

# Bayesian inference for aerosol vertical profiles



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## Motivation

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## Objective

Try to reconstruct aerosol vertical profiles using AOD

# 2D Spatial Disaggregation

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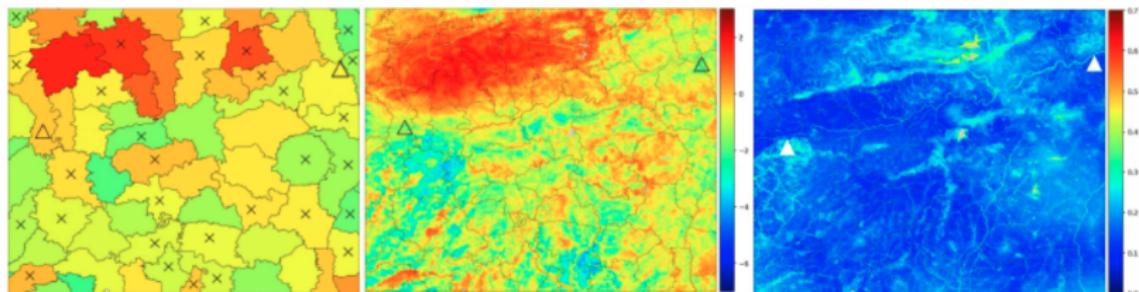


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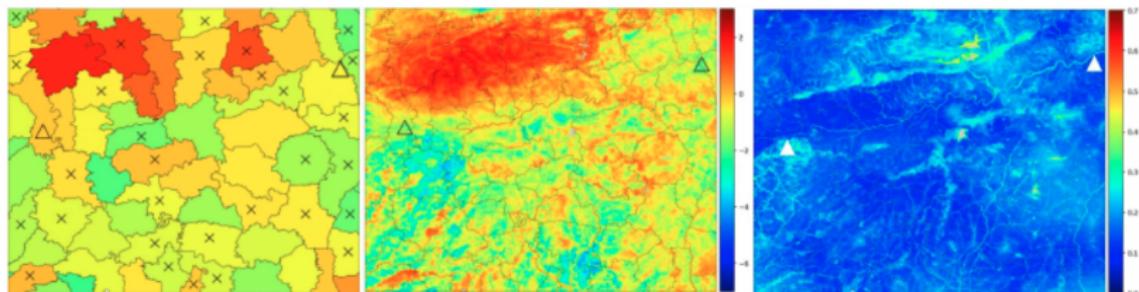


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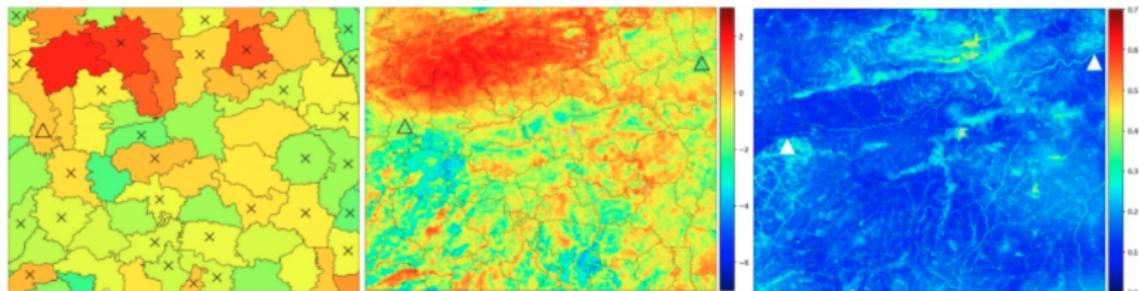


