BAYESIAN INVERSION FOR LONG-PATH SPECTROSCOPIC DATA: ESTIMATION OF VERTICAL PROFILES FOR TRACE GASES

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Introduction

Abstract: *We seek to develop statistical methods for analyzing data collected using long-path spectroscopic techniques which will allow improved quantification of the spatial and temporal distribution of climate-driving atmospheric constituents (i.e., greenhouse gases and aerosols). For this problem, we propose a Bayesian approach. Bayes formula allows us to obtain a high dimensional probability distribution over the space of all vertical profiles, conditional on the data. We can explore this probability density using Markov chain Monte Carlo techniques. Computational issues are dealt with by using delayed acceptance / rejection techniques.*

MAX-DOAS

- we use multi-axis differential optical absorption spectroscopy (MAX-DOAS) as a non-satellite remote sensing technique.
- MAX-DOAS is a long-path spectroscopic method that collects solar radiation spectra using a telescope coupled to an ultraviolet-visible spectrometer
- ground based MAX-DOAS is highly sensitive to absorbers in the lowest few kilometres of the atmosphere and vertical profile information can be retrieved by combining the measurements with Radiative Transfer Model (RTM) calculations.

In current MAX-DOAS literature, typically, a few scenario profiles are chosen and put into the radiative transfer model, and the profile that "best" matches the collected data is reported as the most likely profile.

