Probabilistic Inversion Modelling of Gas Emissions: A Gradient-Based MCMC Estimation of PDE Parameters

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1 | INTRODUCTION

In response to the escalating global concerns regarding air quality and the environmental impact of greenhouse gas emissions, detecting and quantifying sources of emissions has become critical.

AIMS

We present an innovative approach to address the challenging task of estimating parameters in the gas dispersion model, whilst simultaneously estimating the source emission rate, location, background concentration, and the sensors' measurement error variance.

2 | METHODS: MCMC

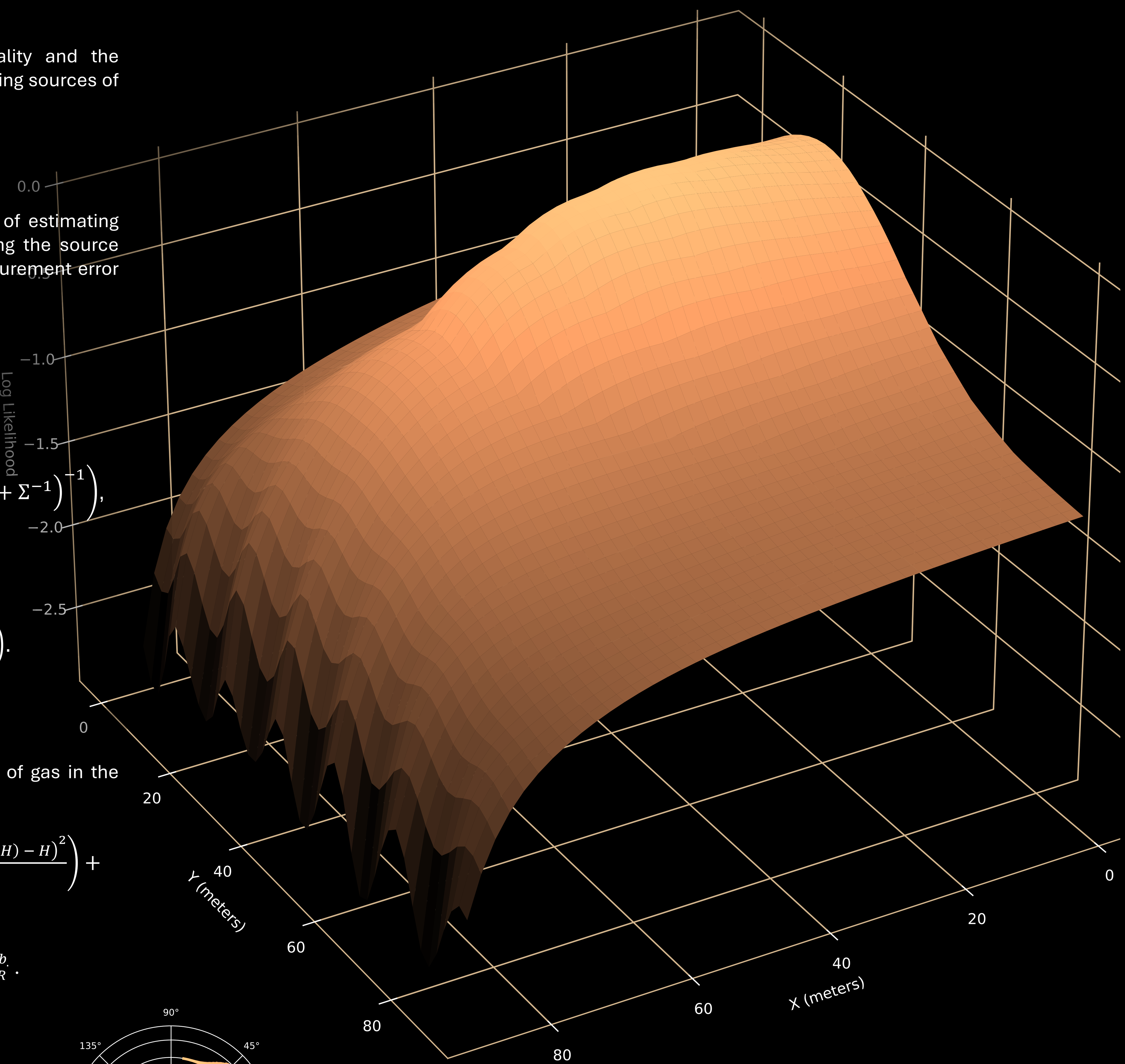
- Parameters are estimated using M-MALA-within-Gibbs.
- Background and measurement error variance using Gibbs:

