Machine Learning-Based Observation Operators to Assimilate Microwave and SIF Satellite Observations into the ECMWF Integrated Forecast System (IFS)

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CORSO
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Outlines

1. Introduction
2. Methodology
3. Active microwave (ASCAT) observation operator
4. Solar Induced Fluorescence (SIF) observation operator
5. Conclusion

Introduction

✓ CORSO project: Reducing the uncertainties in the land carbon budget

- large uncertainties in Gross Primary Productivity (GPP) predictions
- constraint both water and carbon fluxes=> analyze both soil moisture and vegetation variables

✓ Assimilate new type of land satellite observations in the Integrated Forecast System (IFS)

- Level-1 active microwave observations
  - sensitive to both vegetation structure (Petchiappan et al., 2021) and soil moisture (Wagner et al., 2013)
  - more accurate representation of uncertainties compared to retrievals
- Solar Induced Fluorescence (SIF)
  - emission of electromagnetic radiation in the red and far-red by ‘*chlorophyl a*’ molecule under visible light
  - directly related to leaf physiological processes (photosynthesis)
  - correlation with both GPP and Leaf Area Index (LAI) (Guanter et al., 2014; He et al., 2017)

Introduction

✓ Observation operator

- Predict model-simulated counterpart of the satellite observation using the IFS fields as predictors
- Physically based observation operator: large uncertainties over land, complex and computationally expensive,
- ML alternative
  - Generic architectures can be applied to different types of EO
  - Computationally more efficient
  - Quickly test the assimilation of new types of observation

✓ Challenges

- Design simple and robust observation operator for their integration in the IFS at global scale
- Is the information content of the Earth System model fields sufficient to simulate the satellite signal ?
- How to ensure enough sensitivity to the input fields that we want to analyse (LAI, GPP)
- How to represent the uncertainties in the predictors and the output?
- Importance of localization : use latitude and longitude in the predictors ?

Methodology to design the ML-based observation operator

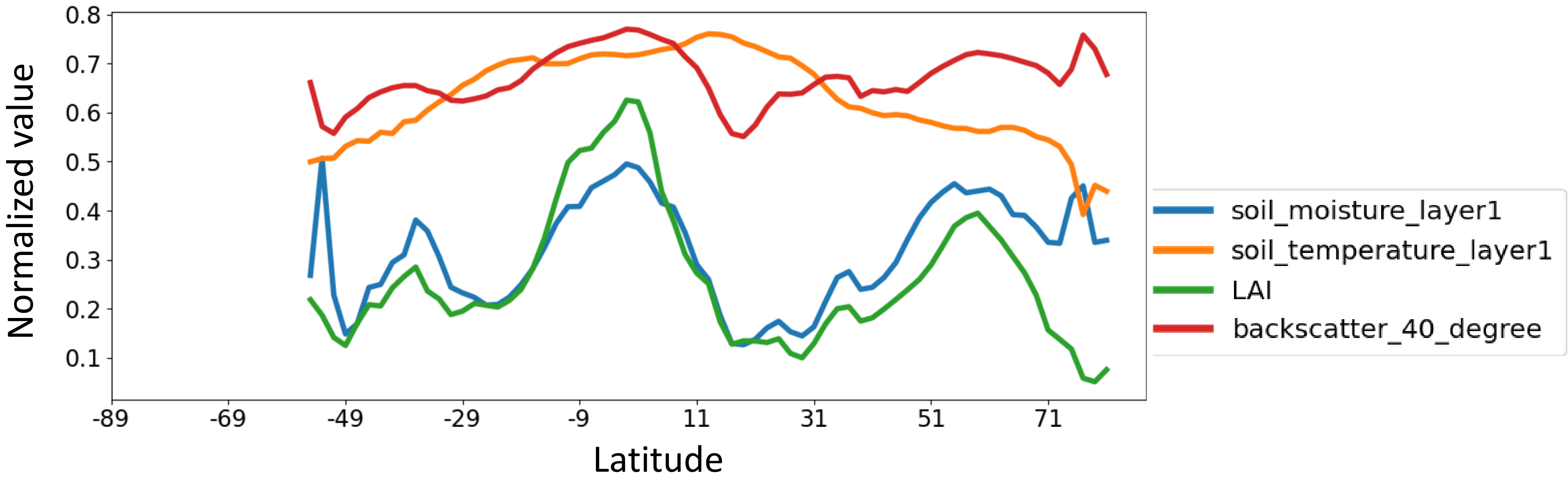
- **Training database**:
  - collocated observation and model fields in the observation space
  - quality control and filtering (snow, frozen soil, orographic surface…)
- **Feature selection**
  - process-based knowledge
  - XAI methods (e.g. SHAP)
- **ML model**:
  - Gradient boosted trees (XGBOOST, Chen et al., 2016) (XGB)
  - Feedforward neural network (NN)
- **Training and hyperparameter** tuning (training and validation set)
- **Evaluation on test set** (temporal profile, spatial distribution, gradient)
- **Implementation and test in IFS – data assimilation experiments**

