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Retrieval of atmospheric CH4 profiles from hyperspectral infrared satellite observations: an inversion approach based on Physically Informed Neural Network

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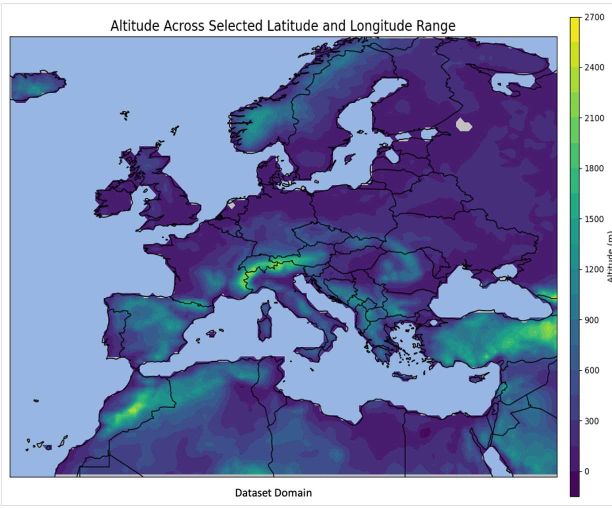
Context and motivation

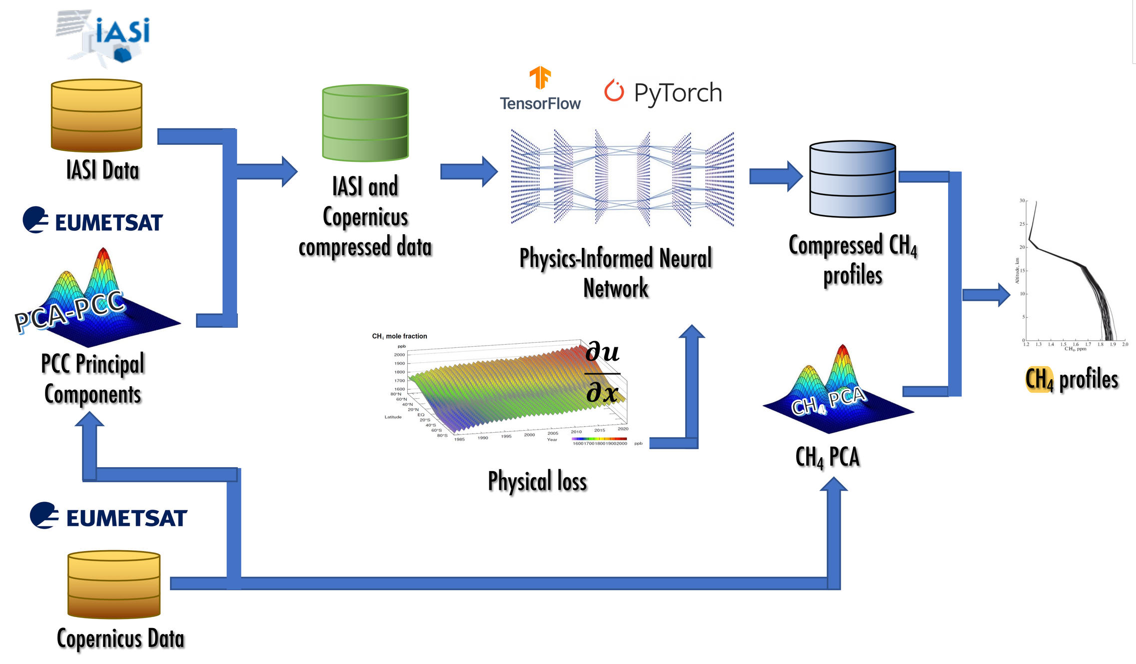
Atmospheric methane (CH_4) plays a critical role in climate change due to its potent greenhouse effect, which is tens of times greater than that of CO_2, with approximately 60% of emissions stemming from human activities. The thawing of Antarctic permafrost, containing an estimated 540 Gt of CH_4, poses a particular threat as its release could significantly intensify global warming. While CO_2's atmospheric cycle and vertical profile are well-documented, CH_4's distribution and profiling remain challenging. Satellite observations in the infrared range, specifically the NIR, MIR, and TIR, are vital for global CH_4 monitoring and analysis of its spatial and temporal variability.