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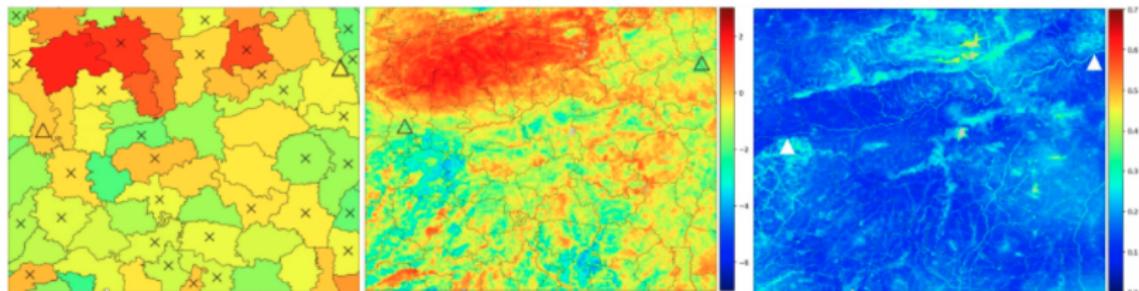
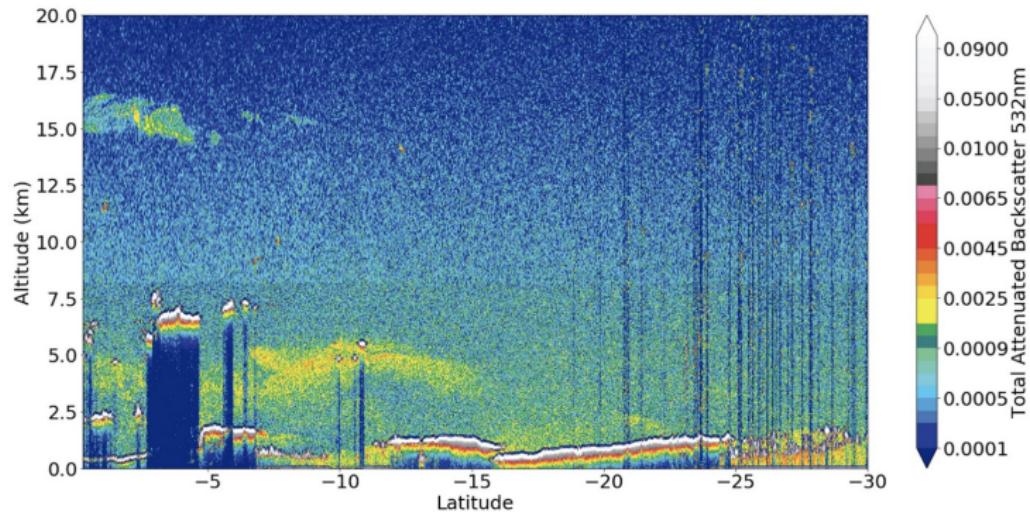


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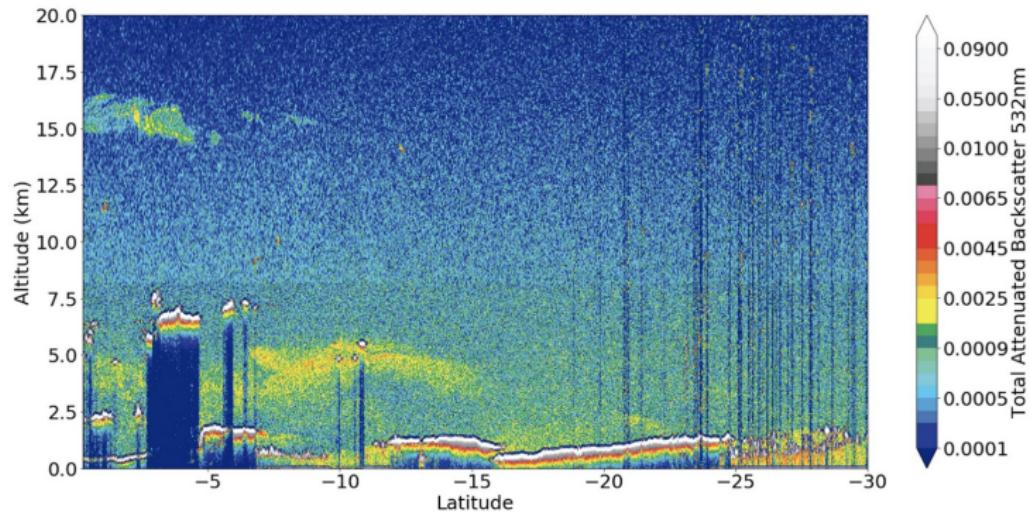
- ▶ **Observations:**  $\text{rate}_{\text{region}}$  and  $x_{\text{fine-grid}}$
- ▶ **Goal:** Infer  $\text{rate}_{\text{fine-grid}}$  as a function of  $x_{\text{fine-grid}}$

# Disaggregating along a 3<sup>rd</sup> dimension?



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- **Observations:**  $\tau_{\text{column}}$  and  $x_{3D}$
- **Goal:** Infer  $b_{\text{ext}}$  as a function of  $x_{3D}$

- ▶ Use **simple, readily available predictors** such as pressure, temperature, humidity → reanalysis data.

For example, for a given altitude  $h$  we can take

$$x = (t, \text{lat}, \text{lon}, P, T, \text{RH}) \quad (1)$$

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## Objective

Using observations of AOD and vertically-resolved meteorological predictors, we want to estimate aerosol extinction

Design of a prior over  $b_{\text{ext}}$

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# An idealized vertical prior

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- Idealized profiles assumed in remote sensing products  
 $b_{\text{ext}}(h) \propto e^{-h/L}$ .