$$\boldsymbol{\beta}|\boldsymbol{y}, A, \boldsymbol{s}, \sigma^2 \sim N\left(\left(\frac{1}{\sigma^2}\mathbb{I} + \Sigma^{-1}\right)^{-1}\left(\frac{1}{\sigma^2}(\boldsymbol{y} - A\boldsymbol{s}) + \Sigma^{-1}\boldsymbol{\mu}\right), \left(\frac{1}{\sigma^2}\mathbb{I} + \Sigma^{-1}\right)^{-1}\right),$$

$$\sigma^2|\boldsymbol{y}, \boldsymbol{s} \sim InvGamma\left(\frac{n}{2} + a, b + \frac{(y-\beta-As)^2}{2}\right).$$

- Emission rate, location, and gas dispersion parameter using M-MALA:

$$X^* \sim N_d\left(\boldsymbol{x} + \frac{h}{2}G^{-1}(\boldsymbol{x})\nabla \log \pi(\boldsymbol{x}) + h\Gamma(\boldsymbol{x}), hG^{-1}(\boldsymbol{x})\right).$$



METHODS: Gas Dispersion Model

- Gaussian plumes are used to describe the spatio-temporal dispersion of gas in the atmosphere, the concentration at location (x, y, z) is given by:

$$c(x,y,z) = \frac{s}{2\pi\sigma_H\sigma_V} exp\left(-\frac{\delta_H^2}{2\sigma_H^2}\right)\sum_{j=0}\left[exp\left(-\frac{1}{2}\frac{\left(2\lfloor(j+1)/2\rfloor P + (-1)^j(\delta_V+H) - H\right)^2}{\sigma_V^2}\right) + exp\left(-\frac{1}{2}\frac{\left(2\lfloor(j+1)/2\rfloor P + (-1)^j(\delta_V+H) + H\right)^2}{\sigma_V^2}\right)\right].$$

- σ_H and σ_V are called wind sigmas and are parametrised by $\sigma_. = \tan(\gamma_.) a_. \delta_R^{b_.}$.
- The PDE parameters estimated are a_H, a_V, b_H, and b_V.

3 | RESULTS

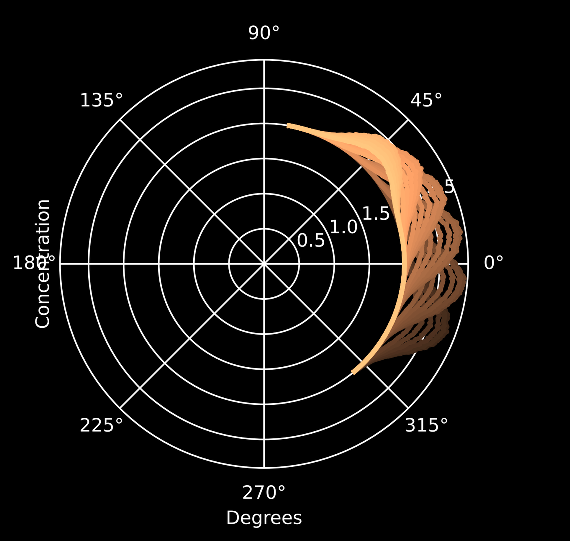


Fig 1 | Polar graph of sensors' measurements.