In the PRIN-MVP project, an innovative methodology based on Physics-Informed Neural Networks (PINNs) [1] was developed and validated to obtain vertical CH_4 profiles from satellite data, allowing accurate identification of methane sources at the surface. We have successfully applied to IASI data, this technique leverages approximately 1,000,000 simulated clear-sky spectra generated by the σ-IASI/F2N radiative model [2], along with ancillary information. Averaging Kernel are used to optimize spectral intervals [3], while PCA reduces dimensionality and noise to achieve consistent projections at each atmospheric level. The results demonstrate the effectiveness of PINNs in reconstructing complete and coherent CH_4 profiles, validated against reference measurements.

Physics Informed Neural Network (PINN)

Radiances were simulated using the σ-IASI/F2N radiative transfer code, which uses a fixed pressure grid. Inputs profiles and parameters are downloaded from the Copernicus databases. The dataset includes clear sky measurements over the 2010-2020 timeframe, considering the 4 synoptic times (00-06-12-18 UTC), with a focus on Europe.



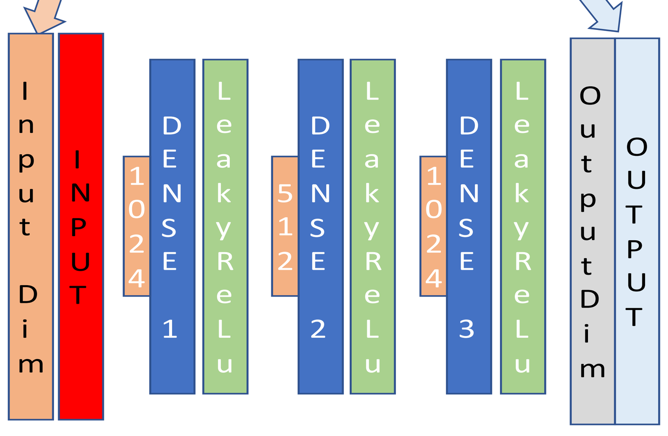


Input Tensor	#
Spectra PC	20
Temperature PC	16
Latitude	1
Longitude	1
Starting Layer	1
Time	1
Vza	1
Input Dimension	41

Output Tensor	#
CH_4 PC	24
Output Dimension	24

The basic structure of the PINN was derived through the Autokeras framework. Starting from this structure, a PINN was trained with the following loss function for each input tensor, where we will call sl the starting layer of the i-th example, y_{pred} the predicted output tensor and y_{true} the reference output tensor.

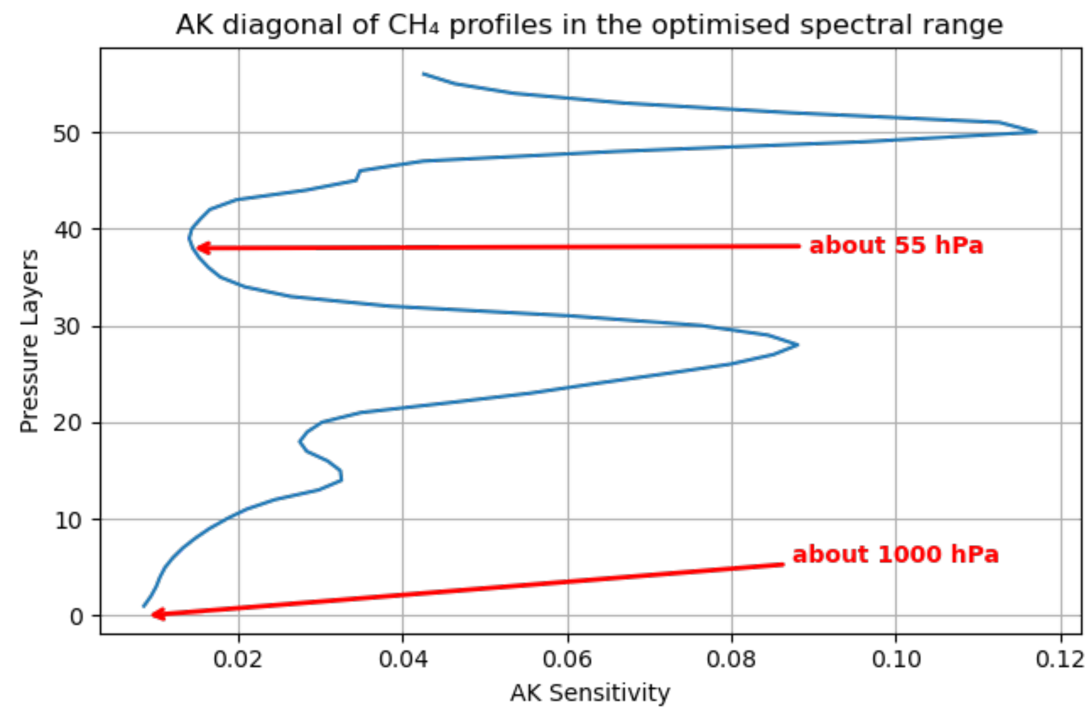
$$S_a = (cov\_matrix(sl))^{-1}$$
$$diff = y_{true}(i) - y_{pred}(i)$$
$$loss(i) = diff * S_a * diff^{T}$$



