

Inferring High-resolution Near-surface NO₂ Concentrations over Belgium through Convolutional Neural Networks

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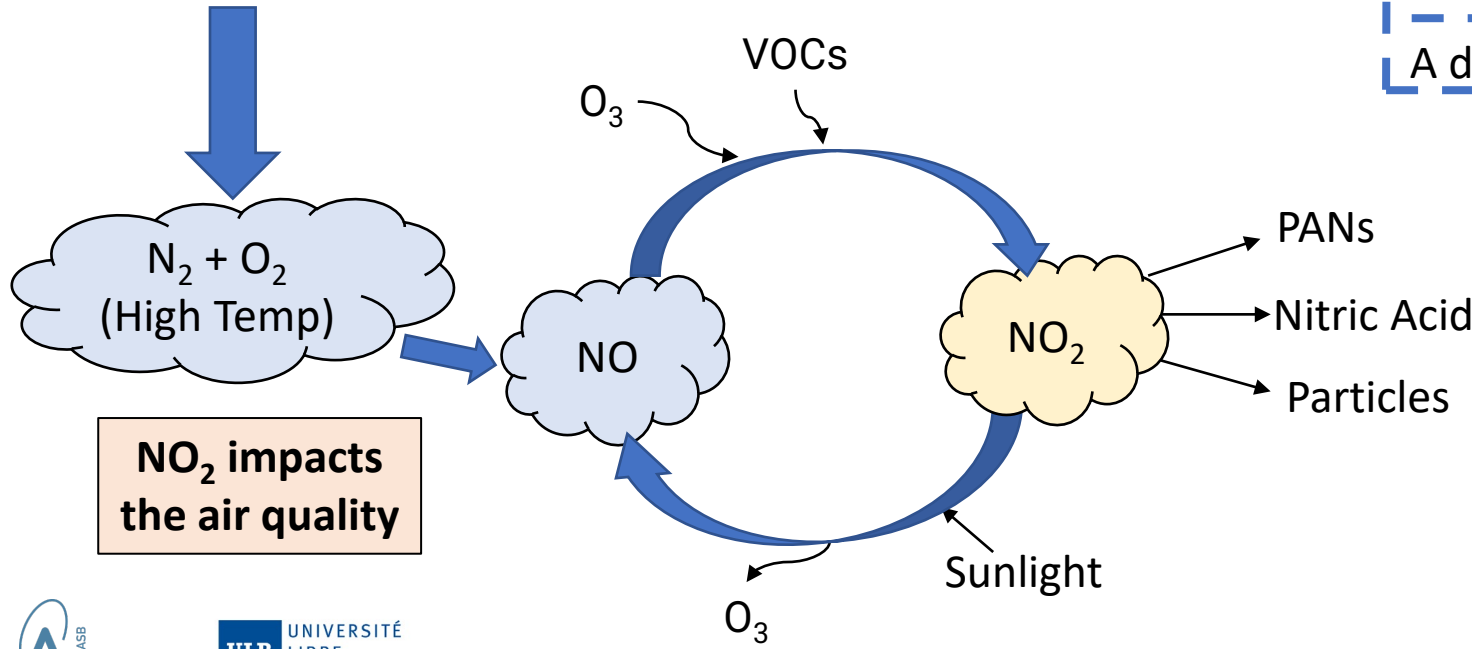
Concerns about NO₂



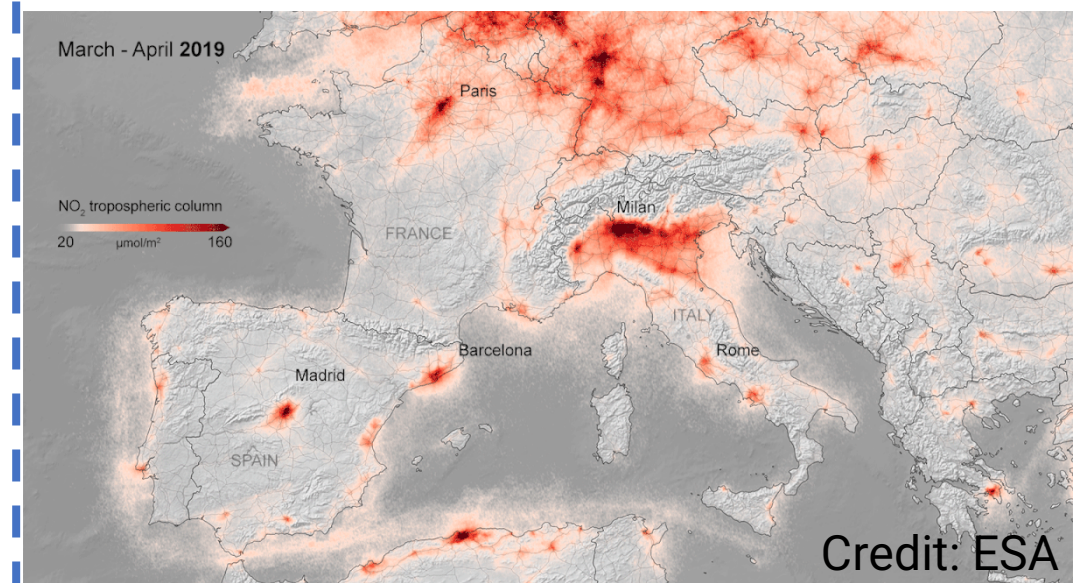
PATHWAY	HEALTH EFFECTS
Exposure to NO ₂ comes from the air we breathe.	Impacts: <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  respiratory system </div> <div style="text-align: center;">  cardiovascular system </div> </div>
	Groups most at risk: <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  elderly </div> <div style="text-align: center;">  those with lung disease </div> <div style="text-align: center;">  children </div> </div>

