Physics informed Transformer-VAE for biophysical parameter estimation: PROSAIL model inversion in Sentinel-2 imagery

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Introduction

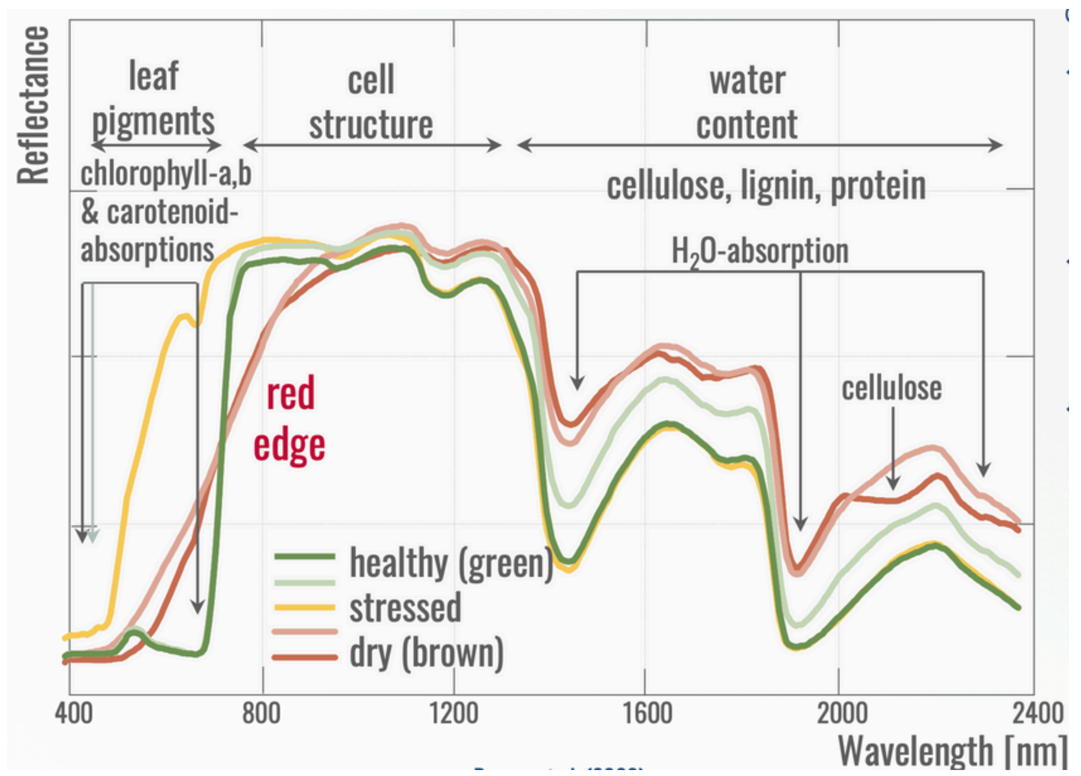
Motivation

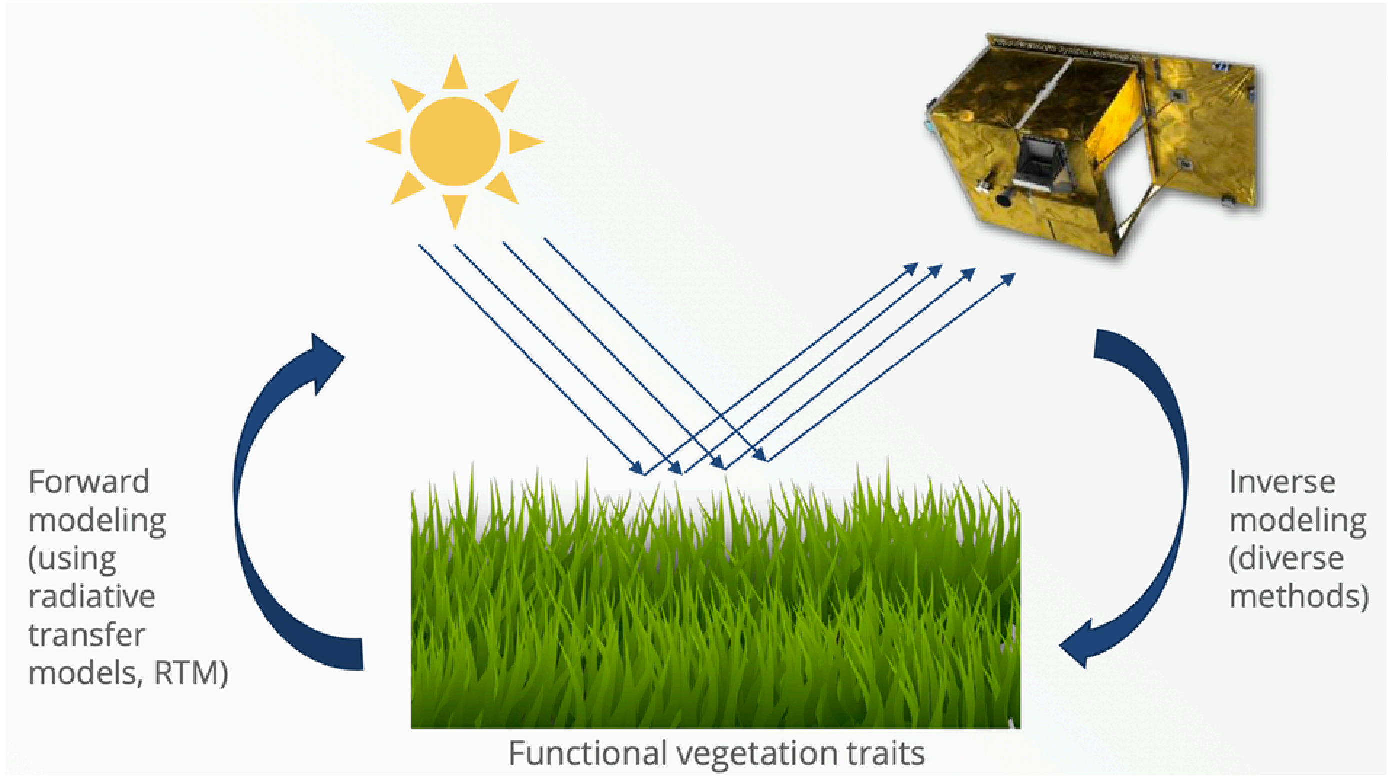
Vegetation BVs → Climate, agriculture, biodiversity