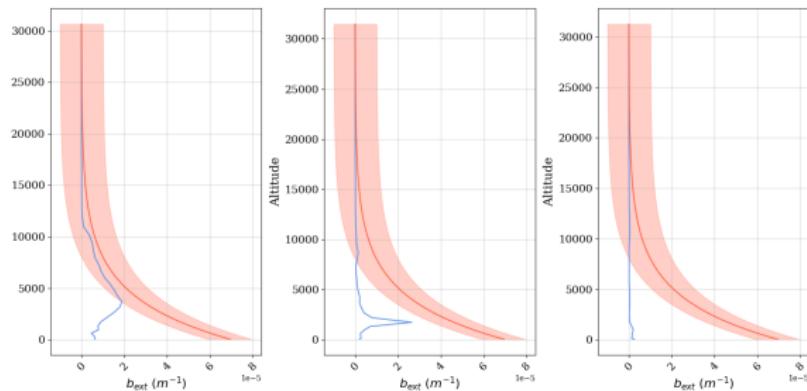


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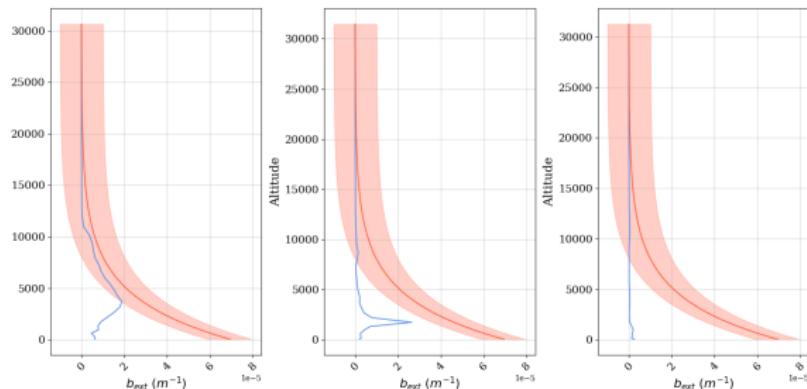


Figure 2: Examples of idealized exponential vertical profiles

- Rough approximation but captures a key structure: **most aerosol lie in *boundary layer* (< 2 km)**

- ▶ Propose to weight the idealized exponential profile with a positive weight function  $w(x|h) > 0$

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Expect relationship between  $x|h$  and  $b_{\text{ext}}(h)$  to be non-trivial and highly non-linear  $\Rightarrow$  learn the weighting  $w(x|h)$

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$$f \sim \text{GP}(m, k) \quad (4)$$

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- ▶ Simple choice  $\psi = \exp$
- ▶  $\psi \circ f$  describes expressive range of probability distribution over complex positive functions
- ▶ Remains interpretable (kernel user-specified determines covariance and functional smoothness)

Connecting  $\varphi(x|h)$  to observations

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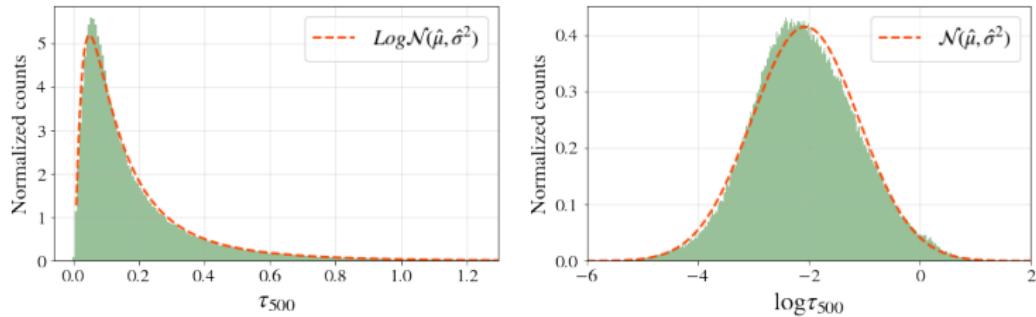