ASCAT observation operator: Training database

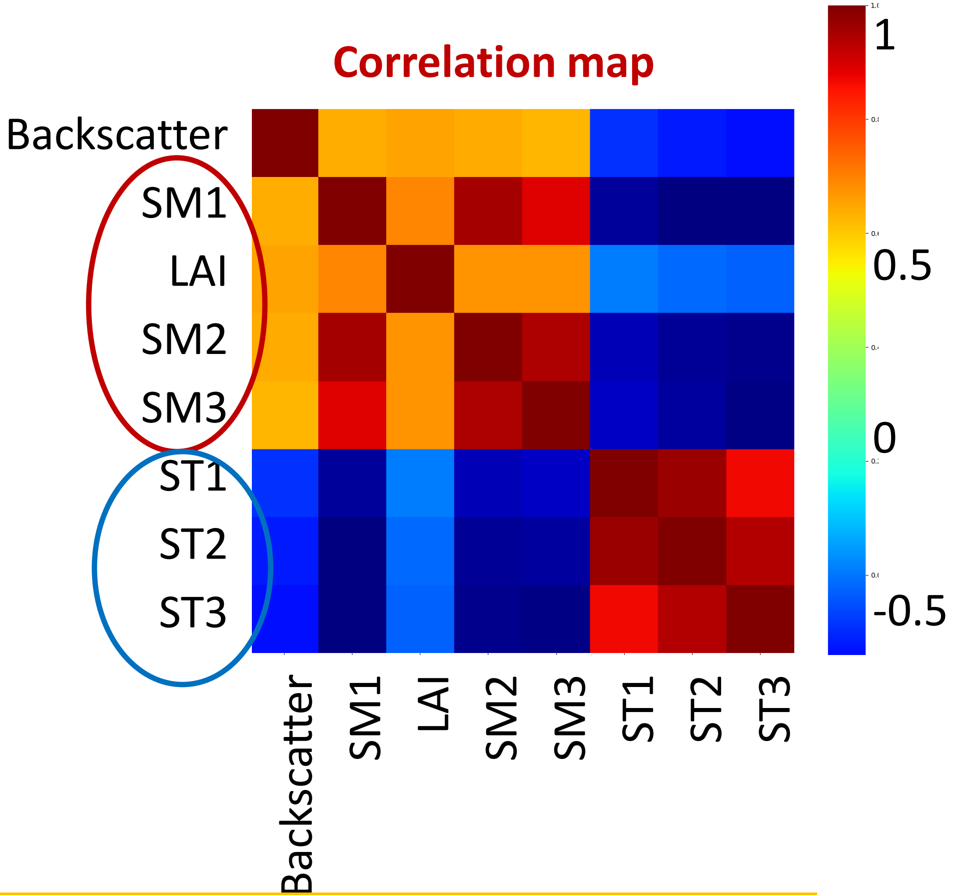
Training database (Aires, et al., QJRS 2021)

- target: ASCAT backscatter normalized at 40°
- model fields (features) from ERA-5: Leaf Area Index (LAI), soil moisture (SM) (3 layers), soil temperature (ST) (3 layers)
- localization : Latitude, longitude (sin/cos transform)
- period: 2016-2018 (training and validation), 2019 (testing)
- resolution: 0.25° grid.