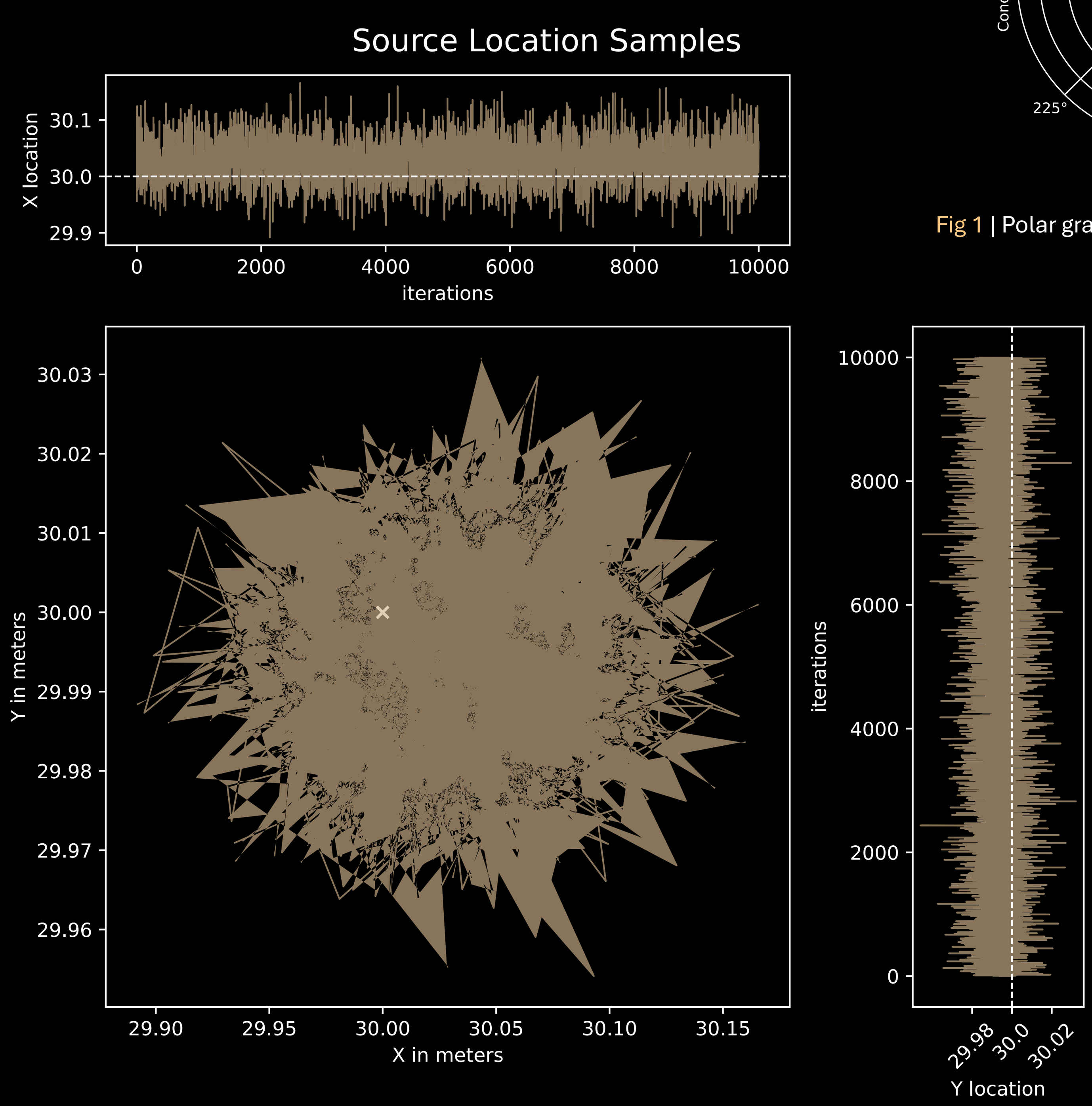


Fig 2 | M-MALA-within-Gibbs samples of the source location. The top and right plots are the MCMC chains of source locations x and y in meters, respectively. The center plot illustrates the spatial uncertainty of the source location estimation . The dotted lines represent the true parameter values.