Data

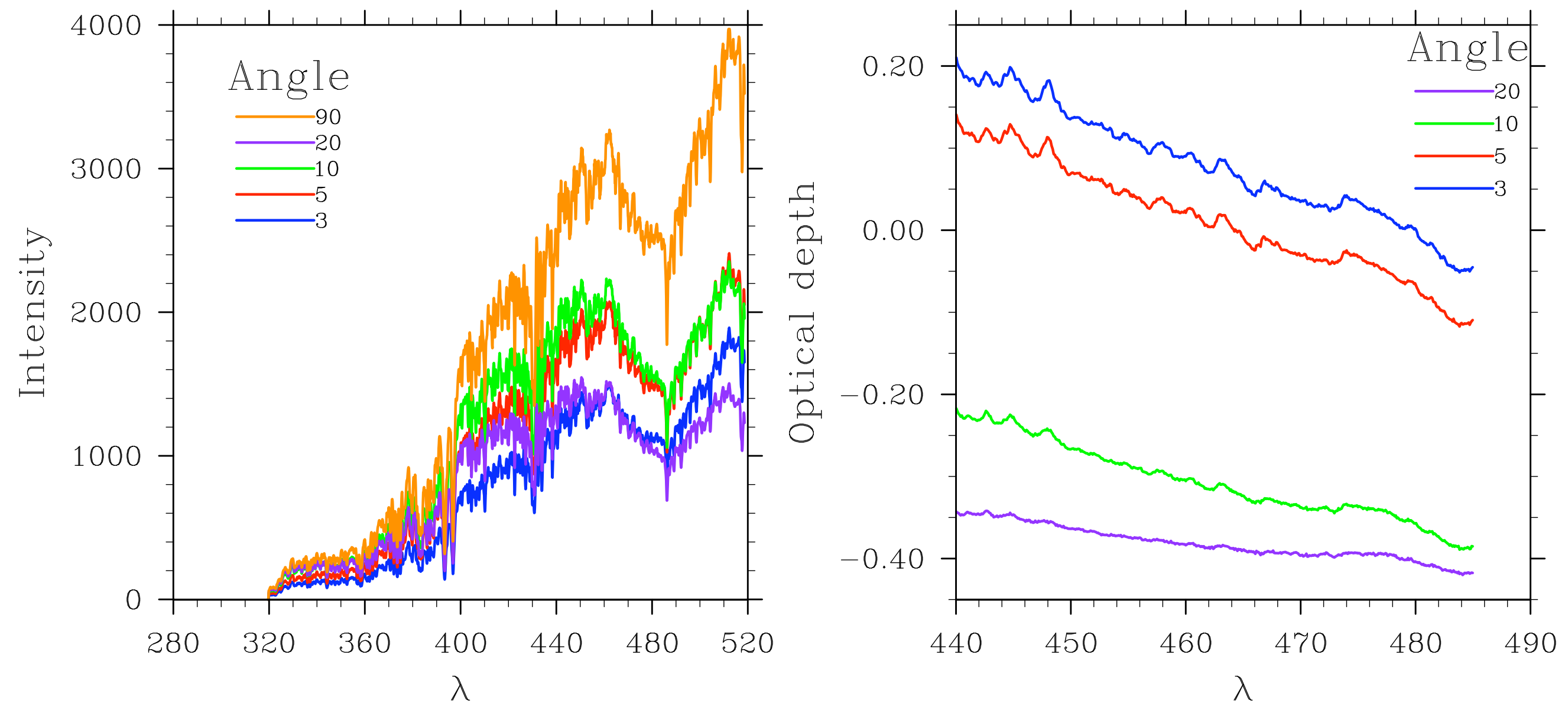

FIGURE 1: Solar radiation intensities at different elevation angles (left) and corresponding optical depths (right).

Beer-Lambert Law:

$$I(\lambda, \alpha) = I_0(\lambda) \exp\left\{ -\sum_i \sigma_i(\lambda) S_i(\alpha) + \sigma_{ray}(\lambda) + \sigma_{mie}(\lambda) \right\}$$

$$OD(\lambda, \alpha) = -\log\left(\frac{I(\lambda, \alpha)}{I_0(\lambda)}\right)$$

Radiative Transfer Model

The connection between vertical profiles and the underlying intensities is made via a *radiative transfer model*.

- the propagation of solar radiation through the atmosphere is affected by absorption, scattering and emission processes.
- aim is to model the change in radiation intensity along a ray path to local absorption, accounting for the above mentioned events;
- available numerical implementations: SCIATRAN, TRACY, UVspec/DISORT, etc.
- SCIATRAN considers multi-scatering events in full spherical geometry and will output intensity spectra given a set of vertical profiles.