PINN Structure Model

Compression Data: Averaging Kernels and Principal Component Analysis

In order to reduce the dimensionality of the data, without reducing the information content of the data itself, compression was done by means of an Averaging Kernel (AK) study and Principal Component Analysis (PCA).



Averaging Kernels

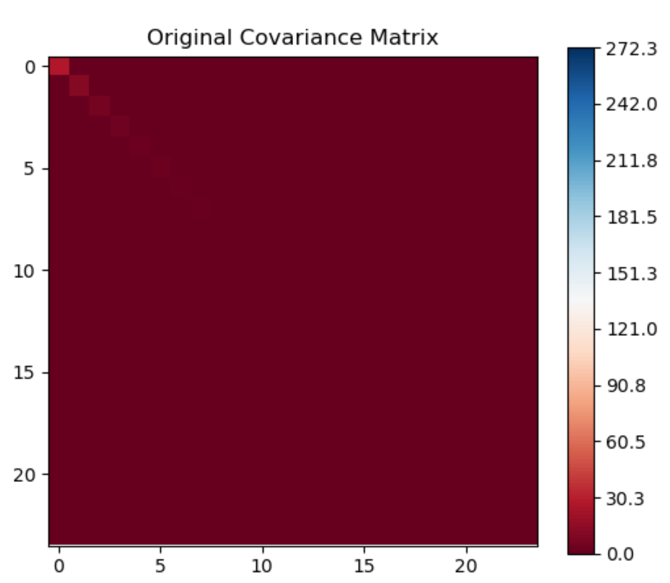
The AK matrix, was calculated starting from the core of the CH_4 band in the infrared (wavelength number 1305 cm^{-1}) by broadening the spectral range under analysis step by step. The study showed that the maximum amount of information, relating to CH_4 profiles, is obtained between the wavenumbers 1180 cm^{-1} and 1430.25 cm^{-1} (1001 channels). We also note that the information from the spectra referring to methane profiles is lacking around 1000 and 55 hPa.

