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

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Abstract

We propose a physics-informed variational autoencoder (VAE) architecture, termed Transformer-PROSAILVAE, for retrieving vegetation biophysical parameters from Sentinel-2 satellite imagery. The model integrates a transformer-based encoder with a fixed PROSAIL radiative transfer model (RTM) decoder, embedding physical knowledge of canopy reflectance into a deep learning framework. This design enables self-supervised training on simulated reflectance data without any ground truth labels – the encoder learns to infer Leaf Area Index (LAI) and canopy chlorophyll content (CCC) by reconstructing spectral reflectances via the PROSAIL decoder. We thoroughly describe the architecture and training pipeline, and compare its performance to the original transformer-VAE approach of Zérah et al. (2023) file-27hzu1p94gn7jorbww3kzm . Experiments on real Sentinel-2 images demonstrate that our Transformer-VAE achieves accurate LAI and CCC retrievals, outperforming both the baseline transformer-VAE and the operational SNAP biophysical processor. The transformer encoder effectively captures complex spectral–spatial context, yielding improved retrieval robustness across diverse landscapes. We report quantitative results on independent in-situ validation datasets (FRM4Veg and BelSAR campaigns) showing that the physics-informed Transformer-VAE attains lower estimation errors and higher consistency with field measurements. The proposed approach illustrates how integrating physical models with advanced deep networks can improve the inversion of RTMs, opening new prospects for large-scale, physically-constrained remote sensing of vegetation traits.

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1. Introduction

Physics-guided deep learning has applied to vegetation parameter retrieval by coupling the prosail radiative transfer model with neural network.

Submission to ICML 2025 will be entirely electronic, via a web site (not email). Information about the submission process and LaTeX templates are available on the conference web site at:

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- References must include page numbers whenever possible and be as complete as possible. Place multiple citations in chronological order.
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```
dvips -Ppdf -tletter -G0 -o paper.ps paper.dvi
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```

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The footnote, "Preliminary work. Under review by the International Conference on Machine Learning (ICML). Do not distribute." must be modified to "*Proceedings of the 42^{nd} International Conference on Machine Learning*, Vancouver, Canada, PMLR 267, 2025. Copyright 2025 by the author(s)."

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```
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You can use footnotes[1] to provide readers with additional information about a topic without interrupting the flow of the paper. Indicate footnotes with a number in the text where the point is most relevant. Place the footnote in 9 point type at the bottom of the column in which it appears. Precede the first footnote in a column with a horizontal rule of 0.8 inches.[2]

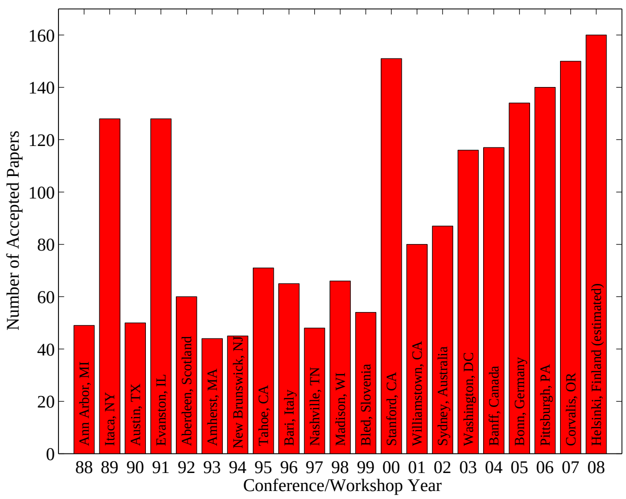

Figure 1. Historical locations and number of accepted papers for International Machine Learning Conferences (ICML 1993 – ICML 2008) and International Workshops on Machine Learning (ML 1988 – ML 1992). At the time this figure was produced, the number of accepted papers for ICML 2008 was unknown and instead estimated.

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You may want to include figures in the paper to illustrate your approach and results. Such artwork should be centered, legible, and separated from the text. Lines should be dark and at least 0.5 points thick for purposes of reproduction, and text should not appear on a gray background.

Label all distinct components of each figure. If the figure takes the form of a graph, then give a name for each axis and include a legend that briefly describes each curve. Do not include a title inside the figure; instead, the caption should

[1]Footnotes should be complete sentences.

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Algorithm 1 Bubble Sort

Input: data x_i, size m
repeat
  Initialize $noChange = true$.
  for $i = 1$ **to** $m - 1$ **do**
    if $x_i > x_{i+1}$ **then**
      Swap x_i and x_{i+1}
      $noChange = false$
    end if
  end for
until $noChange$ is $true$

Table 1. Classification accuracies for naive Bayes and flexible Bayes on various data sets.

Data set	Naive	Flexible	Better?
Breast	95.9± 0.2	96.7± 0.2	√
Cleveland	83.3± 0.6	80.0± 0.6	×
Glass2	61.9± 1.4	83.8± 0.7	√
Credit	74.8± 0.5	78.3± 0.6	
Horse	73.3± 0.9	69.7± 1.0	×
Meta	67.1± 0.6	76.5± 0.5	√
Pima	75.1± 0.6	73.9± 0.5	
Vehicle	44.9± 0.6	61.5± 0.4	√

serve this function.

Number figures sequentially, placing the figure number and caption *after* the graphics, with at least 0.1 inches of space before the caption and 0.1 inches after it, as in **??**. The figure caption should be set in 9 point type and centered unless it runs two or more lines, in which case it should be flush left. You may float figures to the top or bottom of a column, and you may set wide figures across both columns (use the environment `figure*` in LaTeX). Always place two-column figures at the top or bottom of the page.

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Tables contain textual material, whereas figures contain graphical material. Specify the contents of each row and column in the table's topmost row. Again, you may float tables to a column's top or bottom, and set wide tables across both columns. Place two-column tables at the top or bottom of the page.

2.9. Theorems and such

The preferred way is to number definitions, propositions, lemmas, etc. consecutively, within sections, as shown below.

Definition 2.1. A function $f : X \to Y$ is injective if for any $x, y \in X$ different, $f(x) \neq f(y)$.

Using **??** we immediate get the following result:

Proposition 2.2. *If f is injective mapping a set X to another set Y, the cardinality of Y is at least as large as that of X*

Proof. Left as an exercise to the reader. □

?? stated next will prove to be useful.

Lemma 2.3. *For any $f : X \to Y$ and $g : Y \to Z$ injective functions, $f \circ g$ is injective.*

Theorem 2.4. *If $f : X \to Y$ is bijective, the cardinality of X and Y are the same.*

An easy corollary of **??** is the following:

Corollary 2.5. *If $f : X \to Y$ is bijective, the cardinality of X is at least as large as that of Y.*

Assumption 2.6. The set X is finite.

Remark 2.7. According to some, it is only the finite case (cf. **??**) that is interesting.

2.10. Citations and References

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Use an unnumbered first-level section heading for the references, and use a hanging indent style, with the first line of the reference flush against the left margin and subsequent lines indented by 10 points. The references at the end of this document give examples for journal articles (**?**), conference publications (**?**), book chapters (**?**), books (**?**), edited volumes (**?**), technical reports (**?**), and dissertations (**?**).

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Authors are **required** to include a statement of the potential broader impact of their work, including its ethical aspects and future societal consequences. This statement should be in an unnumbered section at the end of the paper (co-located with Acknowledgements – the two may appear in either order, but both must be before References), and does not count toward the paper page limit. In many cases, where the ethical impacts and expected societal implications are those that are well established when advancing the field of Machine Learning, substantial discussion is not required, and a simple statement such as the following will suffice:

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