Key variables:

- LAI (Leaf Area Index), CCC (Canopy Chlorophyll Content)

- Low reflectance across visible wavelengths → pigments absorption.
- High reflectance in the NIR, with only ~ 10% of absorbed radiation.
- Intermediate reflectance in the SWIR, where energy is mainly absorbed by water or plant residues.





- Accurate maps at high resolution (satellite imaging spectroscopy) and frequent revisit are therefore crucial.
- Sun: provides radiation that interacts with vegetation canopies.
- **Forward modeling:** RTMs like PROSAIL to simulate how vegetation with specific traits reflects light: simulate spectral signatures based on known vegetation parameters.
- **Inverse modeling:** Estimating vegetation traits from observed reflectance data captured by satellite sensors.
- **More challenging direction.** Transformer-VAE addresses this by combining deep learning with physics-based constraints.

PROSAIL Inversion

Challenges

Ill-posed problem:

- Many distinct input combinations can produce virtually identical spectra—no unique mathematical “inverse.”

Synthetic-to-Real Gap:

- Training on LUTs (pure PROSAIL simulations) assumes that simulated reflectances mimic all real-world spectral variations.
- In reality, these factors introduce domain shift, so a network trained on “perfect” simulations mis-predicts when faced with actual Sentinel-2 data.

Uncertainty Quantification:

- Providing not just a single LAI or Cab number per pixel, but also a measure of confidence (e.g. a distribution or error bar).
- Without credible uncertainty, downstream decision-making (e.g. crop yield forecasts) can be inaccurate.

Our Contribution

PROSAIL-VAE

- Instead of treating PROSAIL as a “black-box” simulator, we re-implement its entire forward model in PyTorch so that it supports automatic differentiation.
- The decoder is literally the PROSAIL function: it takes a sampled latent vector and outputs the reconstructed Sentinel-2 bands.
- Feed the network a large collection of real, atmospherically-corrected Sentinel-2 image patches and ask it to reconstruct those same pixels via the PROSAIL decoder.

Tranformer-VAE (Proposed approach)

- We fuse PROSAIL as a differentiable decoder with a Transformer-based encoder.
- Most importantly, we train entirely on simulated reflectance data.

- PROSAIL-VAE (MLP or CNN encoder) treats bands either independently or only with local context, so it can miss long-range dependencies—e.g. how red-edge shifts in one part of the spectrum correlate with water absorption features elsewhere.

- Transformer-VAE uses self-attention to learn global relationships across all bands simultaneously. This means it can pick up subtle, non-local spectral cues (tiny shifts, cross-band patterns) that are essential for distinguishing degenerate PROSAIL inputs.