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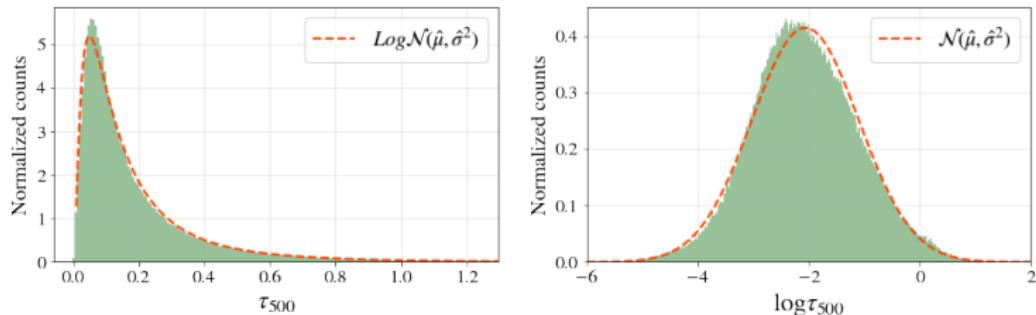


Figure 3: **Left:** empirical distribution of AOD retrievals from AERONET stations; **Right:** logspace version of left plot

Assume **log-normal** model  $\tau|\mu, \sigma \sim \mathcal{LN}(\mu, \sigma)$ .

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Observation model

$$\tau|\eta \sim \mathcal{LN}\left(\log \eta - \frac{\sigma^2}{2}, \sigma\right) \quad (6)$$

$$\eta = \int_0^H \varphi(x|h) \, dh \quad (7)$$

With multiple observations  $\tau_1, \dots, \tau_n$ , scale parameter  $\sigma > 0$  assumed shared among columns but  $\eta$  (or  $\mu$ ) is column-specific.

Model formulation for the  $i^{\text{th}}$  atmospheric column

## Observation Model:

$$\tau_i | \eta_i \sim \mathcal{LN} \left( \log \eta_i - \frac{\sigma^2}{2}, \sigma \right)$$

$$\eta_i = \int_0^H \varphi(x_i | h) dh$$

## Prior:

$$\varphi(x_i | h) = \psi(f(x_i | h)) e^{-h/L}$$

$$f \sim \text{GP}(m, k)$$

|                  |                                  |
|------------------|----------------------------------|
| $\tau_i$         | Observed AOD                     |
| $\mathcal{LN}$   | Log-normal distribution          |
| $\eta_i, \sigma$ | Mean and scale parameters        |
| $\varphi$        | Prior for $b_{\text{ext}}$       |
| $x_i   h$        | Input covariates at altitude $h$ |
| $H$              | Atmospheric column height        |
| $\psi$           | Positive link function           |
| $L$              | Idealized heightscale parameter  |
| $f$              | GP prior                         |

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► **Objective:** Infer distribution of  $\varphi(x|h) | \underbrace{\tau_1, \dots, \tau_n}_{\tau}$

- ▶ Actually...  $f(x|h)|\tau$
- ▶ Access to posterior distribution  $p(f|\tau)$  allows to compute predictive mean and variance of  $\varphi$  at input  $x|h$  following

$$\mathbb{E}[\varphi(x|h)|\tau] = \int \psi(f) e^{-h/L} p(f|\tau) df$$

$$\text{Var}(\varphi(x|h)|\tau) = \mathbb{E}[\varphi(x|h)^2|\tau] - \mathbb{E}[\varphi(x|h)|\tau]^2$$

- ▶ Can be estimated with Monte-Carlo (and admits closed form for  $\psi = \exp$ )

---

## Problem

$$p(f|\tau) = \frac{p(\tau|f)p(f)}{\underbrace{\int p(\tau|f)p(f) df}_{\text{intractable}}}$$

## Solution

- ▶ Approximate  $p(f|\tau)$  (variational approximation)
- ▶ Approximation scheme allows for **sparse representation** which **scales to very large number of data points**

## Experiments

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|                    | Name                         | Notation         | Dimensions                                |
|--------------------|------------------------------|------------------|---|
| <i>Predictors</i>  | Temperature                  | $T$              | $(t, \text{lat}, \text{lon}, \text{lev})$ |
|                    | Pressure                     | $P$              | $(t, \text{lat}, \text{lon}, \text{lev})$ |
|                    | Relative humidity            | $\text{RH}$      | $(t, \text{lat}, \text{lon}, \text{lev})$ |
|                    | Vertical velocity            | $\omega$         | $(t, \text{lat}, \text{lon}, \text{lev})$ |
| <i>Response</i>    | AOD 550nm                    | $\tau$           | $(t, \text{lat}, \text{lon})$             |
| <i>Groundtruth</i> | Extinction coefficient 533nm | $b_{\text{ext}}$ | $(t, \text{lat}, \text{lon}, \text{lev})$ |

Table 1: Gridded variables from ECHAM-HAM simulation data. The grid includes 8 time steps ( $t$ ), 96 latitude levels (lat), 192 longitude levels (lon) and 31 vertical pressure levels (lev). Our objective is to vertically disaggregate the response  $\tau$  using the vertically resolved predictors ( $T, P, \text{RH}, \omega$ ) and spatiotemporal columns locations ( $t, \text{lat}, \text{lon}$ ).