NO₂ health effects

<https://www.epa.vic.gov.au/for-community/environmental-information/air-quality/nitrogen-dioxide-in-the-air>



A dramatic decrease in NO₂ during the Covid-19 outbreak



Inferring NO₂ near-surface concentrations

Surface NO₂ is of great concern due to its adverse impacts on air quality and human health

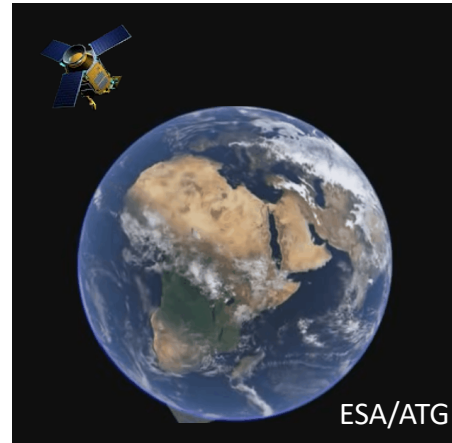
Measurements

- 😊 Accurate and consistent estimations
- 😞 Limited spatial coverage



Satellite observations

- 😊 Large spatial coverage
- 😞 Limited temporal resolution
- 😞 Coarse spatial resolution
- 😞 Low sensitivity to surface NO₂

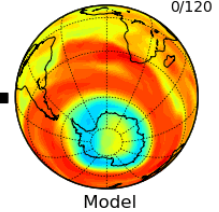
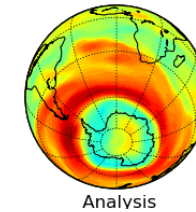
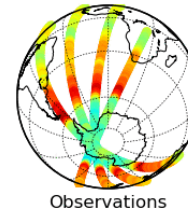


Ancillary datasets

Meteorology Emissions Society
Land information

Physical method

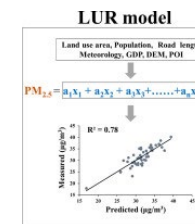
- 😊 Good knowledge (physics and chemistry)
- 😊 Can be constrained by reality (data assimilation)
- 😞 Computationally intensive, coarse spatial resolution
- 😞 Biases caused by mechanism and EMI inventories



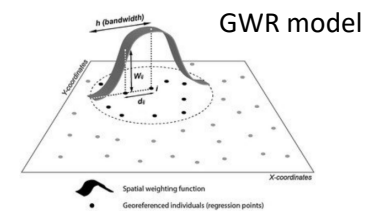
<https://www.issibern.ch/teams/dataassimsphere/>

Empirical statistical method

- 😊 Flexible modeling and can achieve high resolution
- 😞 Limited ability for very complex nonlinear relationship



Mo et al., *Sci. Total Environ.*, (2021)



Feuillet et al., *Int. J. Health Geogr.*, (2015)

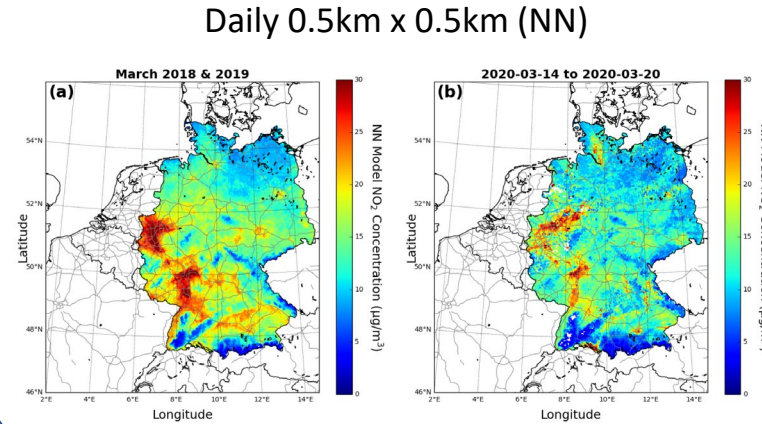
Inferring NO₂ near-surface concentrations by machine learning