Richer Spectral Modeling via Self-Attention Framework

Transformer-VAE Architecture

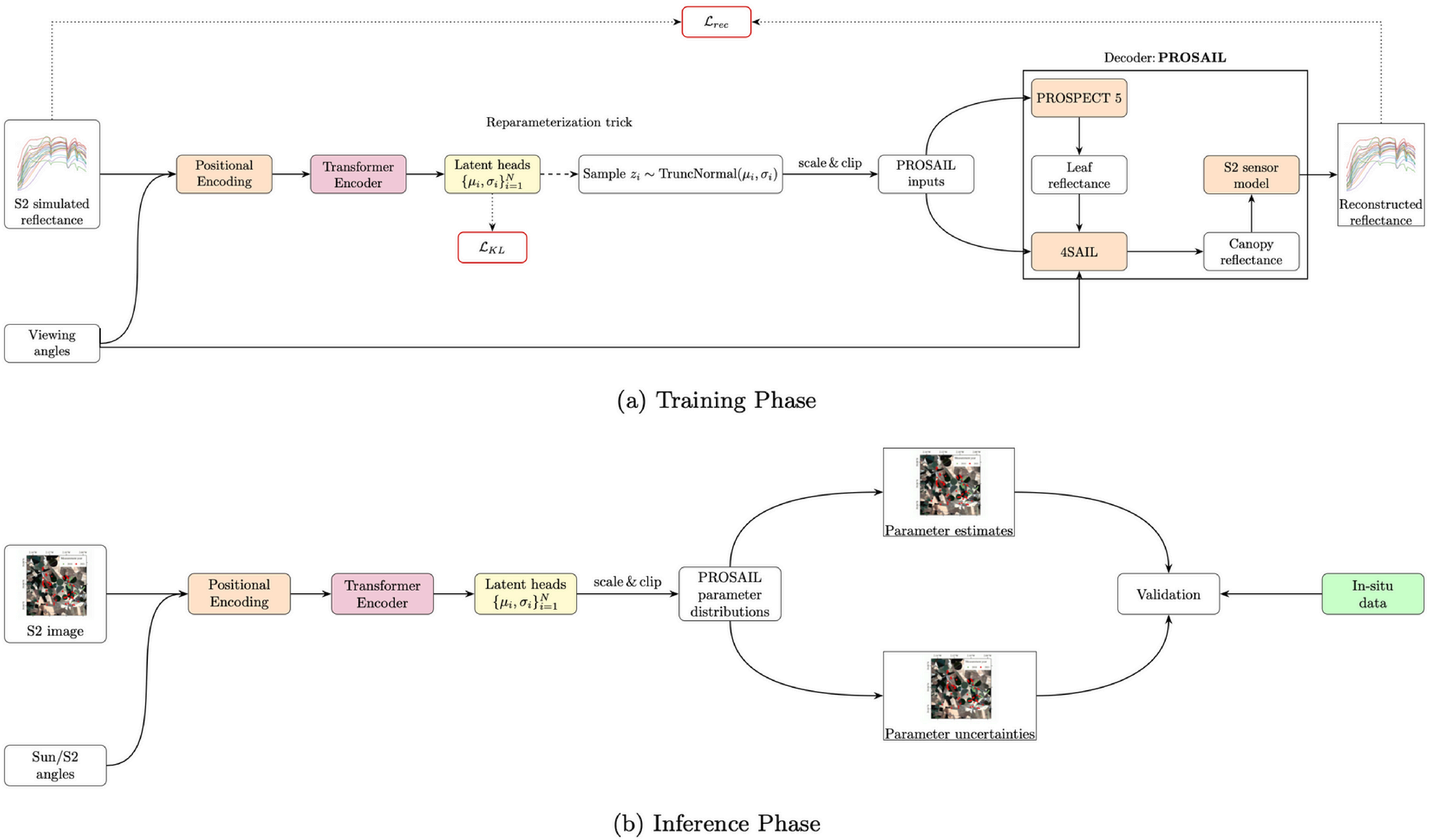
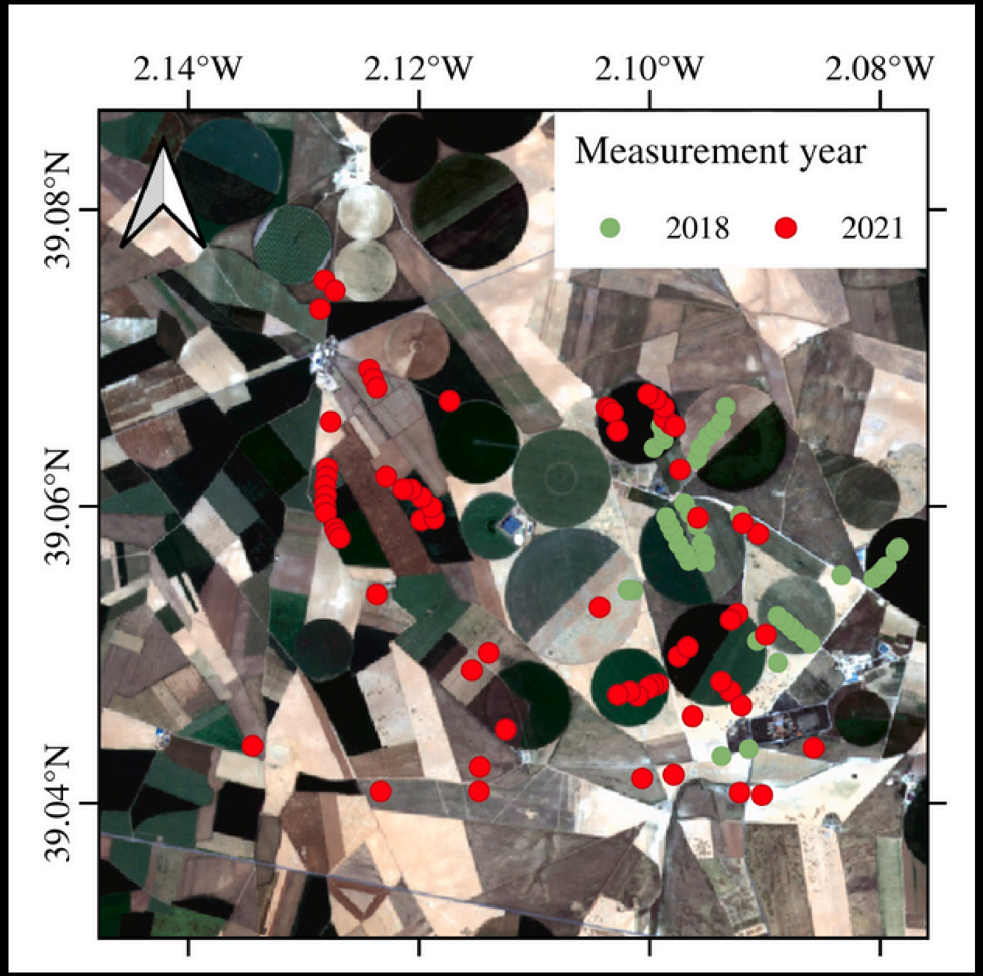