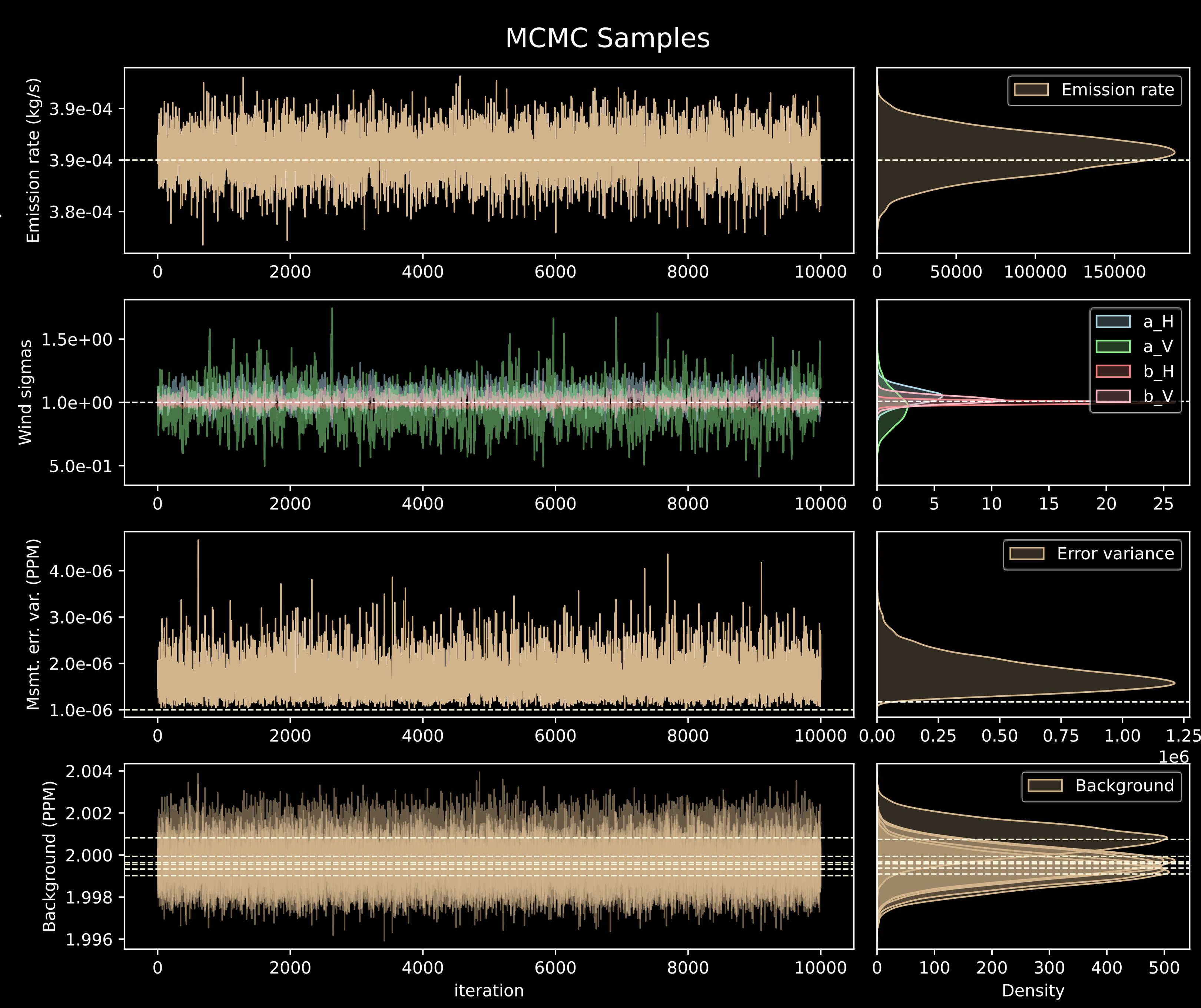


Fig 3 | M-MALA-within-Gibbs samples estimating – from top to bottom – source emission rate (kg/s), gas dispersion parameters, sensors measurement error variances (PPM), and background concentrations (PPM). The left column shows the MCMC chains and the right column shows the corresponding densities. The dotted lines represent the true parameter values.

