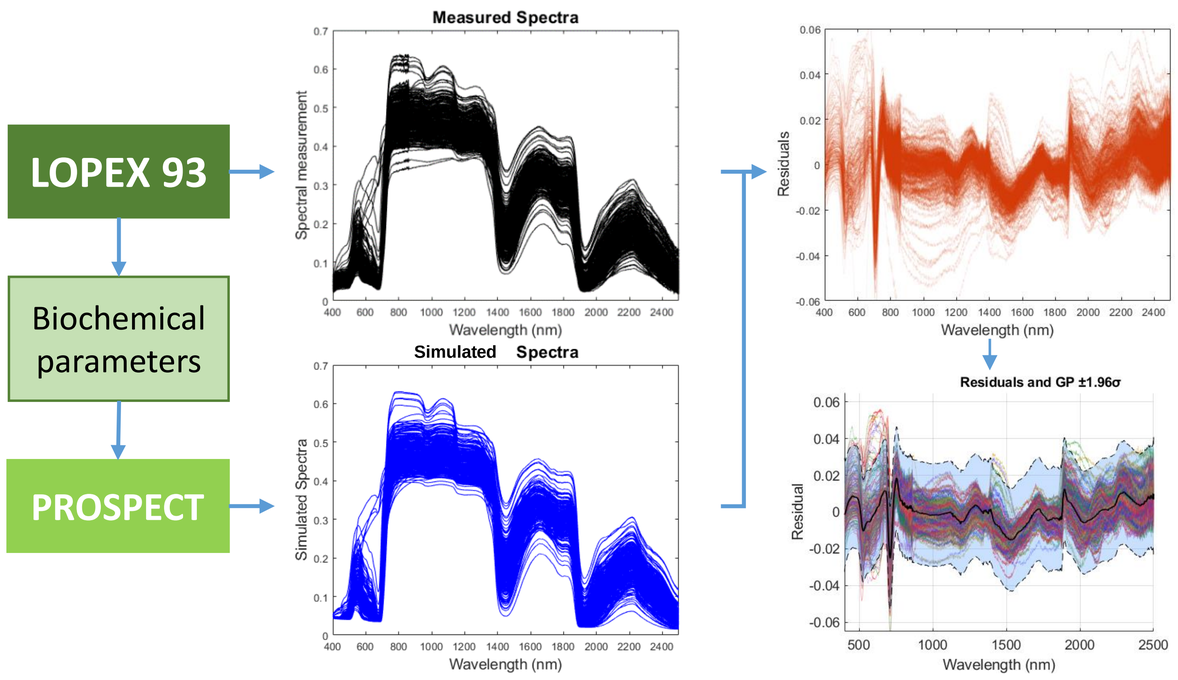
Towards quantifying model error from spectral radiative transfer models

☞An application to PROSPECT

Abstract

Radiative Transfer Models (RTMs) are essential tools for interpreting Earth Observation data, but their **internal uncertainties** are often ignored. While recent efforts in uncertainty quantification have focused on propagating measurement errors, the **structural uncertainty** of the models themselves remains unexplored. In this work, we assess the inherent uncertainty in the PROSPECT leaf model by comparing model outputs to reflectance spectra generated using ground-truth biochemical parameters. We model the residuals using a zero-mean Gaussian Process, allowing us to characterise the spectral uncertainty of the model across a range of conditions. This approach offers a practical route to integrating model error into uncertainty-aware EO applications.

PROSPECT spectral uncertainty as a GP



1. Use ground-truth input parameters $\vec{\theta}$ to generate model predictions of reflectance $\rho(\lambda)$ and transmittance $\tau(\lambda)$:

$$\mathcal{M}_x(\vec{\theta}),\ \text{with}\, x \in \rho,\ \tau$$

2. Compute residuals between model and measurements:

$$r_x(\lambda) = x_{meas}(\lambda) - \mathcal{M}_x(\vec{\theta})$$

3. Fit two independent zero-mean Gaussian Processes across all samples:

$$r_x(\lambda) \sim \mathcal{GP}\left(0,\ k_x(\lambda, \lambda')\right)$$

4. The two GPs encode the model uncertainty

$\Rightarrow$ GPs capture smooth, structured residuals for $\rho(\lambda)$ and $\tau(\lambda)$.

$\Rightarrow$ Posterior GP variance serves as a spectral estimate of model error.

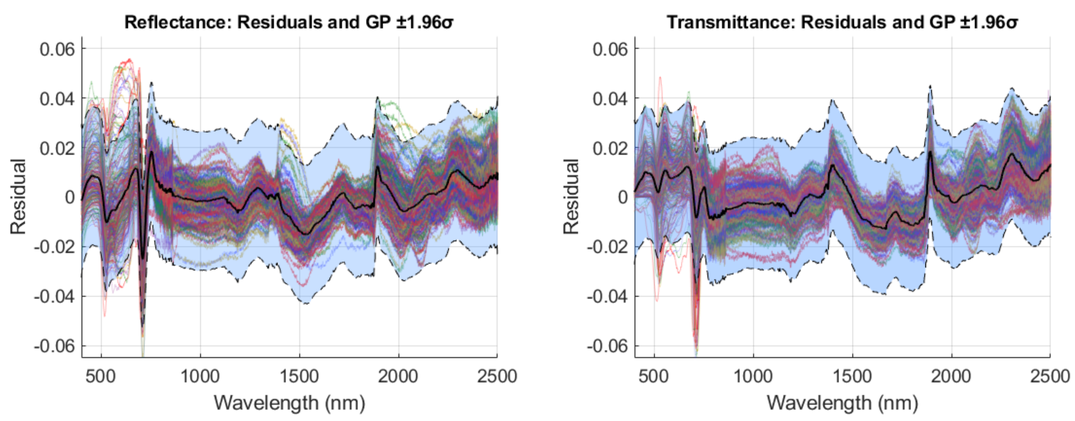
$\Rightarrow$ Can extend to non-zero mean