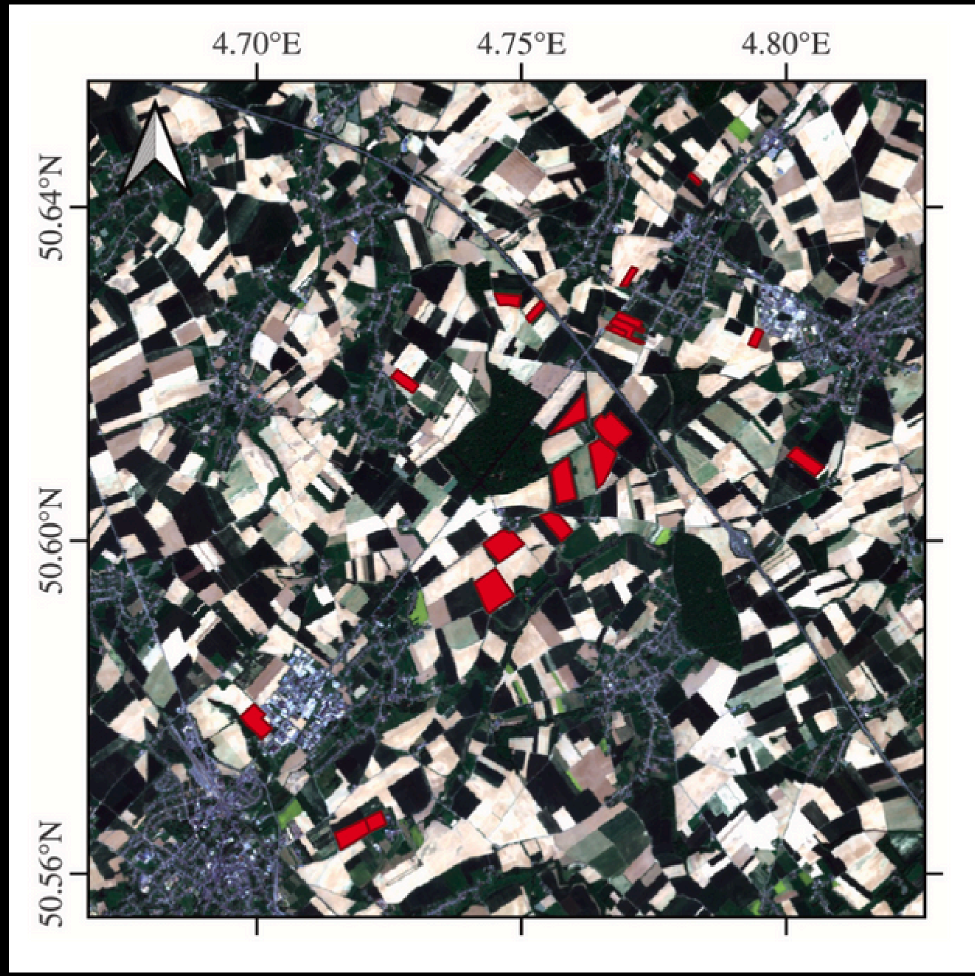
Figure 1: End-to-end architecture: (a) training with transformer-VAE & PROSAIL decoder, (b) inference and validation.

Test Dataset (In-situ)