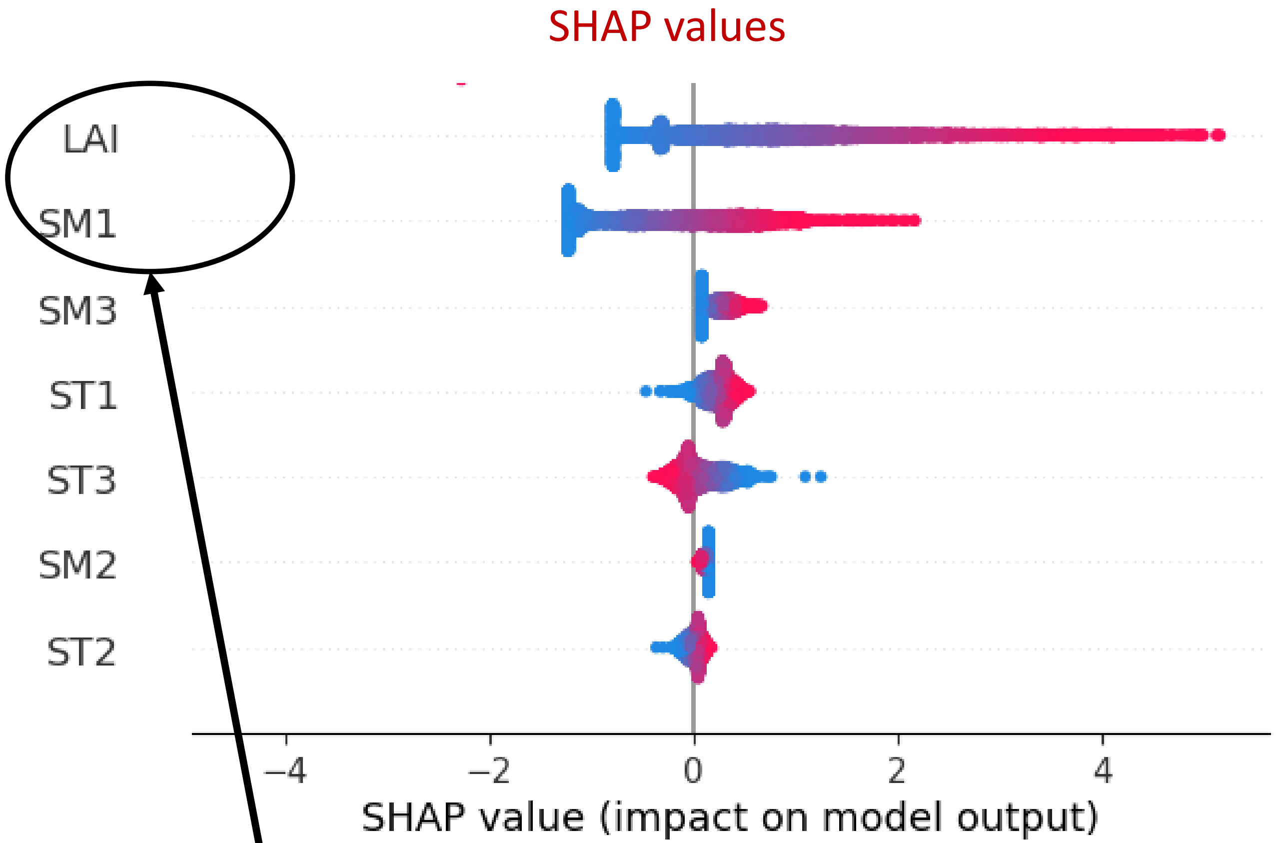
Latitude transect



ASCAT observation operator: Information content and explainability analysis



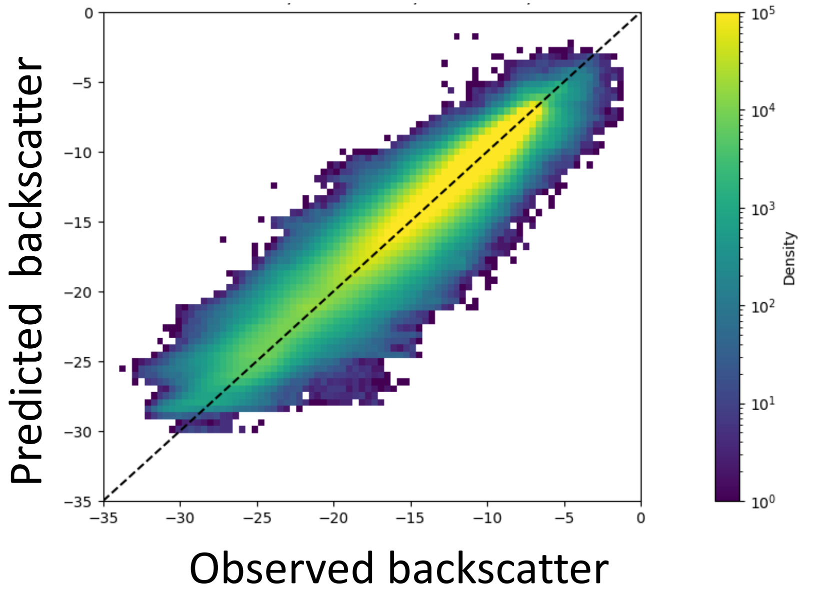
Contrasted correlation with backscatter:
- SM, LAI: positively correlated
- ST: negatively correlated



Vegetation (LAI) and surface soil moisture (SM1) are the most influent variables

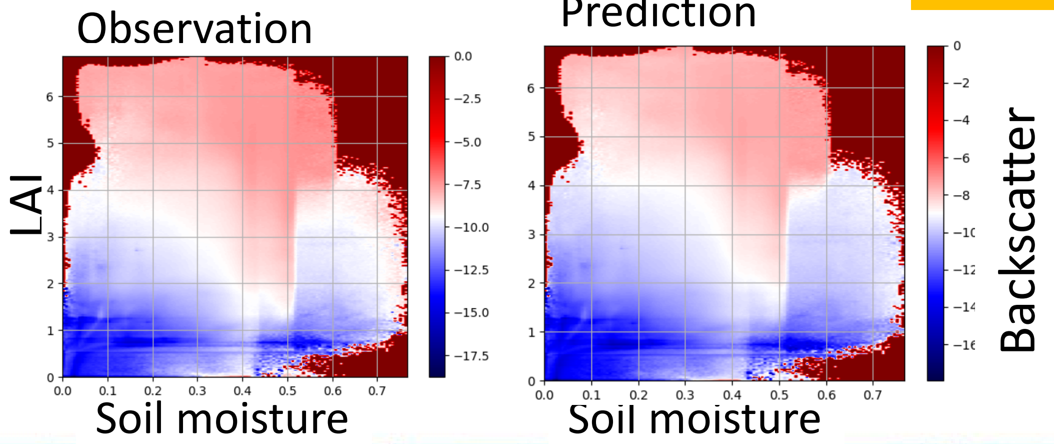
ASCAT observation operator: Performance evaluation

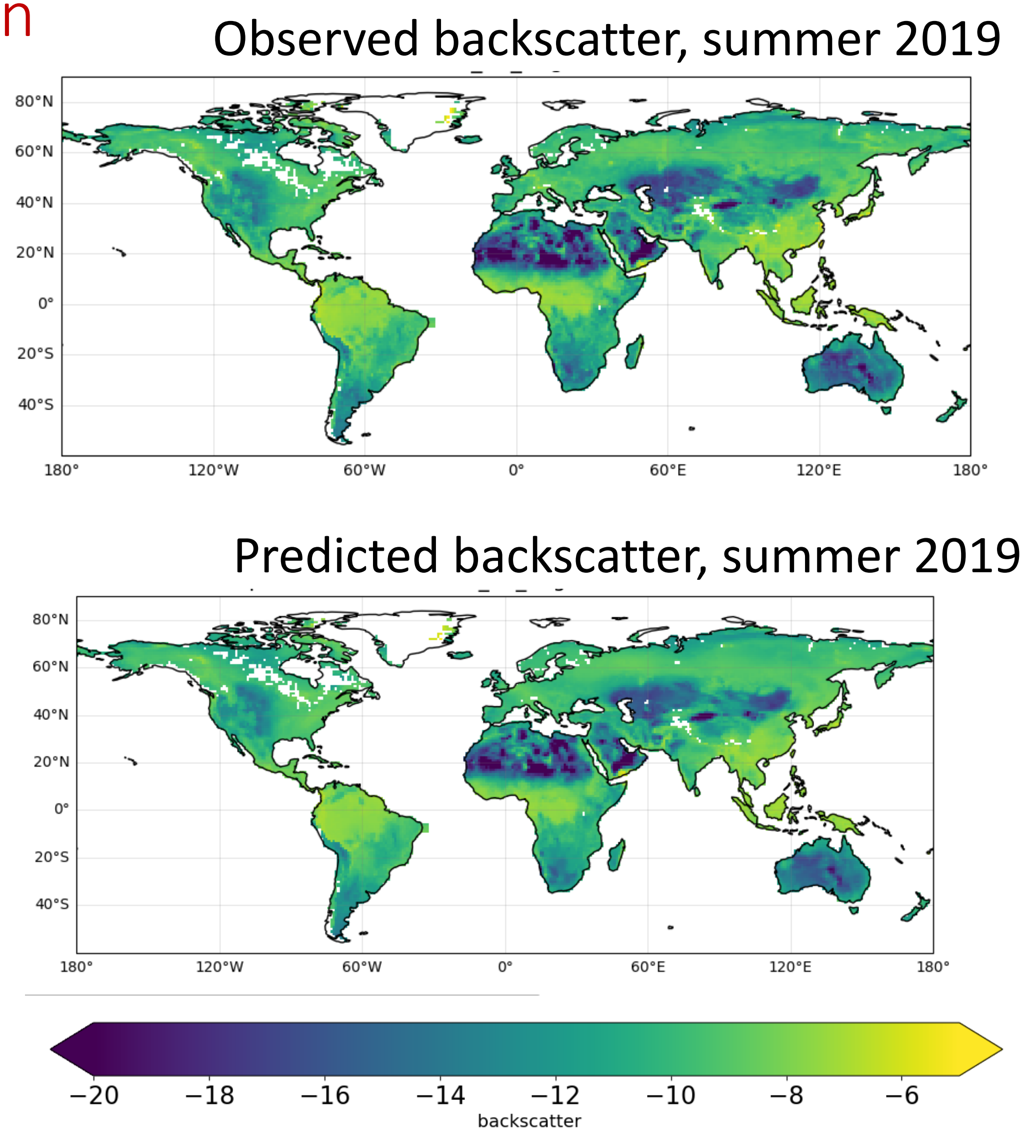
Test: R^2=0.93; RMSE=0.87;MAE=0.78;SD=0.87