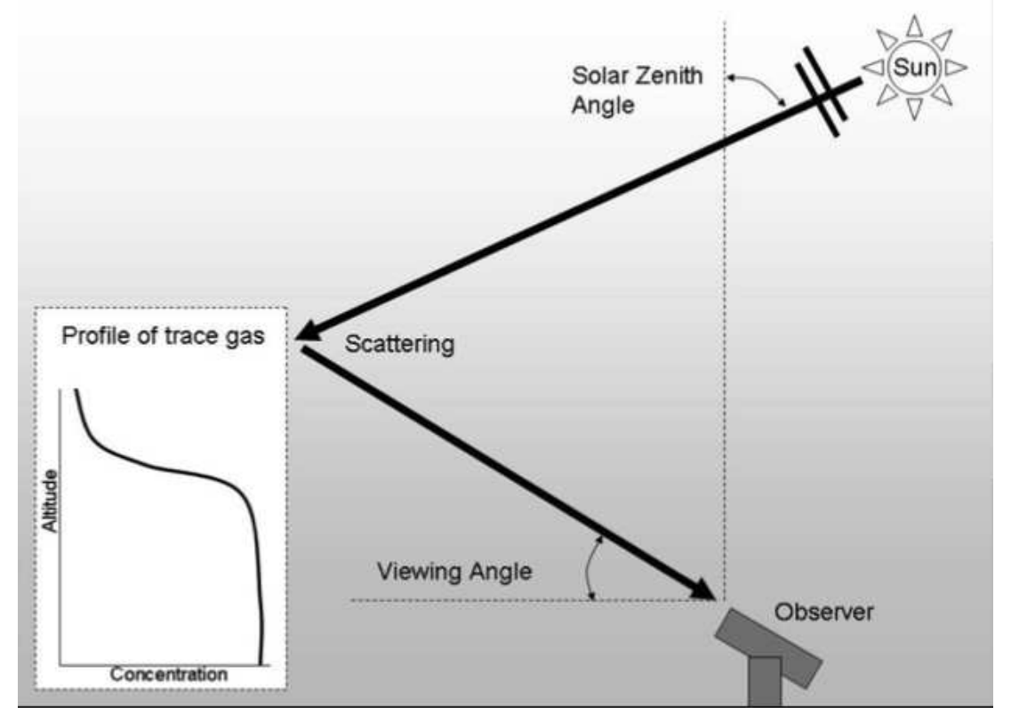

FIGURE 2: Scattered light enters the observer's telescope elevated at a viewing angle α.

Bayesian Formulation

Observational model:

$$I^{\text{obs}}_{\alpha,\lambda} \overset{iid}{\sim} N\left(I^{\text{true}}_{\alpha,\lambda}, \sigma^2\right), \quad I^{\text{true}}_{\alpha,\lambda} = cI^{\text{model}}_{\alpha,\lambda}$$

where c is a scaling parameter.

Given vertical trace gas profiles $\theta_i = \{\theta_i(z); z \geq 0\},\ i = 1, \ldots, M$,

$$I^{\text{model}}_{\alpha,\lambda} = \tilde{F}(\lambda; \alpha; \theta_1, \ldots, \theta_M, \Psi),$$

where $\tilde{F}$ denotes the numerical approximation of the radiative transfer model, and Ψ comprises all "other" parameters influencing the intensities, such as climate parameters (temperature, atm. pressure, scattering, solar geometry). For now, Ψ is assumed fixed.

Posterior distribution:

$$\pi(\theta_1, \ldots, \theta_M | I^{\text{obs}}) \propto L(I^{\text{obs}} | \theta 1, \ldots, \theta_M) \prod_{i=1}^{M} \pi(\theta_i)$$

where

$$L(I^{\text{obs}} | \theta_1, \ldots, \theta_M, c) = \prod_{\alpha} \prod_{\lambda} \exp\left\{ -\frac{(cI^{\text{model}}_{\alpha,\lambda} - I^{\text{obs}}_{\alpha,\lambda})^2}{2\sigma^2} \right\}$$