- Total of  $8 \times 96 \times 192 = 147\,456$  columns.

# Predictors slices

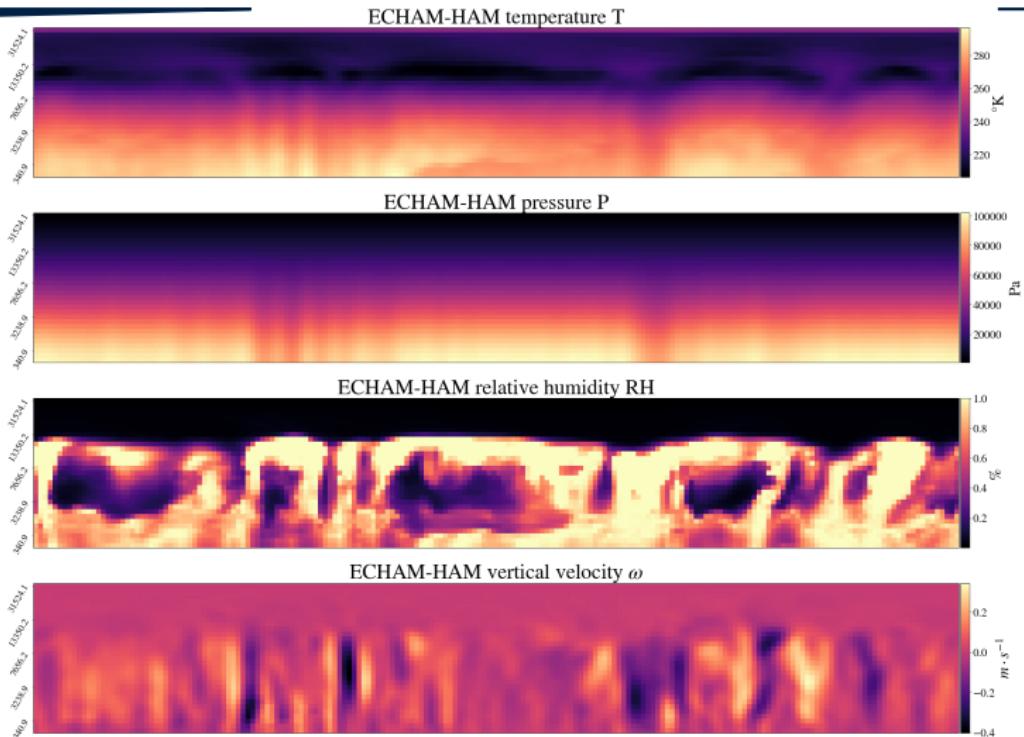


Figure 4: Vertical slices at latitude  $51.29^{\circ}$  of meteorological predictors