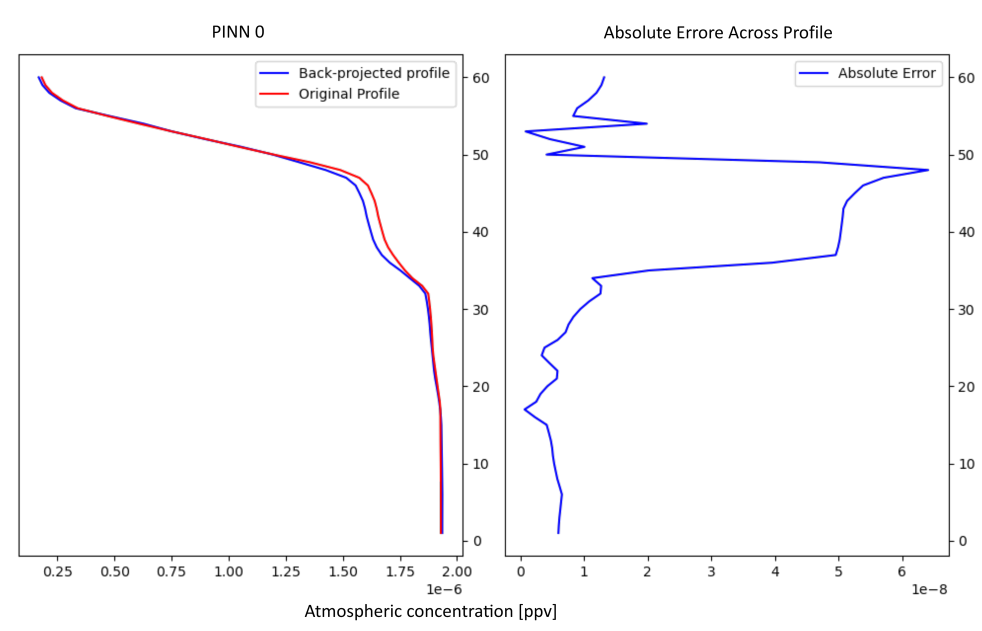
Principal Component Analysis

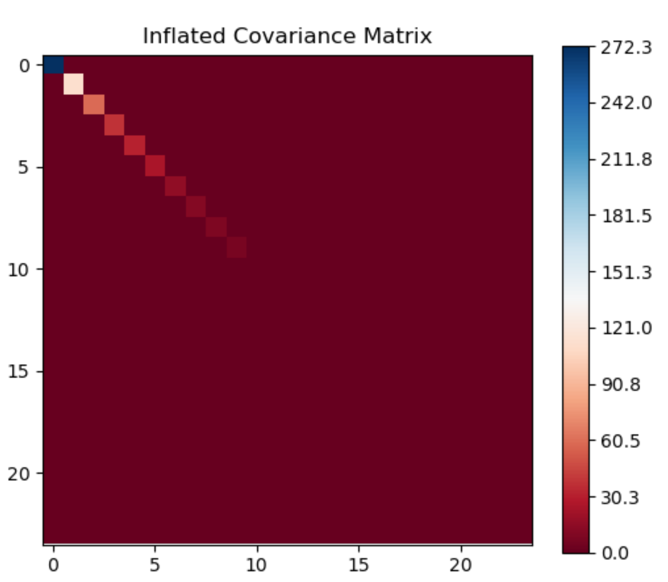
PCA was applied to both spectra and vertical profiles of methane and temperature, for which a different projection basis was calculated for each starting layer in the dataset. To obtain 99.99% of the variance explained, 20 PCs for the spectra, 24 PCs for the methane profiles and 16 PCs for the temperature profiles, respectively, are required.

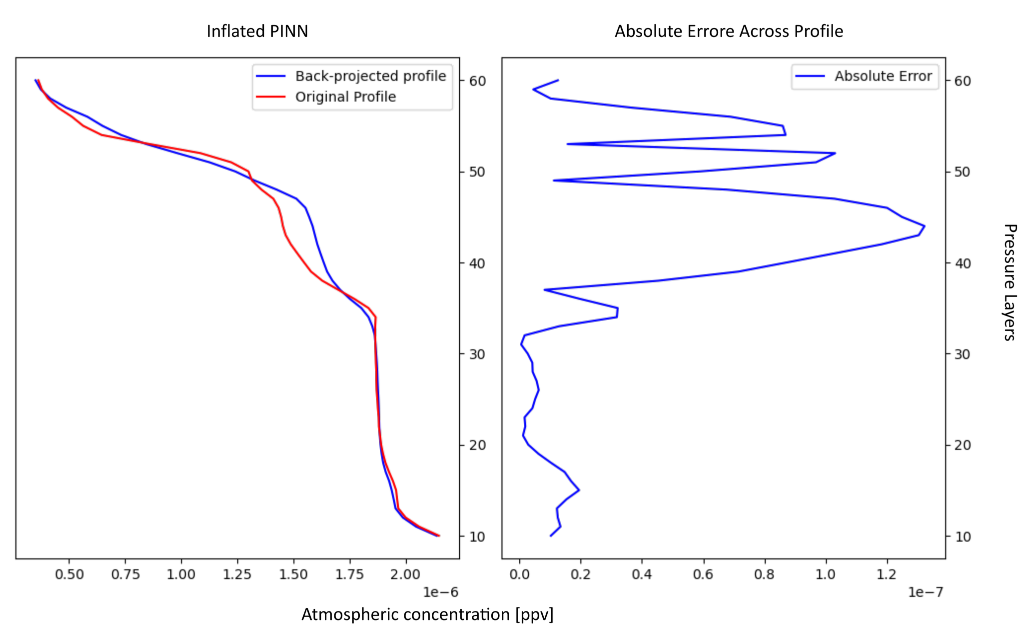
Results

Two different PINN models were implemented, "PINN 0" to accurately find the vertical gas profile and "**Inflated** PINN" to find CH_4 sources. The substantial difference between the two networks is in the covariance matrix used in the cost function. For the PINN inflated, the first 10 values of the first 10 rows of the covariance matrix were inflated by a factor of 10, so as to give the network more freedom in finding the minimum error at the sources , i.e. the first pressure layers.