Prior Specification

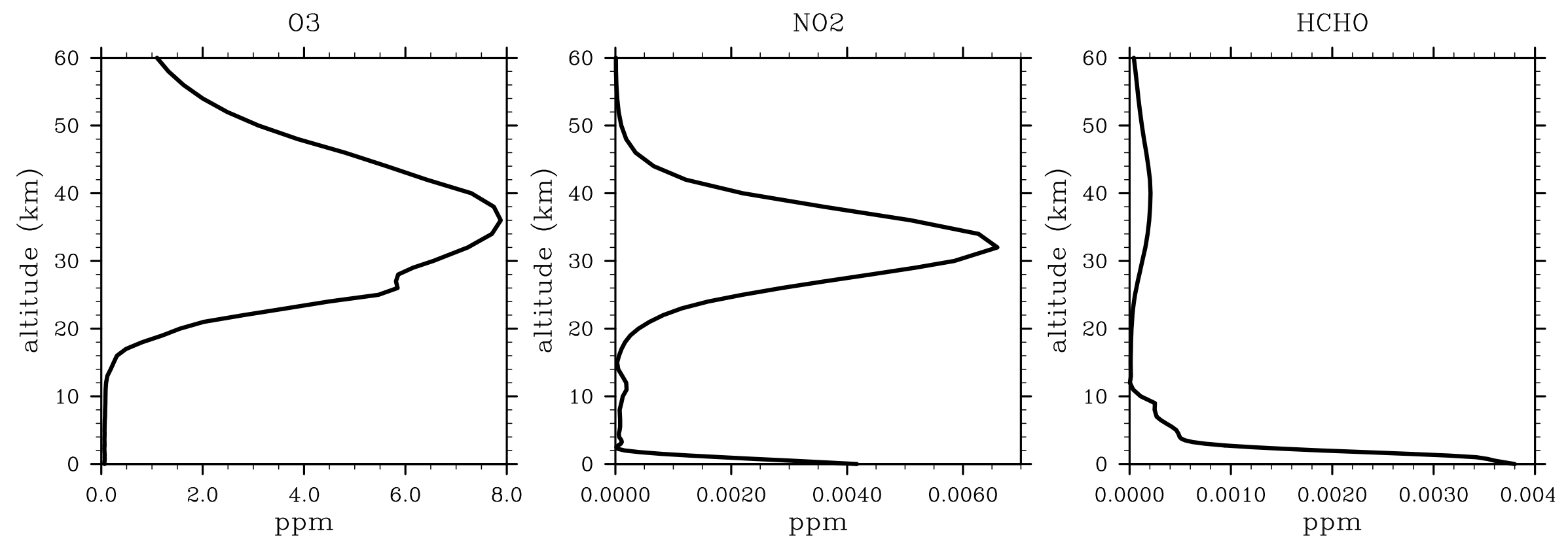

FIGURE 3: Estimated vertical profiles for different tracers available in the literature.

- Informative priors
  - −Parametric representation

$$\theta_i(z) = \sum_{j=1}^{k} w_{ij} K_{ij} \left(\frac{z - \mu_{ij}}{\psi_{ij}} \right);$$

  - −Interpolated knots of a point process restricted to a buffer zone;
- Non-informative priors (work in progress)
  - −Basis function representation.

Results and Conclusions

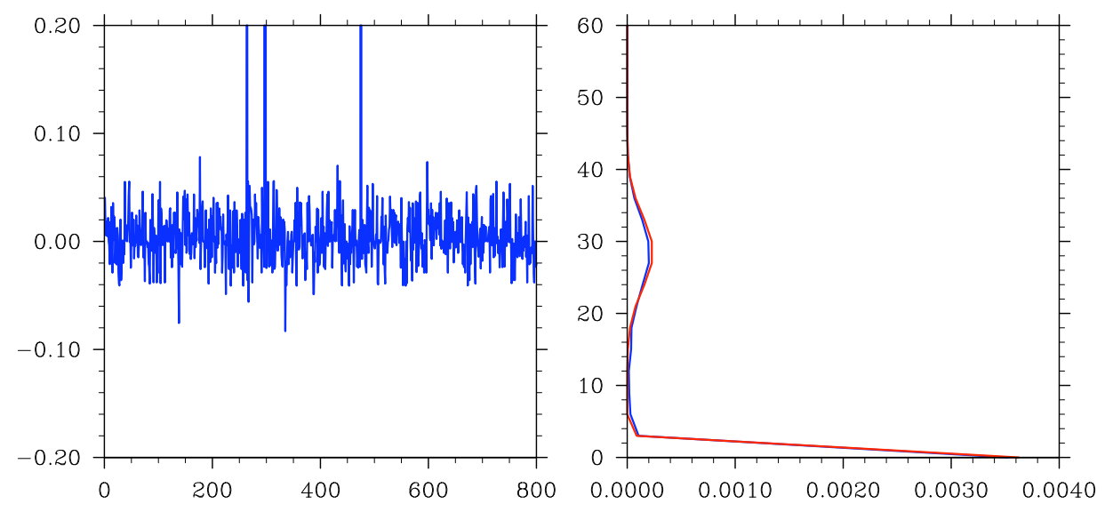

FIGURE 4: Simulation study results: Trace plot of a location parameter (left panel) and a comparison (right panel) between the target profile (red) and estimated profile (blue).

Conclusions:

- We develop statistical methodology for estimating vertical trace gas profiles and their uncertainties.
- Attractive feature: the data-collection process is very low-cost, compared to other remote sensing devices.
- Simulation study success offers confidence in future developments.

Work in Progress:

- Low acceptance rate; Computational time (likelihood computation takes about 20 seconds);

This research is supported in part by The Climate, Water and Carbon Program at The Ohio State University