Experimental setup

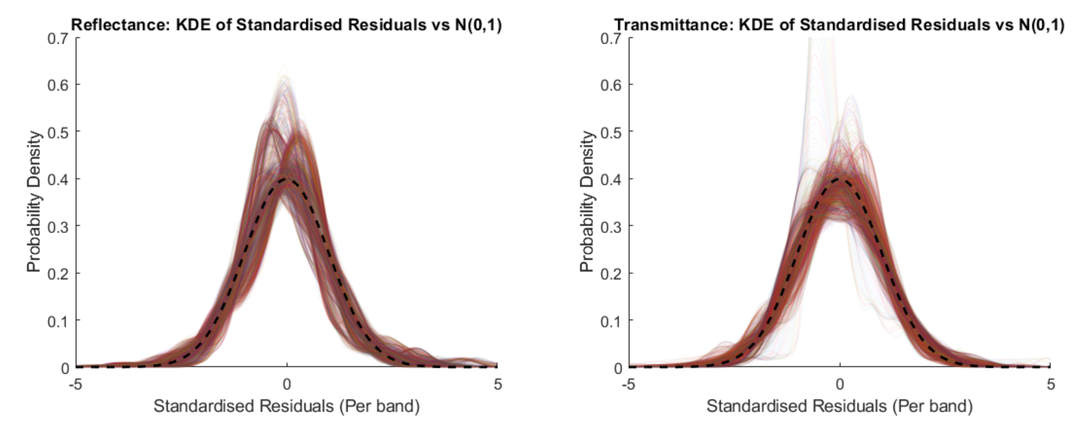
- **LOPEX93**: High-resolution **VIS–NIR spectra (400–2500nm)** from various leaf species
- Includes measured **biochemical** and **biophysical traits**
- Simulated spectra with PROSPECT-PRO using lab-measured traits
  - Leaf thickness, Equivalent water thickness
  - Chlorophyll and carotenoids concentration, protein content, ...
- Goal is to **quantify PROSPECT predictive error**

Results

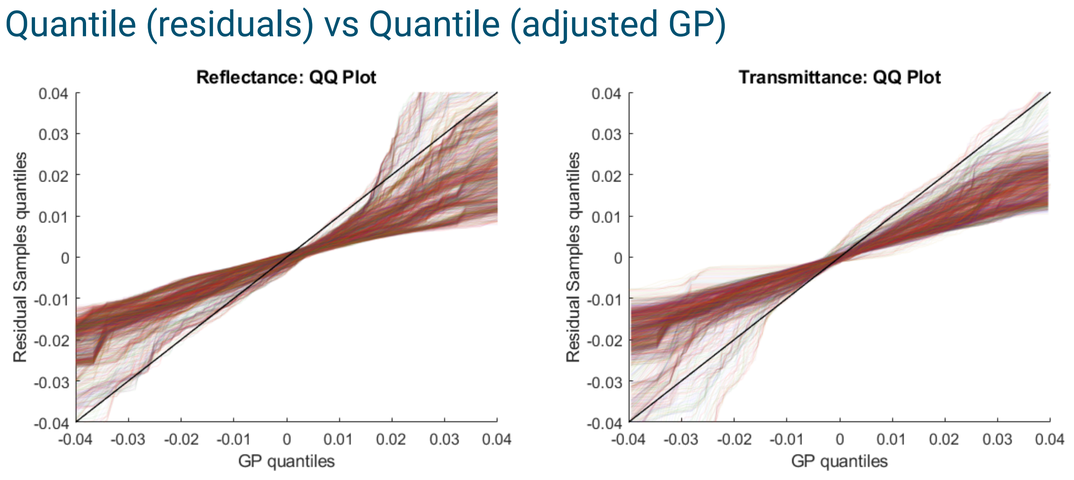
- Spectral plot of training residuals and shaded GP $\pm 1.96\sigma$ interval.



- Residuals against $N(0,1)$



- Quantile (residuals) vs Quantile (adjusted GP)



Conclusions

- **Simple method** to quantify RTM uncertainty, demonstrated with **PROSPECT-PRO**
- Adds **model error estimates** alongside observational uncertainty for **inversion** and **simulation**
- **Current model likely overestimates uncertainty** due to **wavelength-dependent bias** in residuals
- Use a **simple spectral model** to remove bias & **normalise residuals**
- Next: test on a **larger spectral dataset** to check **robustness**
- **Want to test this on your data? Get in touch!**

Contact

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