NN model:
3 years training,
4 hidden layers,
60 neurons,
global scale

Good training and generalization performances

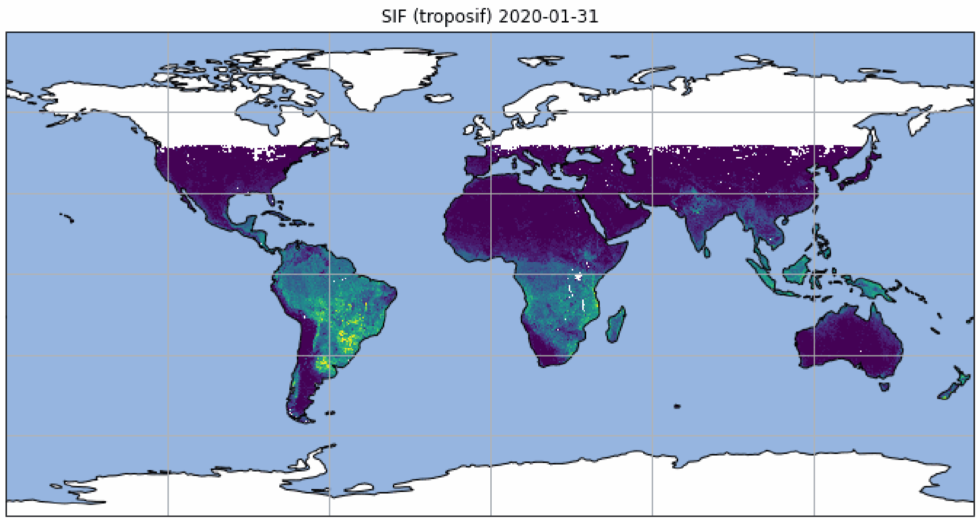




SIF observation operator: Training database

✓ Data

- Predictors: fields from ECLand land model offline simulations (IFS Cyc49r1)
- Target: SIF at 740nm satellite observations from TROPOMI/Sentinel-5p, Troposif dataset (Guanter et a., ESSD 2021)
- Resolution: 0.1° grid and at 8-day temporal frequency
- Filters: Large view and solar zenith angles, orography area, snow area, frozen soil
- Training: 2019-2020; Validation:2021; Test:2022



SIF observation operator: Feature selection

SIF canopy drivers

$$SIF_{canopy} = \underbrace{f_{esc} \quad x \quad APAR}_{\text{Canopy structure (LAI)}} \quad x \quad \phi_F$$

Canopy structure (LAI)

Leaf physiological characteristics (GPP)

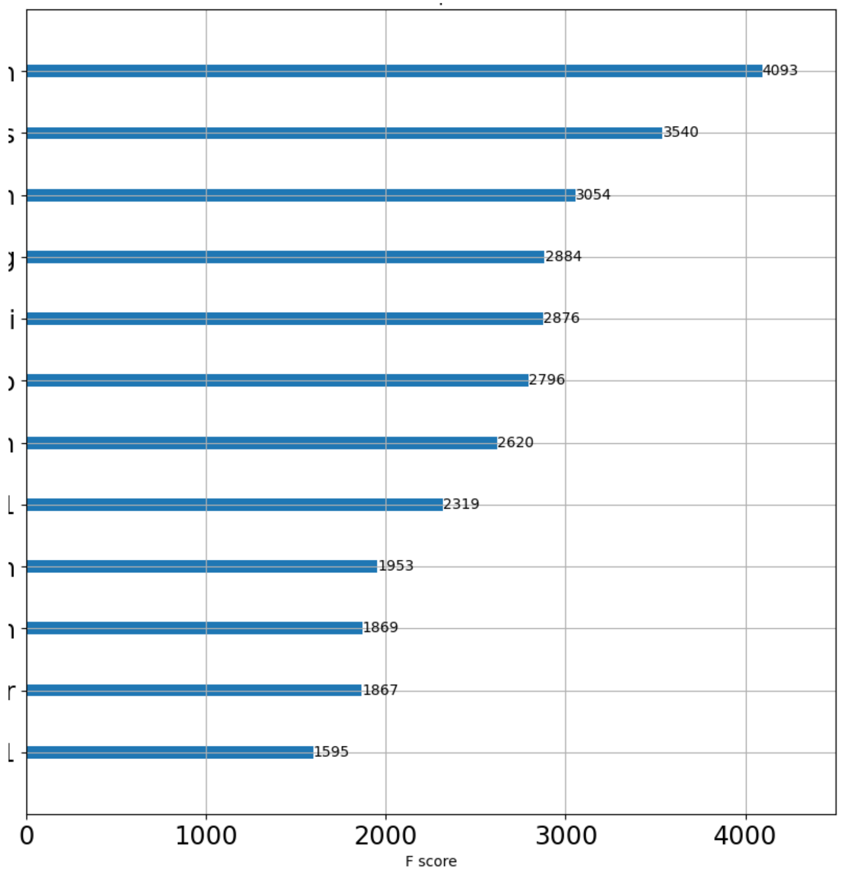
Regulated by environmental factors:
soil moisture, solar radiation, 2m temperature and humidity

+ Temporal dependency: week of the year (cyclic transform)