4 | CONCLUSION

Efficient estimation of source emission rate and location, coupled with accurate quantification of uncertainties, stands as a cornerstone achievement. This entails mitigating biases in wind sigmas, measurement error variance, and background concentration. Furthermore, imposing positivity constraints and sparsity on source emissions enhances the fidelity of the estimation process. These steps collectively refine inversion techniques, with particular emphasis on estimating wind sigmas, thereby enhancing the overall accuracy and reliability of the methodology.

By enforcing positivity constraints and sparsity on source emissions, the estimation process gains precision and robustness. Moreover, the refinement of inversion methods, notably through the estimation of wind sigmas, marks a significant advancement towards achieving more accurate and reliable outcomes in source emission estimation.

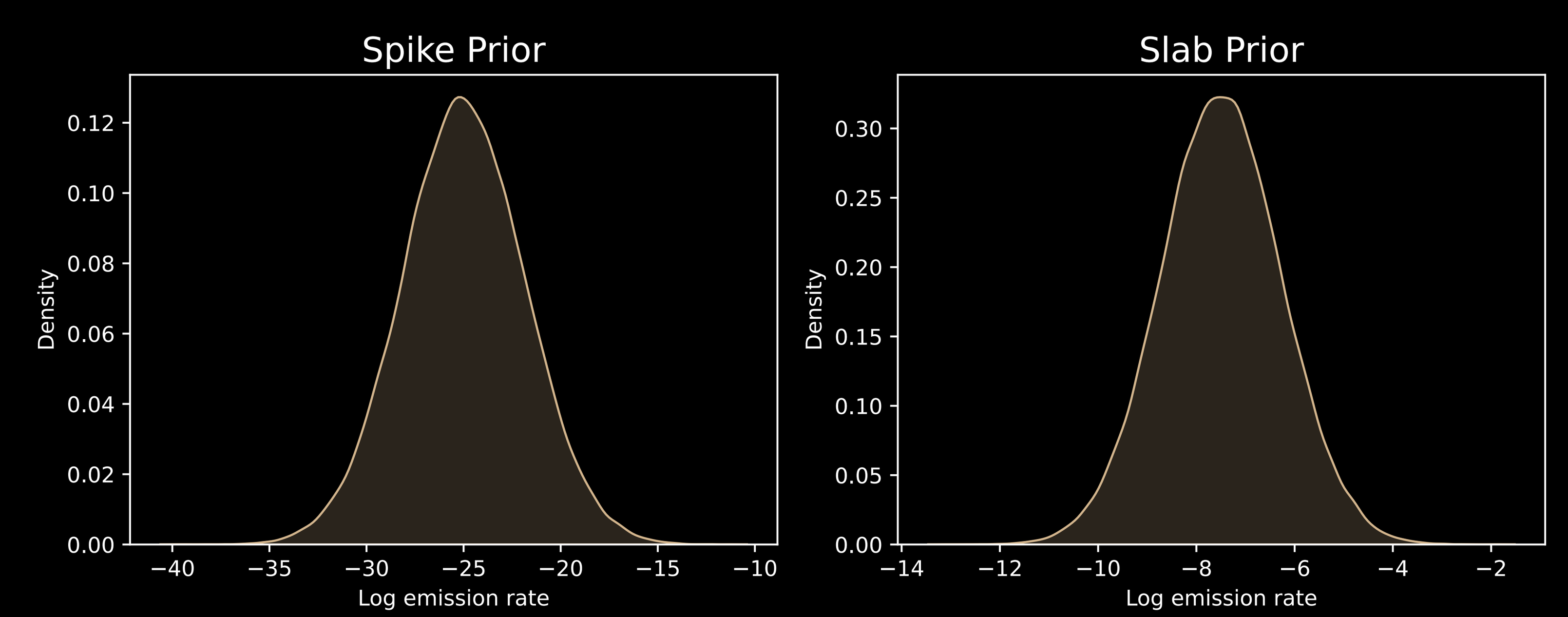


Fig 4 | Sparse and positively constrained prior for emission rate parameter. The spike and slab prior is used to enforce sparsity in the number of sources detected during the inversion process.

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