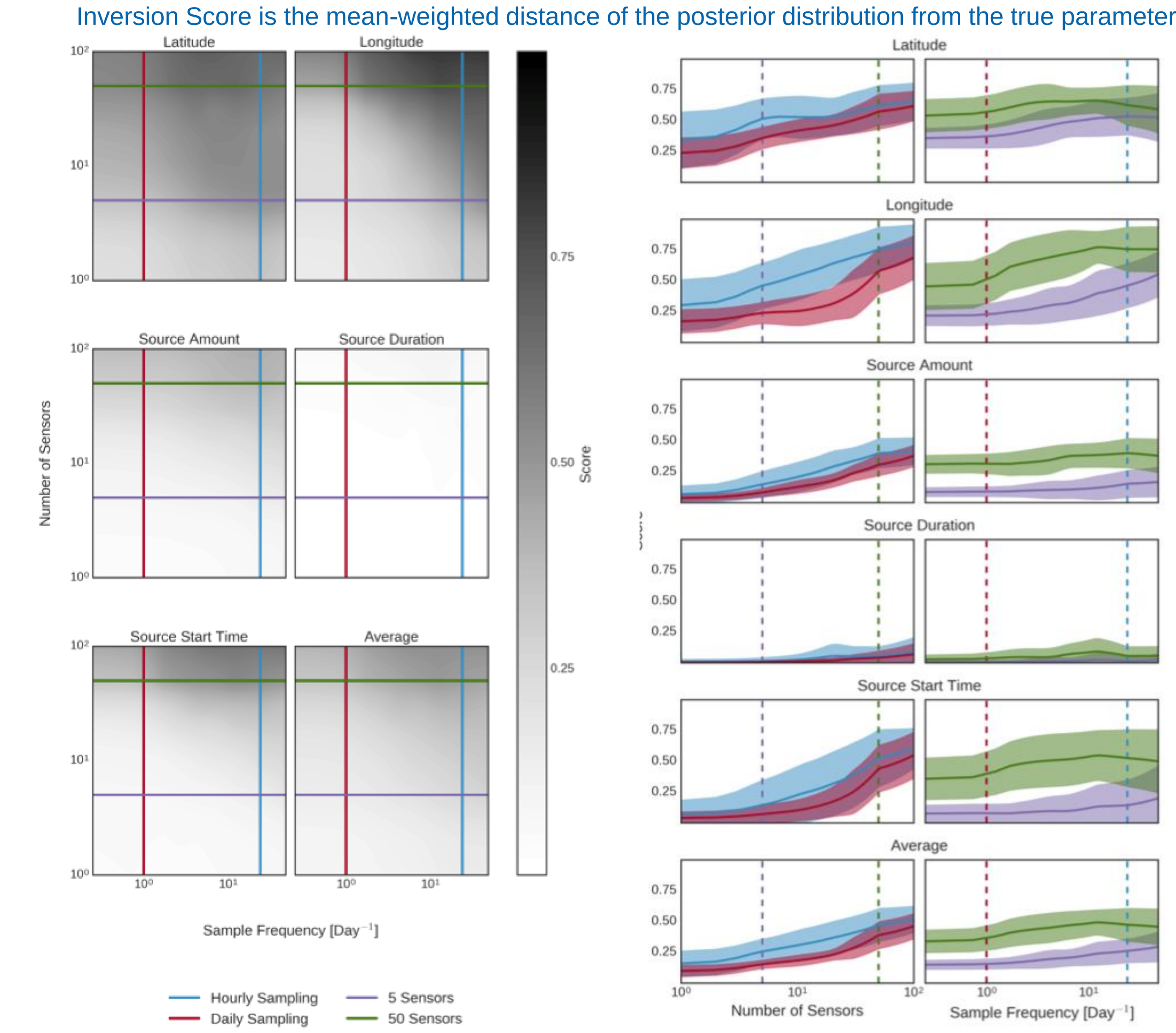
$$Posterior = \frac{Likelihood \cdot Prior}{Evidence}$$

$$\Rightarrow P(\boldsymbol{\theta}|\boldsymbol{J}) = \frac{P(\boldsymbol{J}|\boldsymbol{\theta}) * P(\boldsymbol{\theta})}{P(\boldsymbol{J})} \propto P(\boldsymbol{J}|\boldsymbol{\theta}) * P(\boldsymbol{\theta}) \qquad \ln L = 0.5[\tilde{f}(\boldsymbol{\theta}) - \boldsymbol{\mu}]^T \boldsymbol{\Sigma}^{-1} [\tilde{f}(\boldsymbol{\theta}) - \boldsymbol{\mu}]$$

Sensor Density is Important



Posterior distributions of source parameters constrained by dense (top) and course (bottom) sensors networks. The Inversion Score is the mean-weighted distance of the posterior distribution from the true parameter.



Inversion Score contours (left) and transects (right) for 7,488 inversion runs testing the STE algorithm for the release illustrated in the leftmost column

CONCLUSIONS

- The regression f_1 score and the Spearman rank r_r robustly and resiliently gauge the disparity between model and observational data
- The inversion algorithm is robust and able to accurately estimate the source for the majority of the randomly configured sensor networks.
- The large ensemble of forward model runs and the extensive STE evaluation are both computationally expensive. The work would be very difficult without the computational resources available at LLNL

1. Lucas, Donald D., et al. "Bayesian inverse modeling of the atmospheric transport and emissions of a controlled tracer release from a nuclear power plant." *Atmospheric Chemistry and Physics Discussions* 2017 (2017): 1-36.
2. Torgo L., Ribeiro R. (2009) Precision and Recall for Regression. In: Gama J., Costa V.S., Jorge A.M., Brazdil P.B. (eds) Discovery Science. DS 2009. Lecture Notes in Computer Science, vol 5808. Springer, Berlin, Heidelberg

Deep Learning can be leveraged to probabilistically infer release parameters from an unknown atmospheric source

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