Feature importance (xgboost)

features

SWDOWN
TIME
D2M
MEAN OROG
LAI
GPP
TIME
SM1
T2M
1m SM
SD OROG
ST1

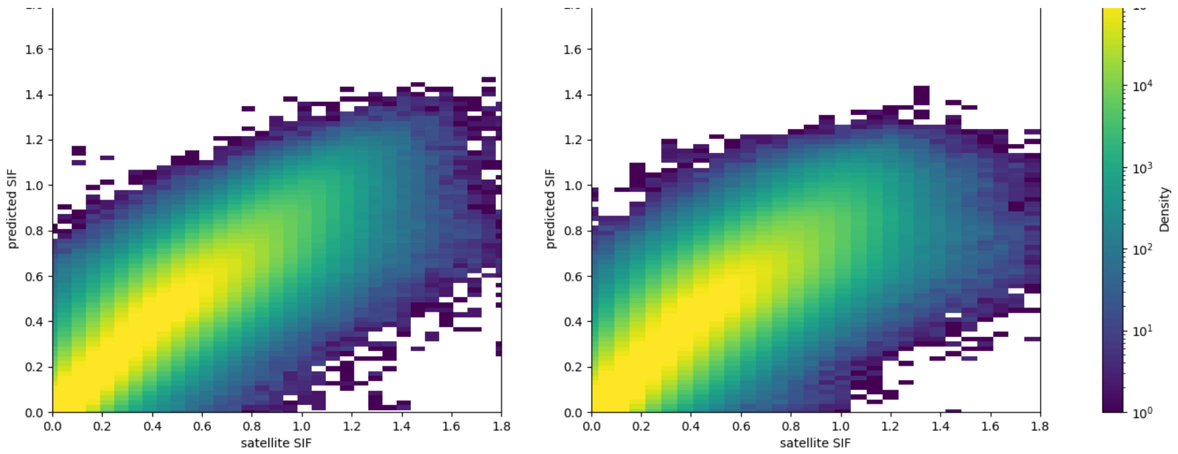


SIF observation operator: ML model comparison

Training year=2019-2020, test=2022

Training R^2=0.88, RMSE=0.09, MAE=0.25

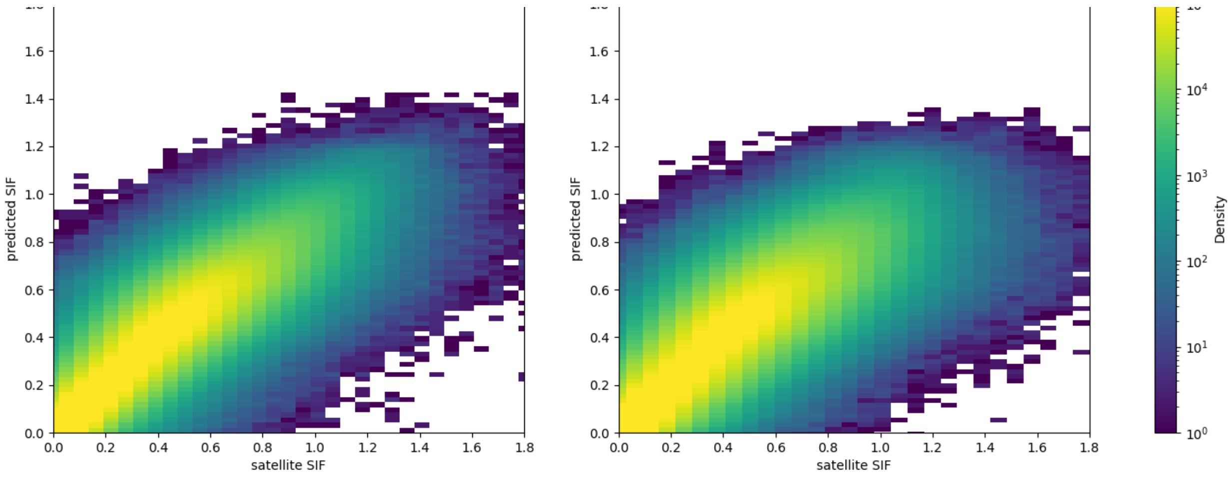
Test R^2=0.85, RMSE=0.1, MAE=0.26



XGBOOST (ntrees=500, optimized hyperparameters)

Training R^2=0.87, RMSE=0.09, MAE=0.25

Test R^2=0.84, RMSE=0.1, MAE=0.27



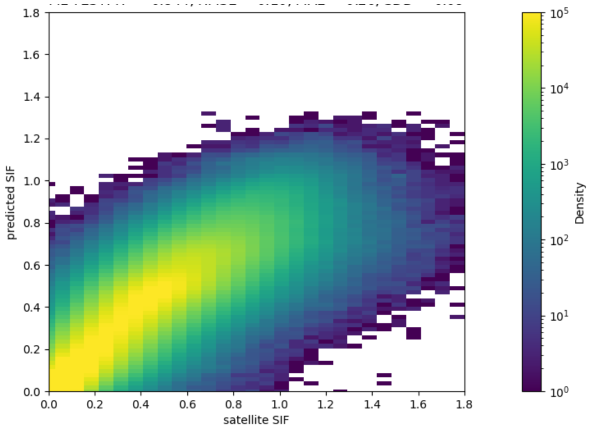
Feedforward NN (6 layers, 60 neurons, batch size=128, lr=0.001)