## Ideal slices

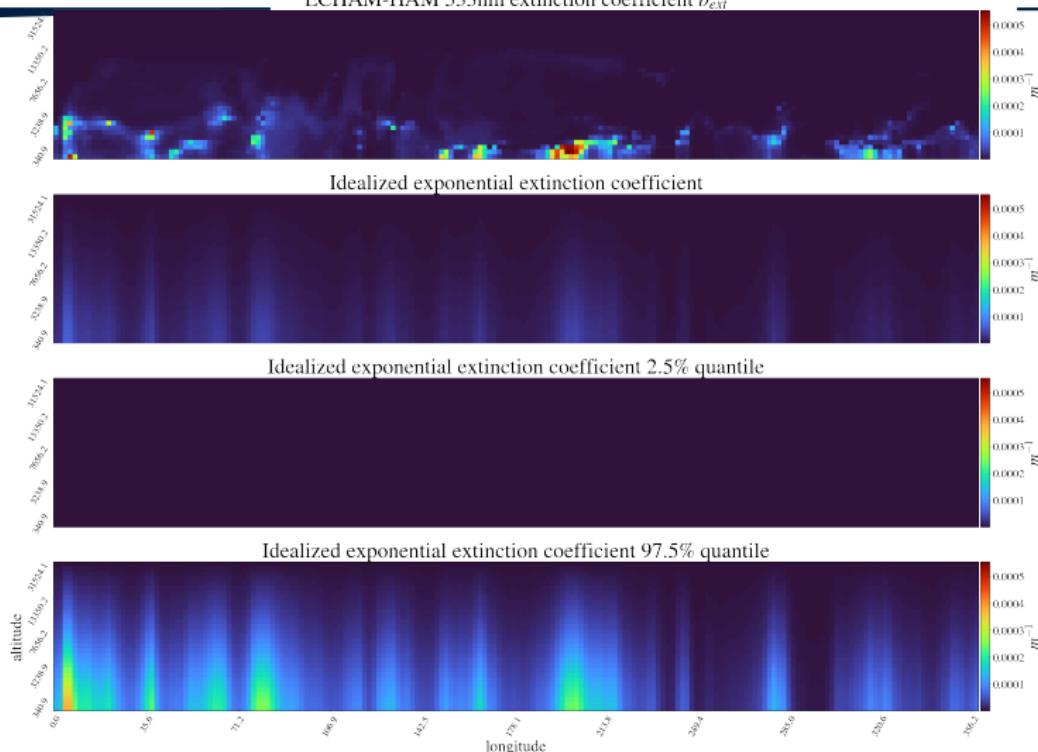


Figure 5: Vertical slices at latitude  $51.29^\circ$  of idealized profiles

# Predicted slices

21

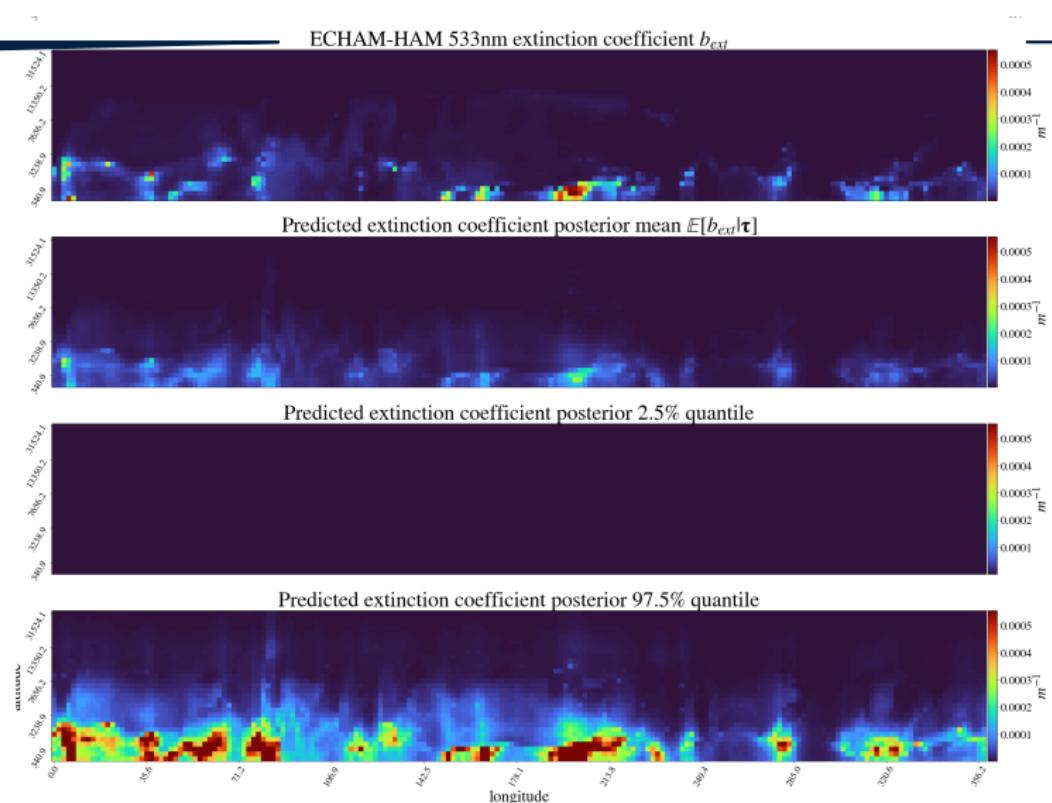
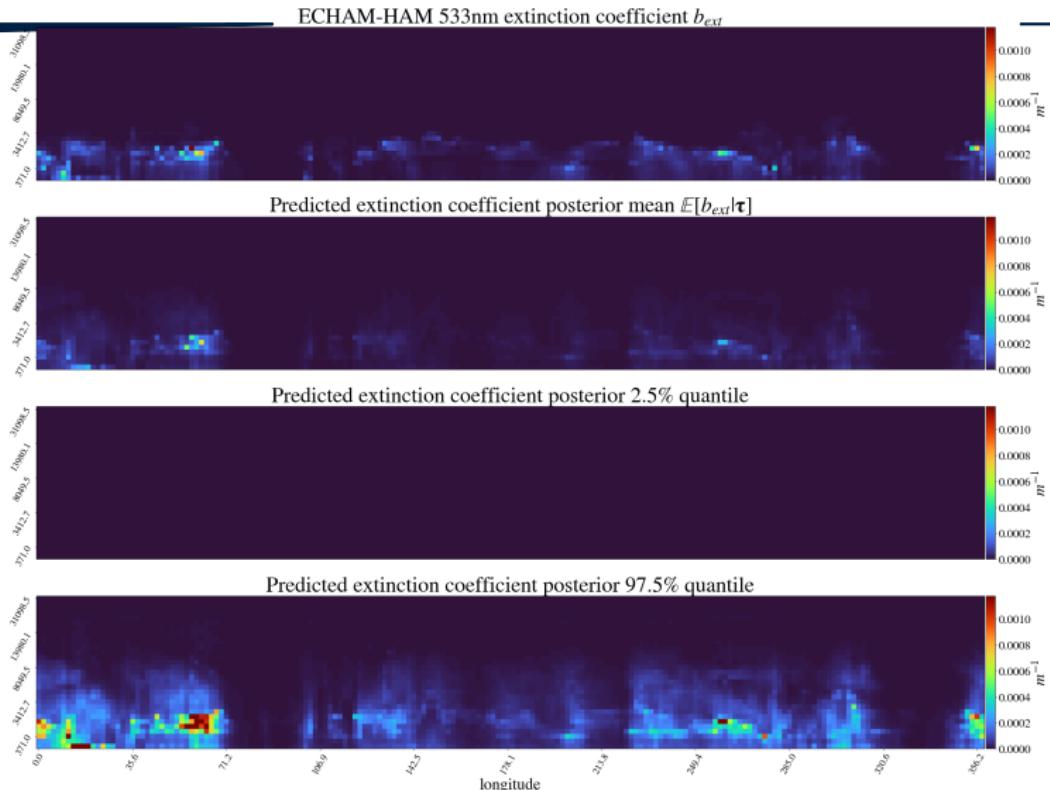