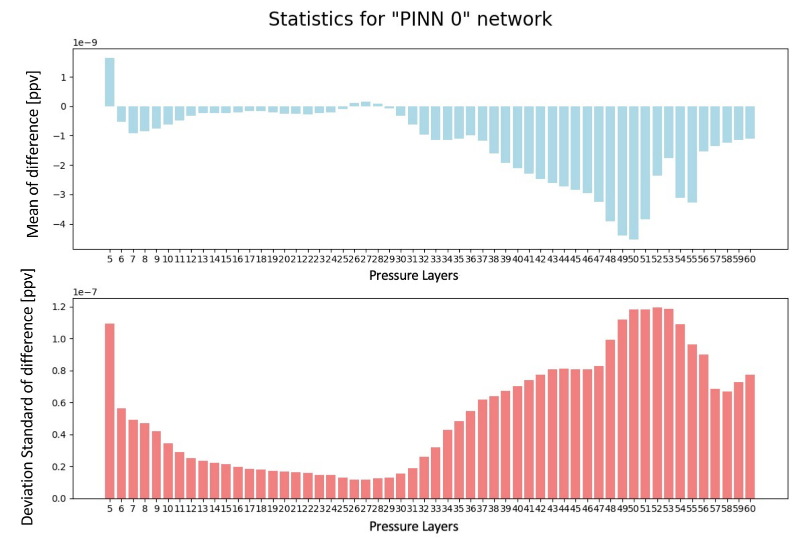


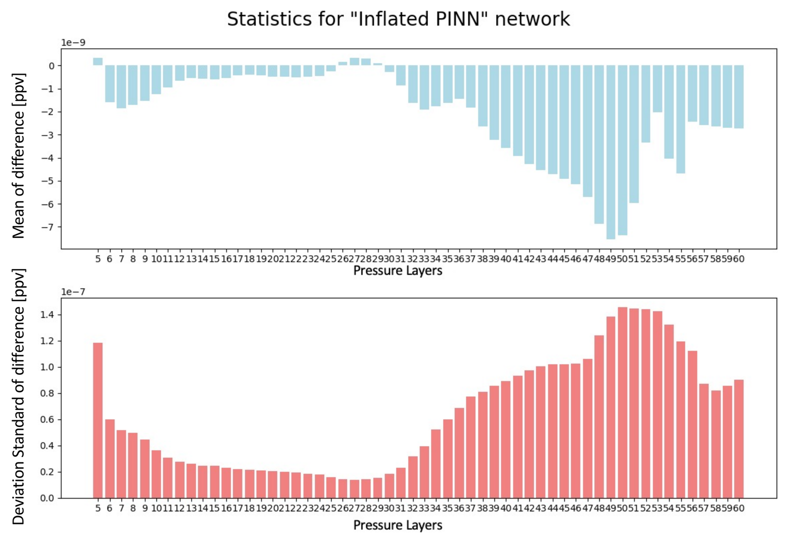




"PINN 0" model:

The "PINN 0" model is most accurate when evaluated over all pressure layers, while it performs slightly worse in finding sources. The mean absolute error, calculated on all IASI pressure levels, is equal to 30 ppbv. This model is therefore useful for estimating the column content of methane.





"Inflated PINN" model:

The "Inflated PINN" model appears to be adequately accurate for the prediction of sources with small to medium emissions, while although it is able to identify them, it tends to slightly underestimate very large emissions. An analysis on the test set produced an average error relative to the first pressure layer (i.e. the initial layer of each profile) of 200 ppbv, or ~10% of the value.

Future Developments

- We would like to further validate the network with IASI data related to sources and background;
- We intend to expand the training dataset by adding more sources. This increase would provide the network with more examples and greater variability, allowing it to better learn the characteristics of the methane sources and, consequently, make more accurate predictions.

Consiglio Nazionale delle Ricerche

[1] Cuomo et al. (2022), GSC, doi: 10.1007/s10915-022-01939-z
[2] Masiello et al. (2024), JQSRT, doi:10.1016/j.jqsrt.2023.108814
[3] Serio et al. (2019), JQSRT, doi: 10.1016/j.jqsrt.2018.10.020

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