Equivalent performances between XGBOOST and NN

SIF observation operator: Global vs vegetation type ML model

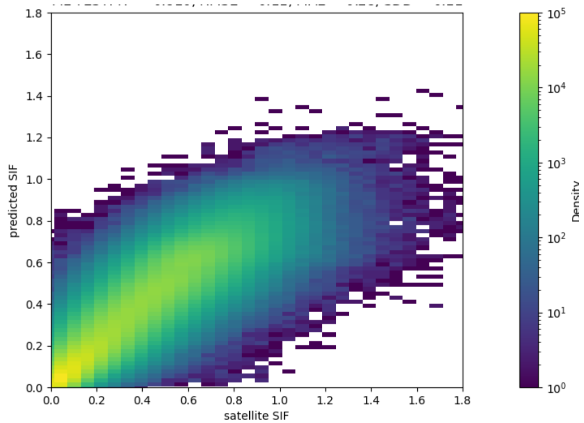
global

R^2=0.85, RMSE=0.1, MAE=0.26



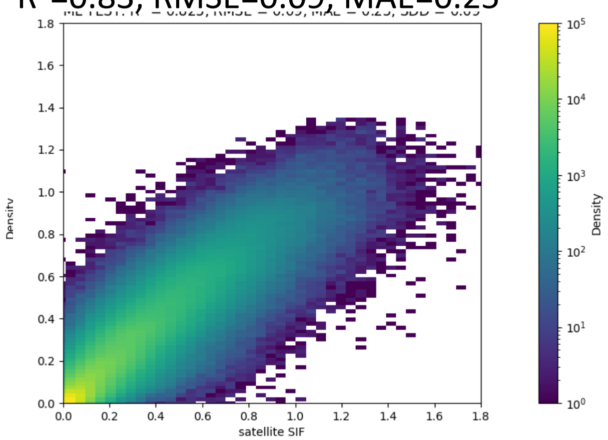
crop

R^2=0.82, RMSE=0.11, MAE=0.28



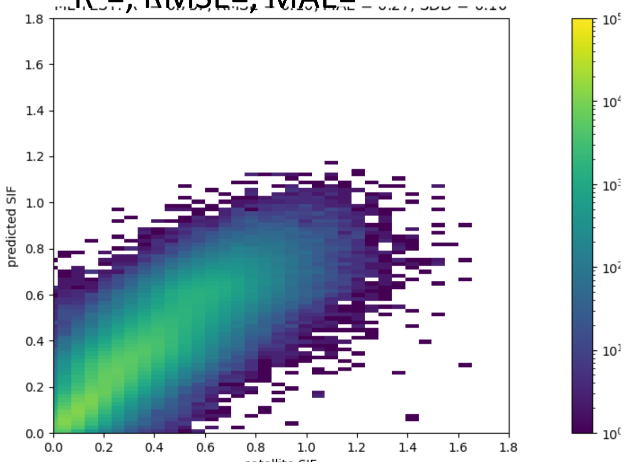
grassland

R^2=0.83, RMSE=0.09, MAE=0.25



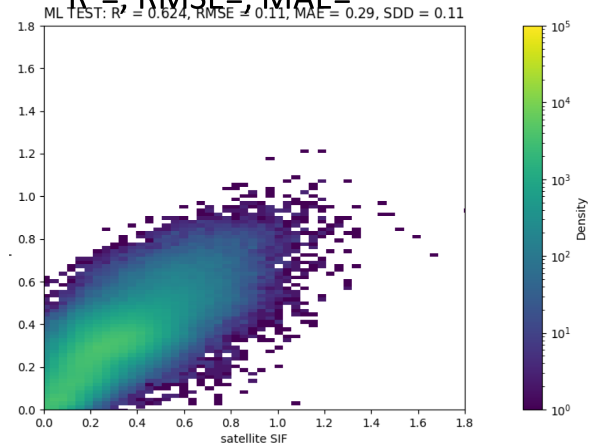
ENF

R^2=, RMSE=, MAE=