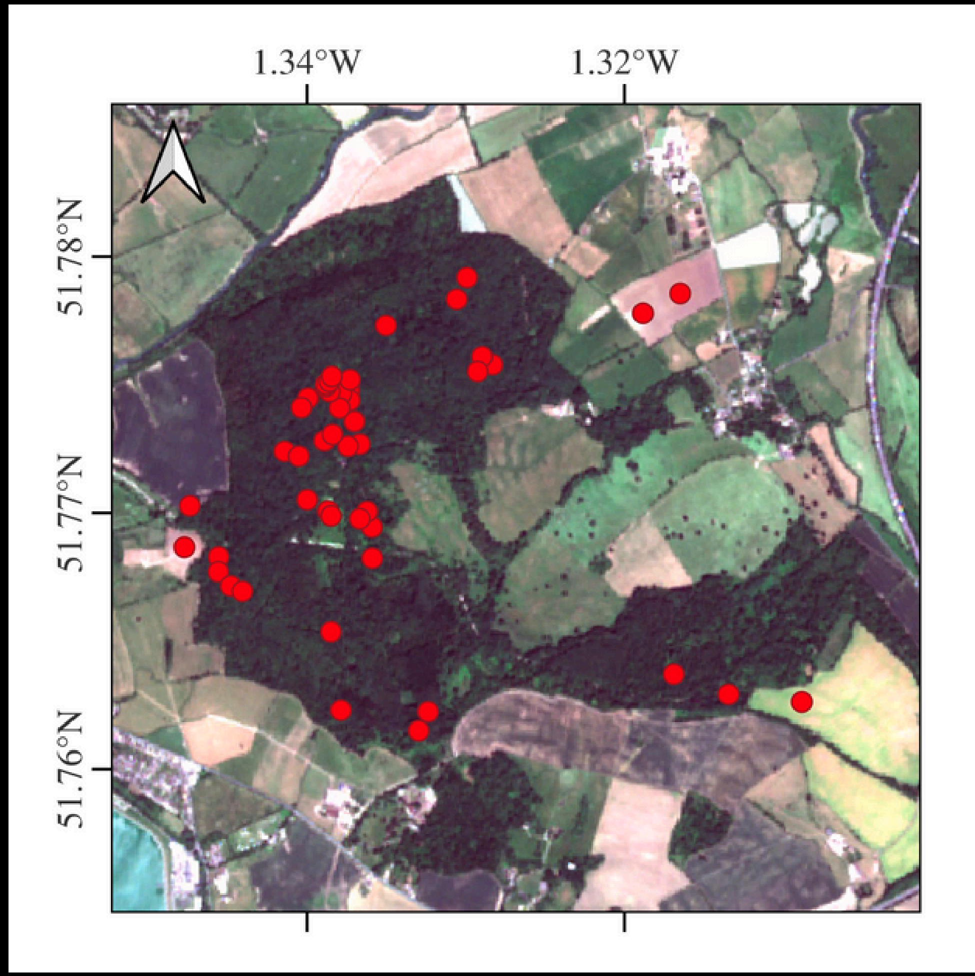
In-situ



Barrax, Spain



BelSAR, Belgium



Wytham, UK

- Barrax campaigns conducted in 2018 (green points) and 2021 (red points). Includes LAI and CCC across various crop types.
- BelSAR include both wheat fields and maize fields. Plant Area Index (PAI) measured for wheat fields and Green Area Index (GAI) measured for maize fields.
- Wytham Woods represents a complex natural forest ecosystem dominated by deciduous species. Includes Leaf LAI and CCC measurements.