Figure 6: Vertical slices at latitude  $51.29^{\circ}$  of predicted profiles

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22



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23

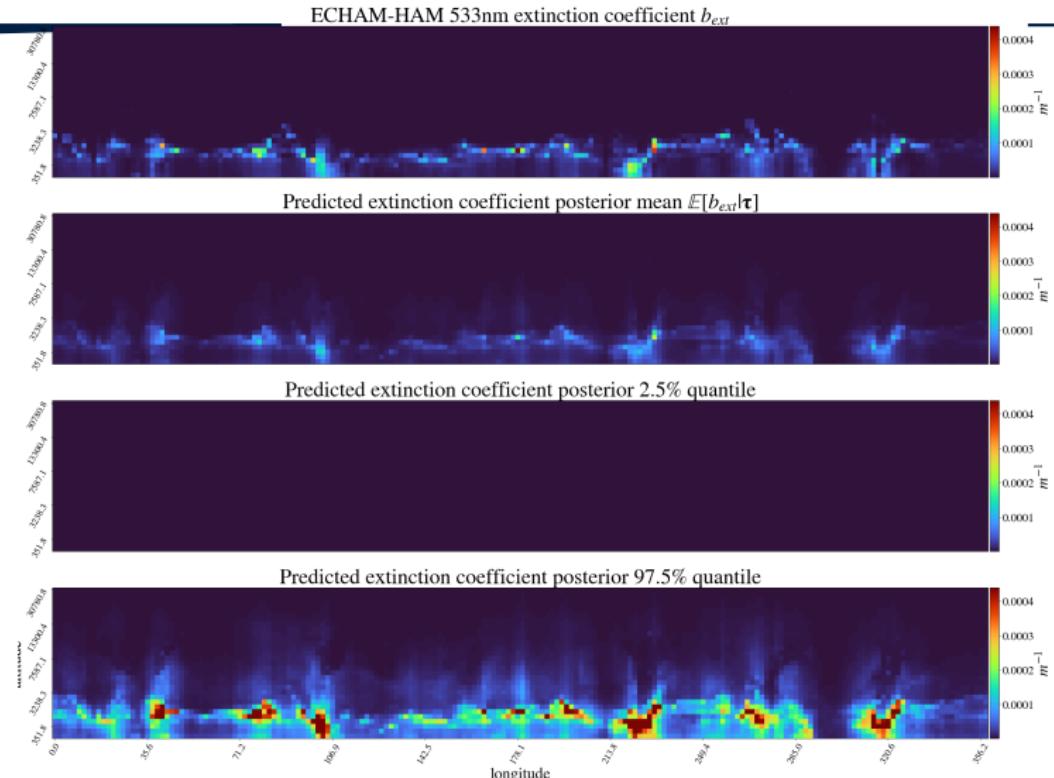


Figure 8: Vertical slices at latitude  $-38.2^{\circ}$  of predicted profiles

Table 2: Scores of our method (Our) compared to an idealized exponential baseline (Ideal)