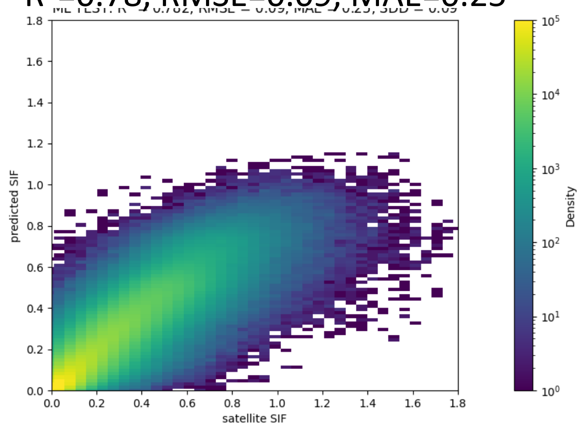
DNF

R^2=, RMSE=, MAE=



Shrubland

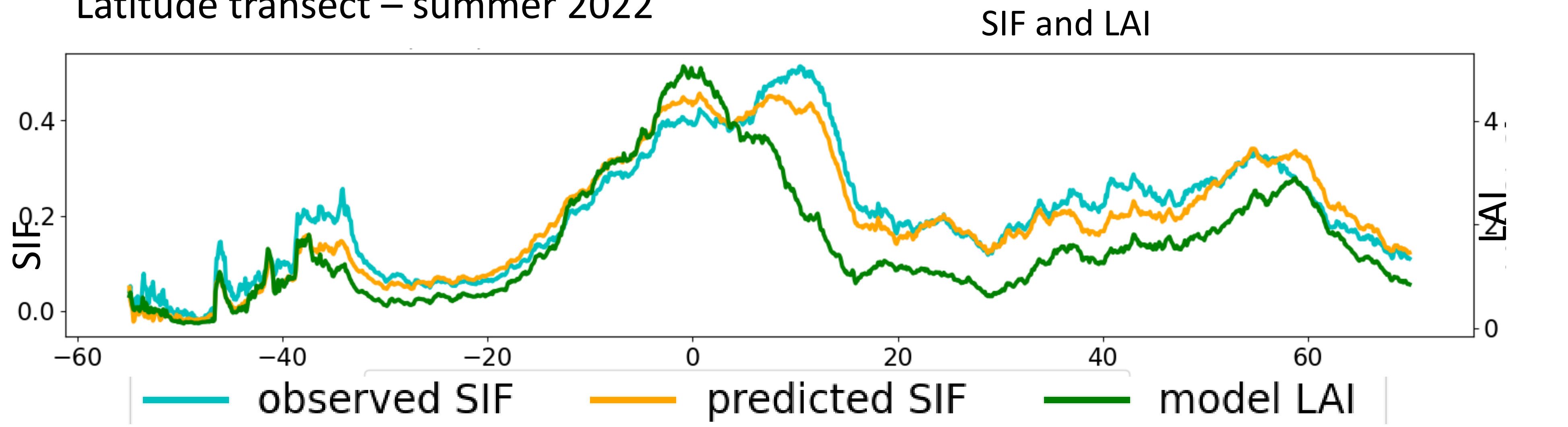
R^2=0.78, RMSE=0.09, MAE=0.25



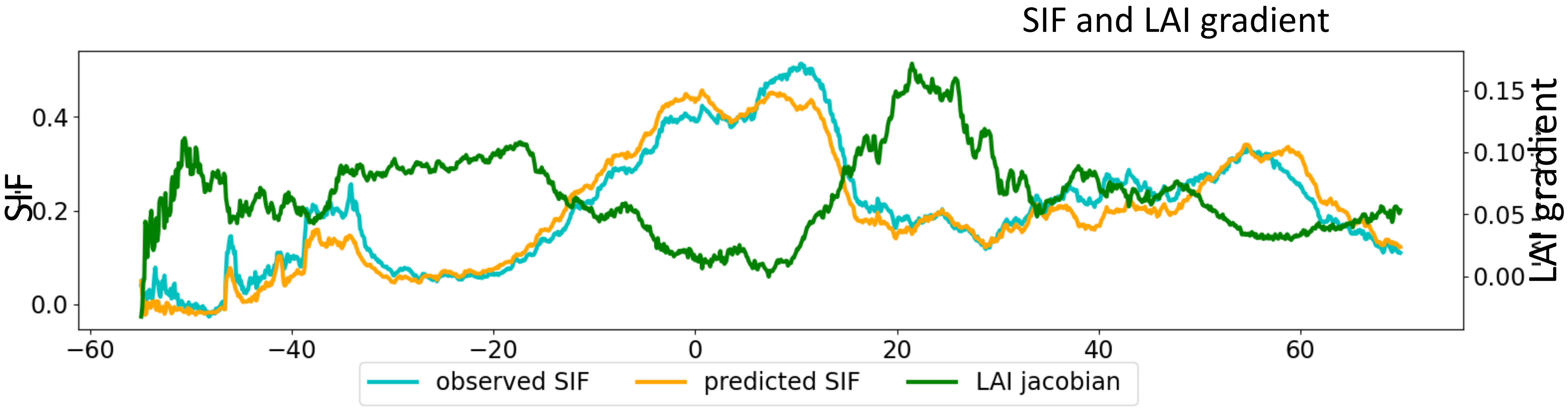
Little benefit of training the model on distinct vegetation types

SIF observation operator: Evaluation

Latitude transect – summer 2022



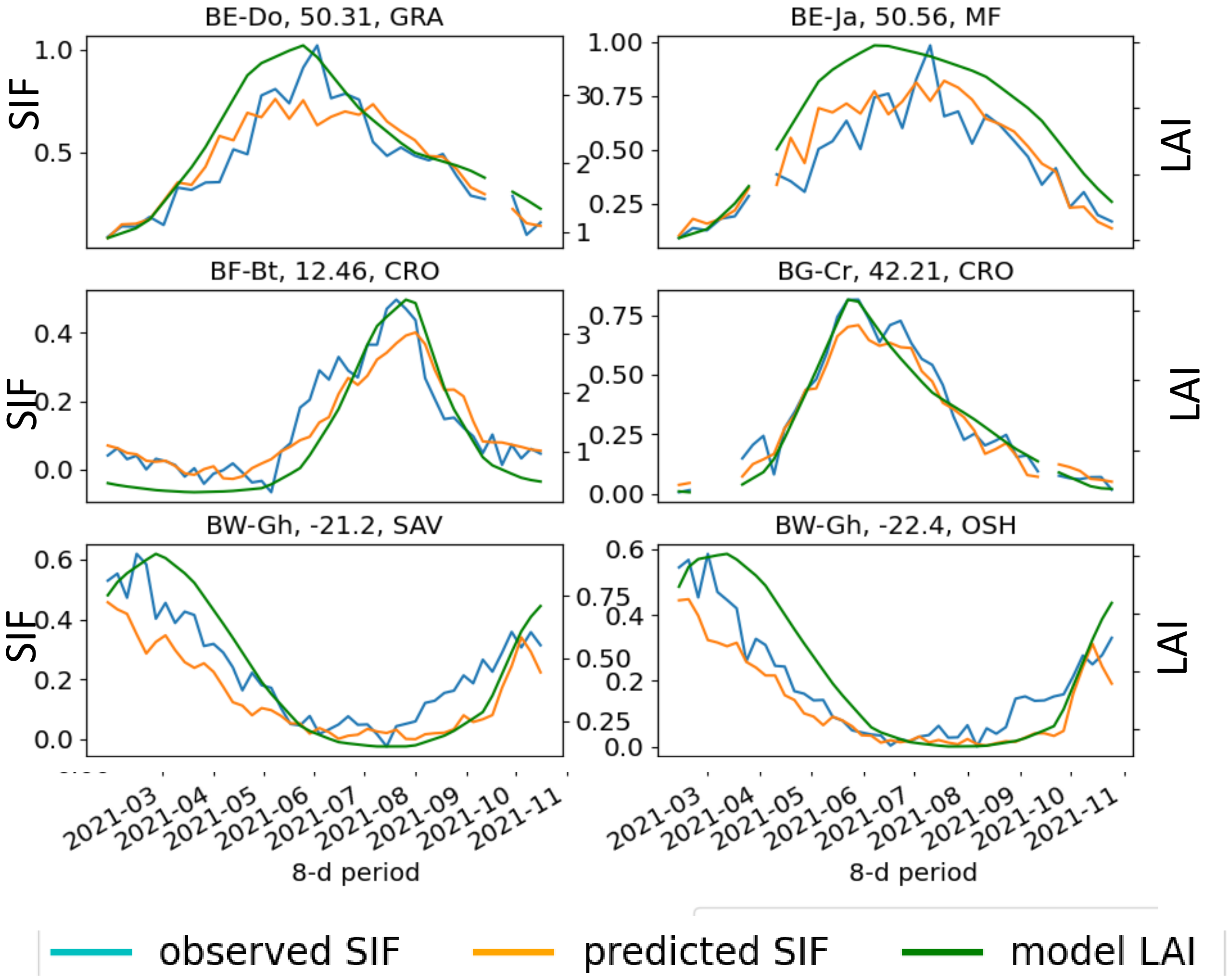
Accurate prediction of SIF spatial distribution