Results and Comparison

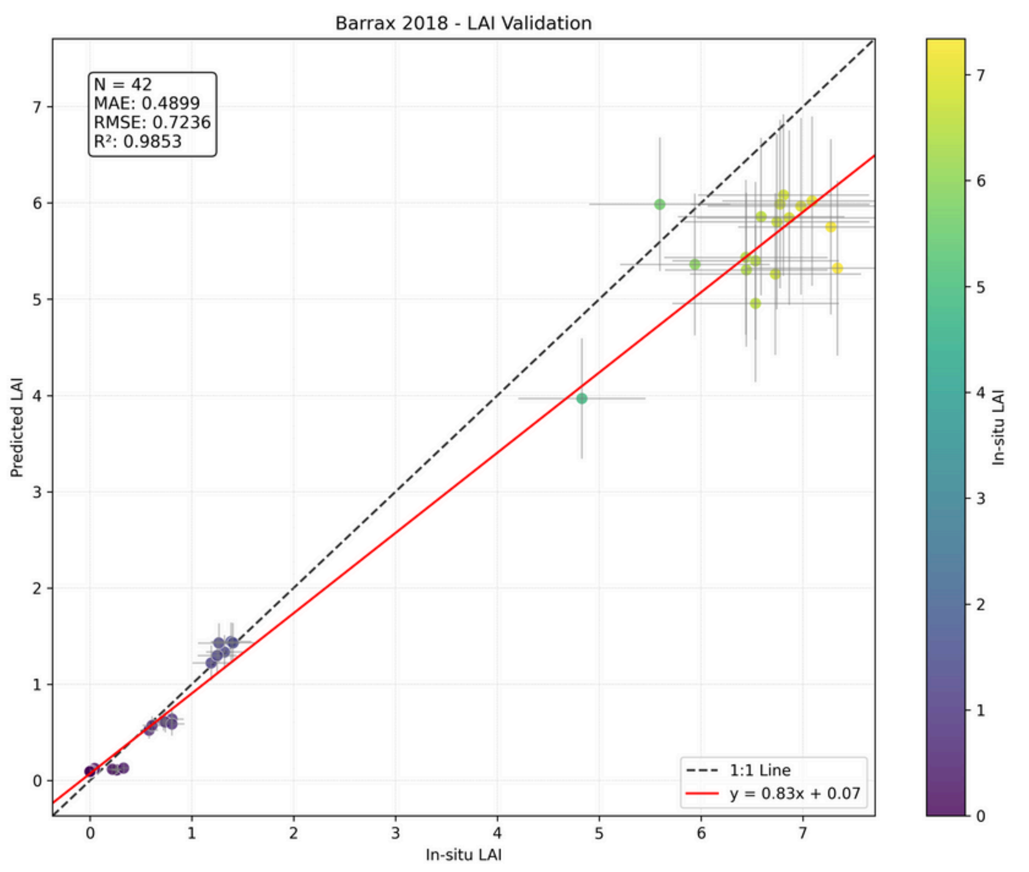
Results

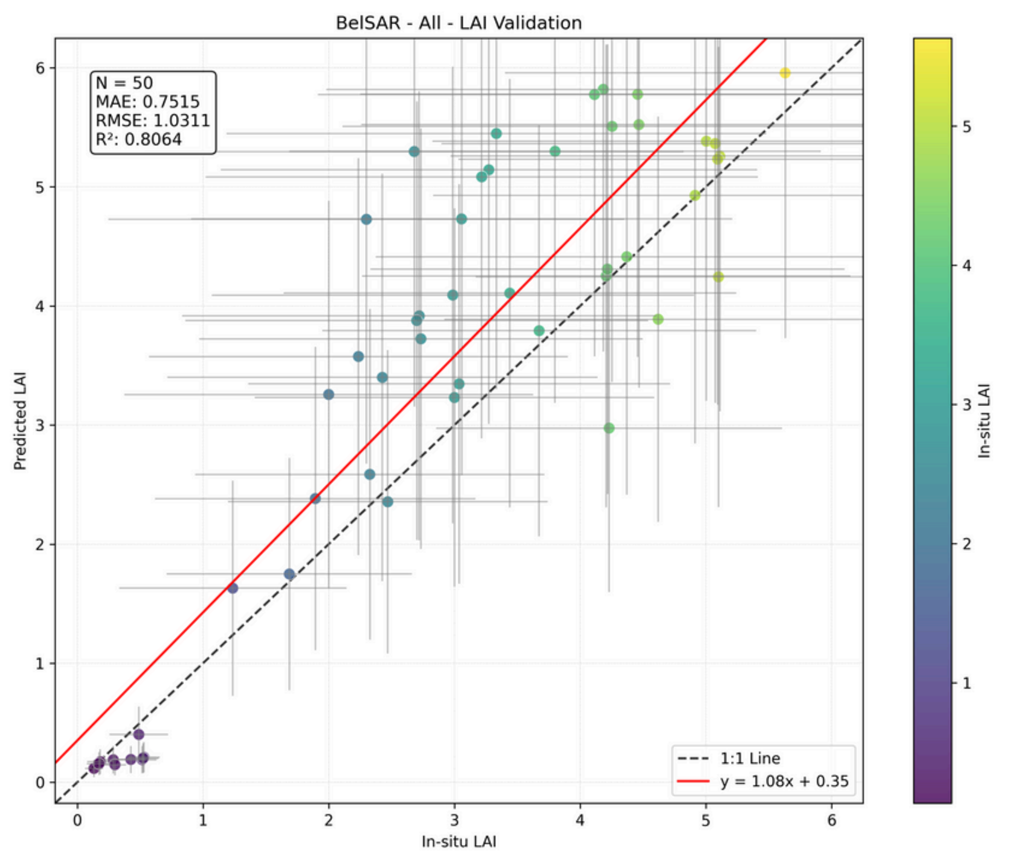
Table 1. LAI and CCC prediction performance on in-situ data for SNAP, PROSAIL-VAE and Transformer-VAE.

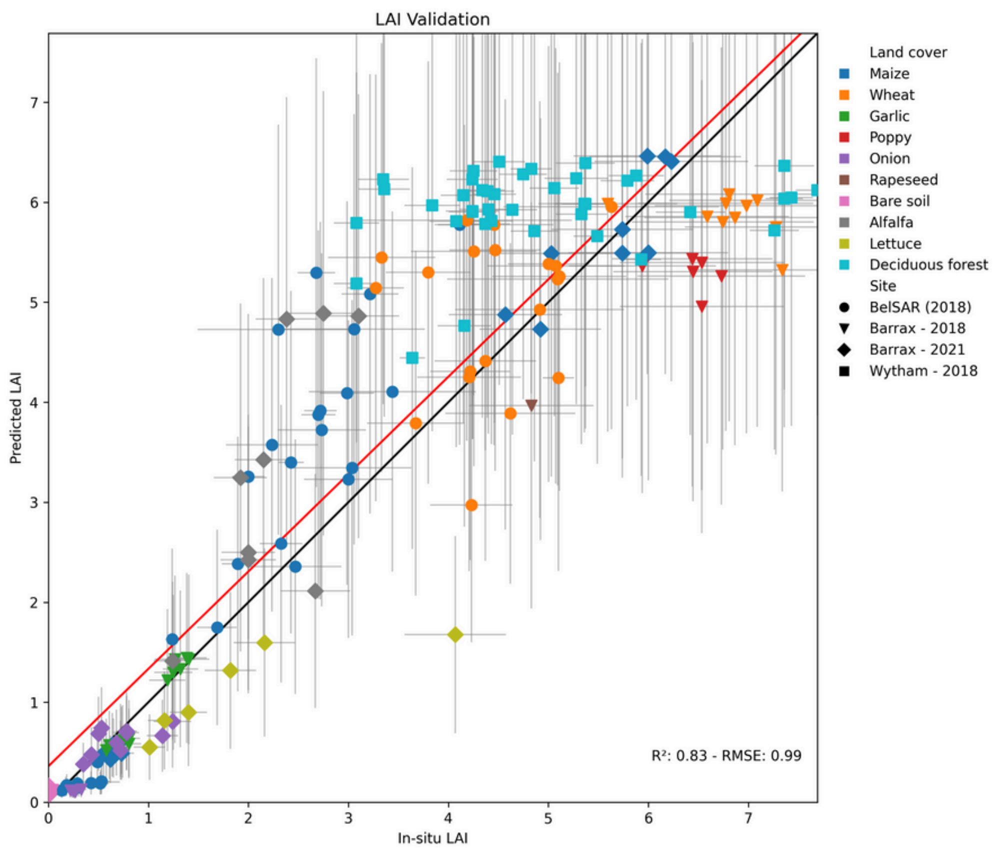
		LAI					CCC			
Method	Metric	BelSAR	Barrax (2018)	Barrax (2021)	Wytham	All	Barrax (2018)	Barrax (2021)	Wytham	All
SNAP	RMSE	1.22	1.43	0.48	1.77	1.24	83.92	84.53	101.35	88.08
PROSAIL-VAE	RMSE	1.30	1.42	0.72	1.21	1.16	27.60	20.51	80.78	42.33
	MPIW	4.74	3.74	2.72	5.45	4.04	140.53	94.02	235.20	138.18
	PICP	1.00	0.88	0.96	0.95	0.95	0.95	0.98	0.84	0.94
T-VAE	RMSE	**1.03**	**0.72**	**0.63**	1.53	**0.99**	63.43	41.56	134.75	76.56
	MPIW	6.04	**1.52**	**0.72**	**0.96**	5.15	**56.09**	**30.11**	**77.89**	310.55
	PICP	0.92	0.67	0.37	0.10	0.95	0.21	0.19	0.16	0.88