| Region                | Method | RMSE ( $10^{-5}$ )     | Corr (%)              | Bias ( $10^{-6}$ )        | Bias98 ( $10^{-5}$ )      |
|-----------------------|--------|------------------------|-----------------------|---------------------------|---------------------------|
| <i>Entire column</i>  | Our    | <b>3.29</b> $\pm 0.02$ | <b>70.9</b> $\pm 0.4$ | <b>-0.167</b> $\pm 0.105$ | <b>-0.646</b> $\pm 0.151$ |
|                       | Ideal  | 4.10                   | 51.2                  | -2.40                     | -4.08                     |
| <i>Boundary layer</i> | Our    | <b>6.06</b> $\pm 0.03$ | <b>69.8</b> $\pm 0.5$ | <b>-1.25</b> $\pm 0.45$   | <b>-4.64</b> $\pm 0.32$   |
|                       | Ideal  | 7.55                   | 53.6                  | -12.9                     | -11.7                     |

| Region                | Method | ELBO                  | Calib95 (%)           | ICI ( $10^{-2}$ )      |
|-----------------------|--------|-----------------------|-----------------------|------------------------|
| <i>Entire column</i>  | Our    | <b>13.1</b> $\pm 0.1$ | <b>94.9</b> $\pm 0.1$ | $5.29 \pm 0.59$        |
|                       | Ideal  | <b>13.1</b>           | 96.0                  | <b>5.05</b>            |
| <i>Boundary layer</i> | Our    | <b>10.6</b> $\pm 0.1$ | $98.8 \pm 0.1$        | <b>8.27</b> $\pm 0.29$ |
|                       | Ideal  | 10.2                  | <b>93.5</b>           | 19.1                   |

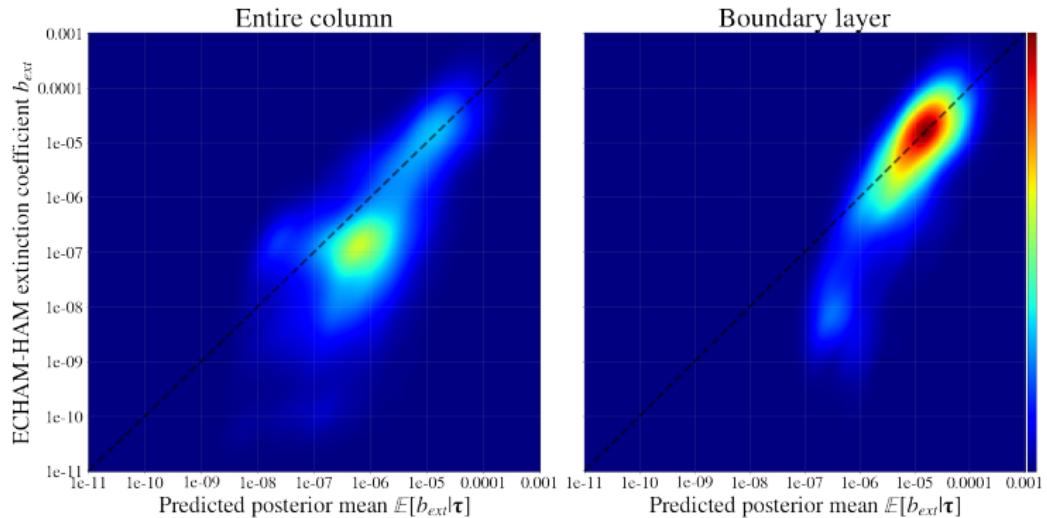


Figure 9: Density plots of groundtruth extinction coefficient values against predicted posterior mean extinction coefficient; **Left:** entire column; **Right:** boundary layer only

## Conclusion

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## Limitations and Directions

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- ▶ Can only capture extinction due to aerosol swelling (missing mass concentration, particle size and radiative properties extinction which would require additional predictors harder to obtain)
- ▶ Methodological extensions (use multiple wavelengths, allow unmatched data setting)
- ▶ Different use case: investigation on aerosol mode/species contribution to extinction using model data only

- [1] Leon Ho Chung Law, Dino Sejdinovic, Ewan Cameron, Tim C.D. Lucas, Seth Flaxman, Katherine Battle, and Kenji Fukumizu. Variational learning on aggregate outputs with Gaussian processes. In *Advances in Neural Information Processing Systems*, 2018.