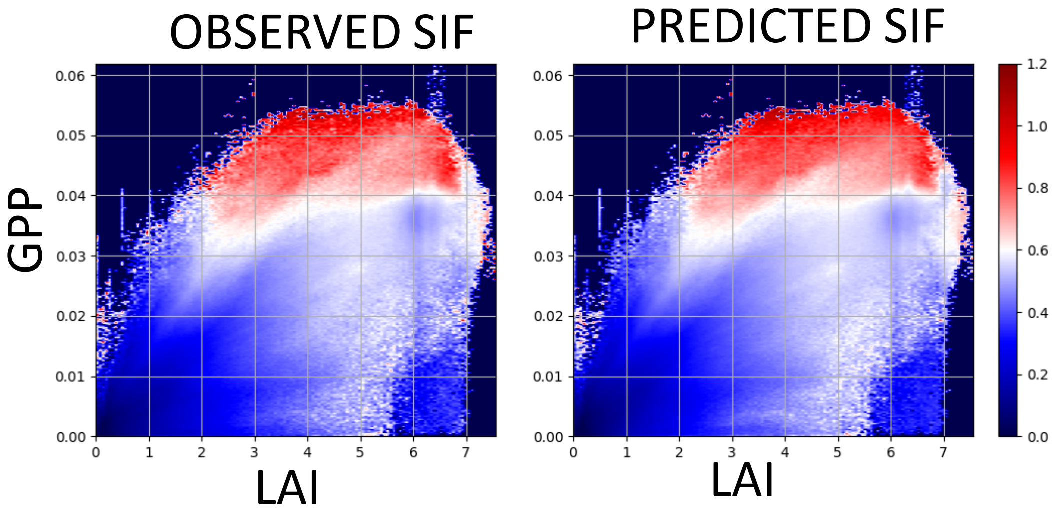
Good sensitivity to LAI

SIF observation operator: Evaluation

Seasonal evolution



GPP and LAI patterns



Accurate prediction of
- SIF seasonal evolution
- SIF patterns in GPP vs LAI spaces.

Conclusions

- **Simple feedforward NN** provides **accurate enough prediction of backscatter and SIF** satellite signals from the **ECMWF/IFS NWP model fields**

- Nex step : **test the assimilation in the IFS** and **evaluate the impact** on carbon fluxes, water fluxes and NWP near surface variables

- **ML-based observation operator** allows to **quickly test the assimilation** of **new types of observations, generic framework can be applied to other observations** (e.g. passive microwave observation)

- **Challenges and lesson learned**
  - Important to evaluate the sensitivity of the input fields that will be analyzed
  - Representation of uncertainties in both input features and satellite target
  - Risk of overfitting due to the use of latitude and longitude

Thanks for your attention

Acknowledgements

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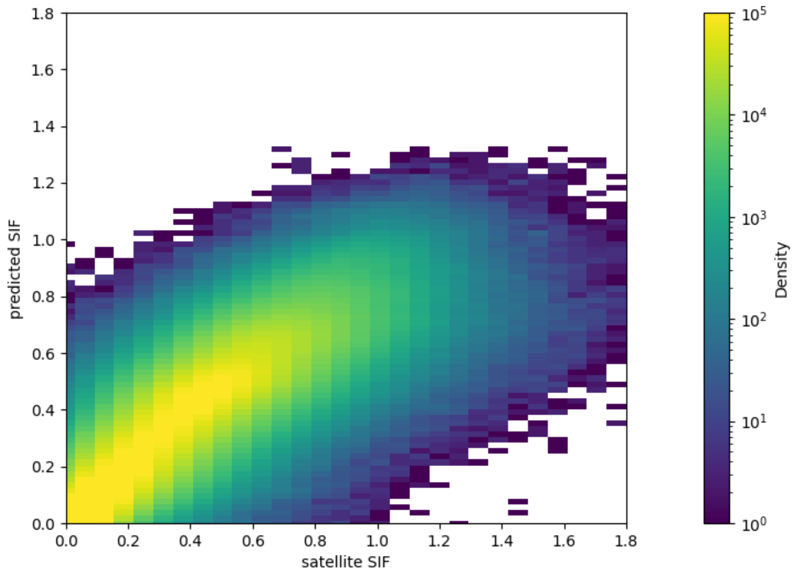
SIF observation operator: Impact of target variable

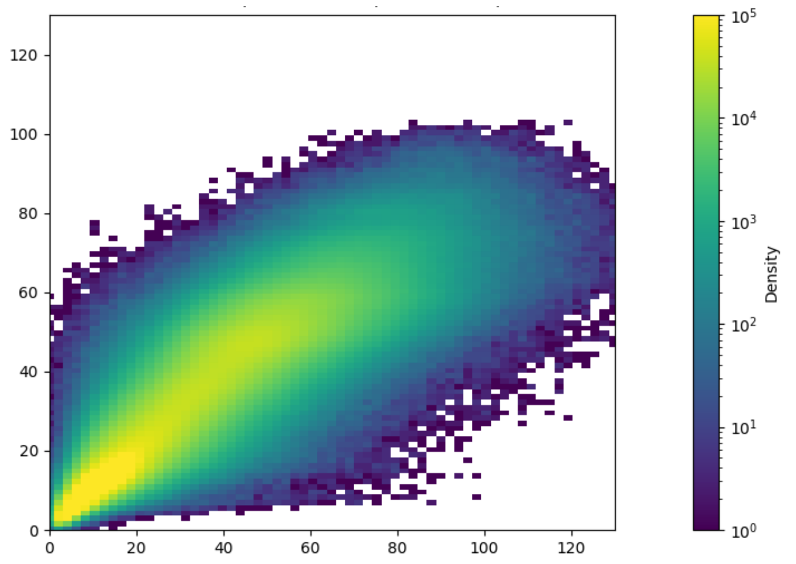
Target= SIF

Target= NIRVp (product of the near infrared reflectance of vegetation (NIR_V) over the NIR region and incoming PAR

R^2=0.85, RMSE=%, MAE=%



R^2=0.86, RMSE=%, MAE=%



SIF signal is more moisy than NVIRp
=> Reduced prediction performances