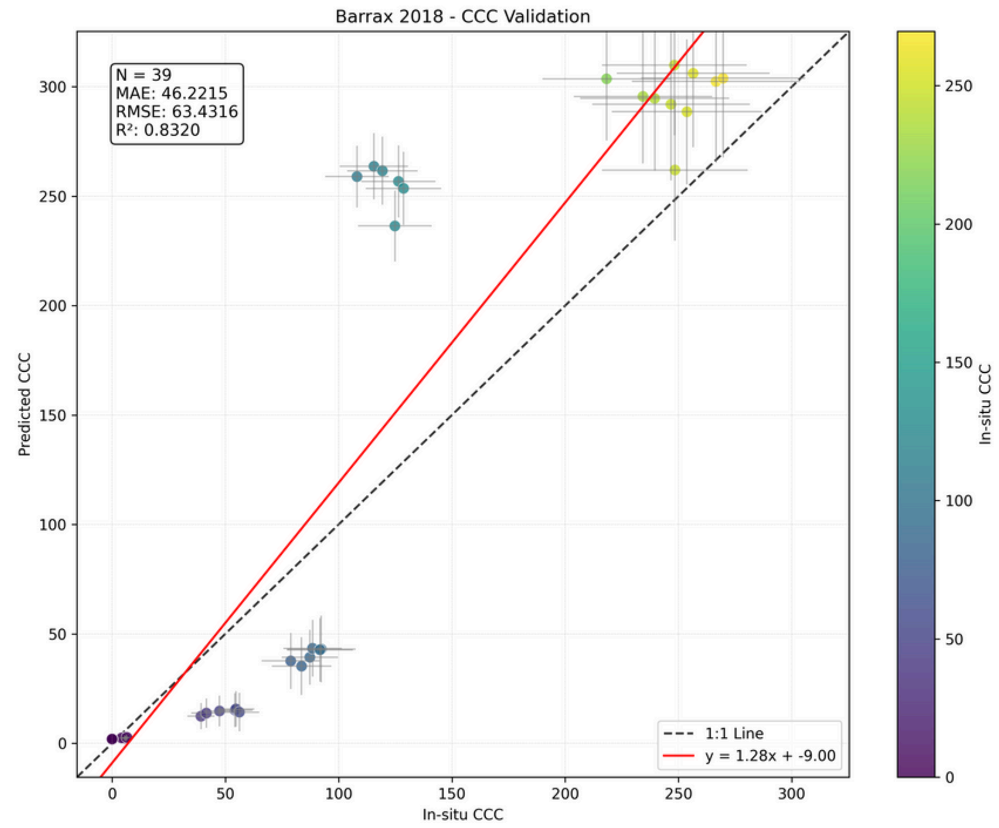
- Transformer-VAE trained on purely simulated data achieves the lowest RMSE values **(bold numbers)** across most sites.

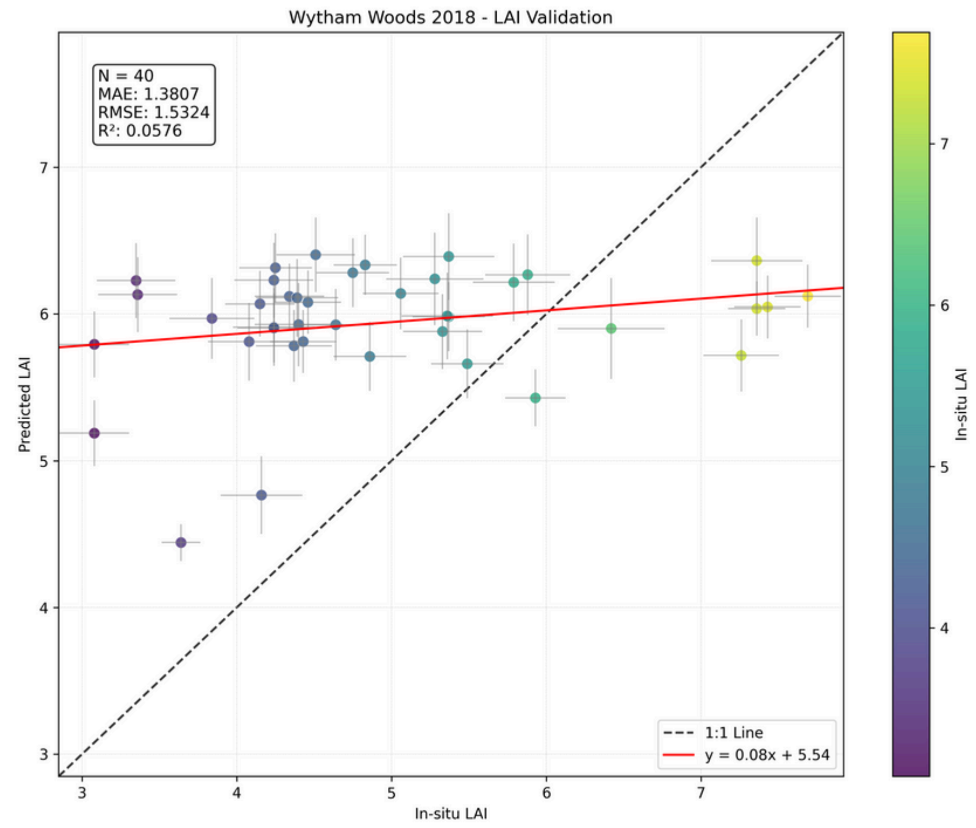
Results and Comparison

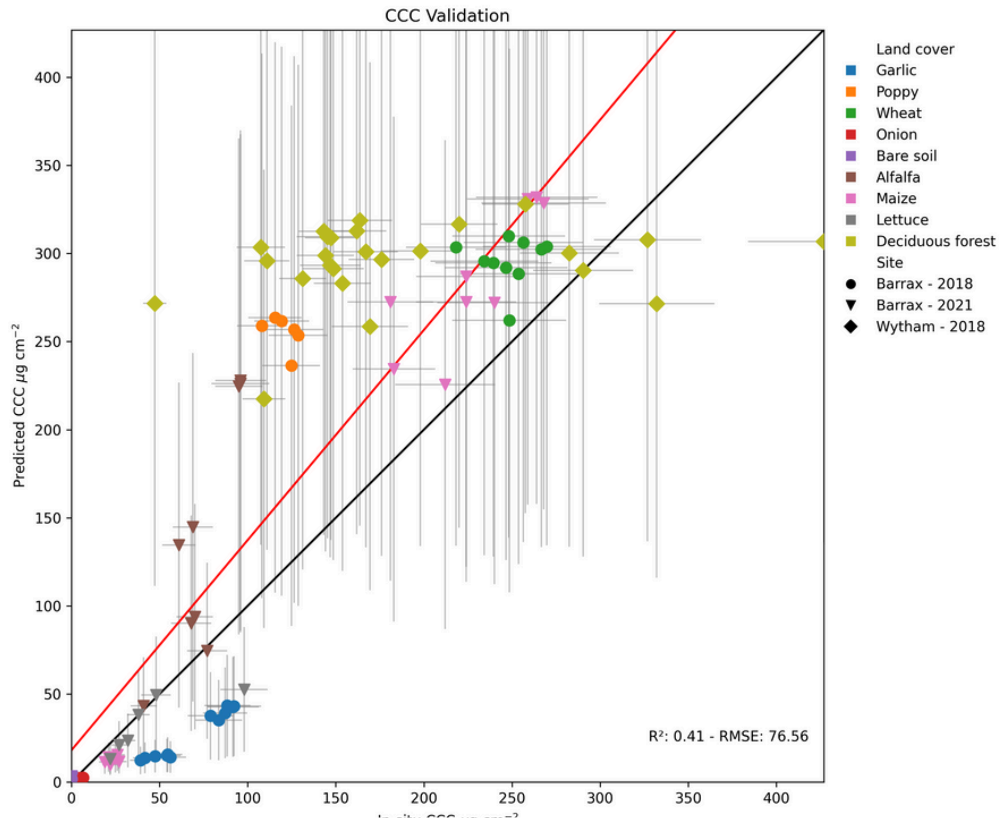












Conclusion

Key Takeaways

- This approach removes the need for costly in-situ or real-image calibration, making it ideal for global operational mapping.
- The Transformer excels at modeling subtle spectral features, while PROSAIL ensures every prediction adheres to physical laws. The VAE latent variances give us trustworthy confidence bounds.”

Future Works

- Extend to hyperspectral (HyMap, AVIRIS) + advanced RTMs
- Transformer-priors: model interdependencies, across different parameter values.

Thank You

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