Current ML methods

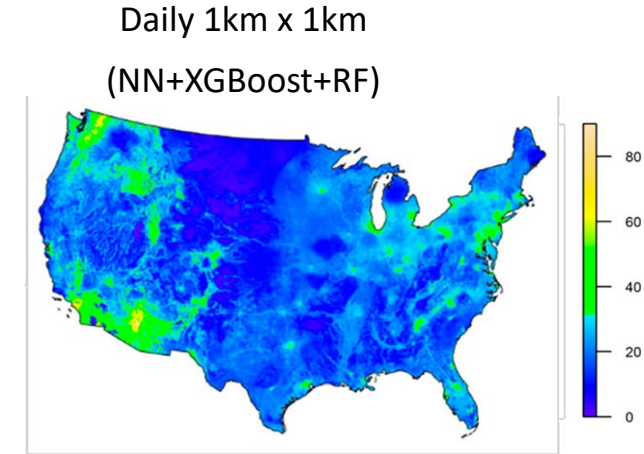
- Random Forest (RF)
- eXtreme Gradient Boosting (XGBoost)
- Neural Network (NN)
-

Machine learning method

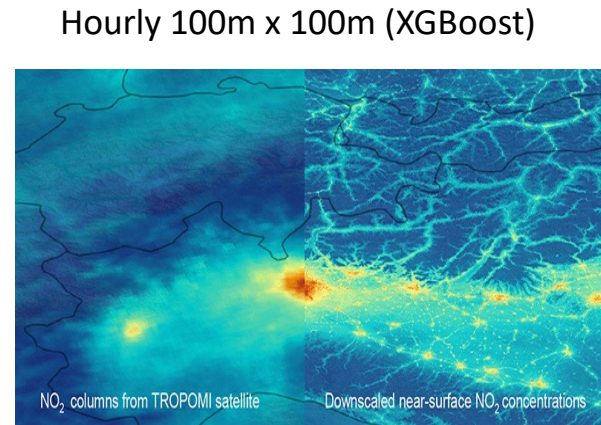
- 😊 Can establish a complex nonlinear mapping
- 😊 High accuracy, efficiency, and fine resolution
- 😞 Risk of manufacturing artifacts when mapping



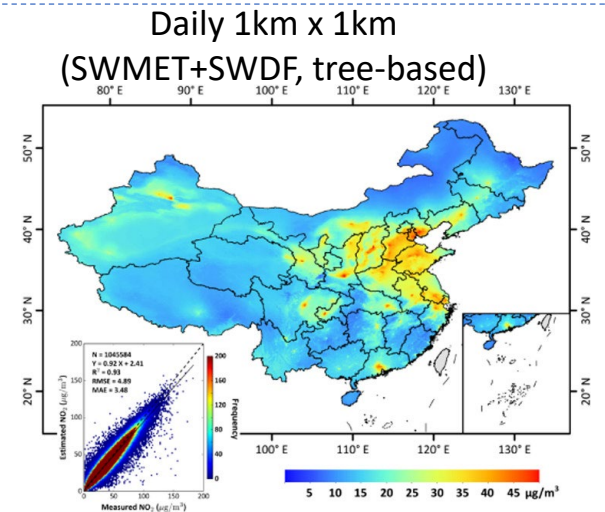
Chan *et al.*, *Remote Sens.*, 2021



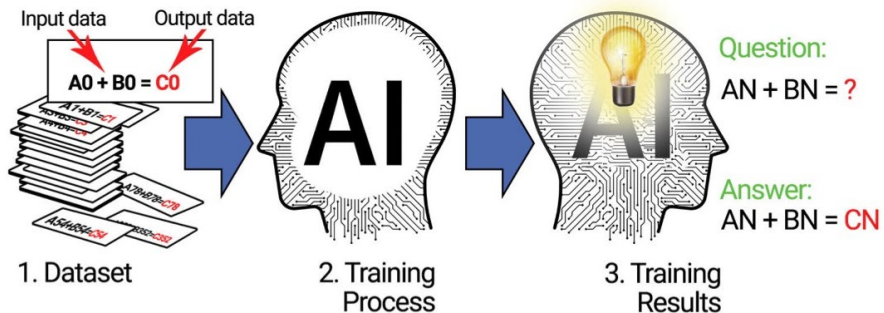
Di *et al.*, *Environ. Sci. Technol.*, 2020



Kim *et al.*, *Remote Sens. Environ.*, 2021

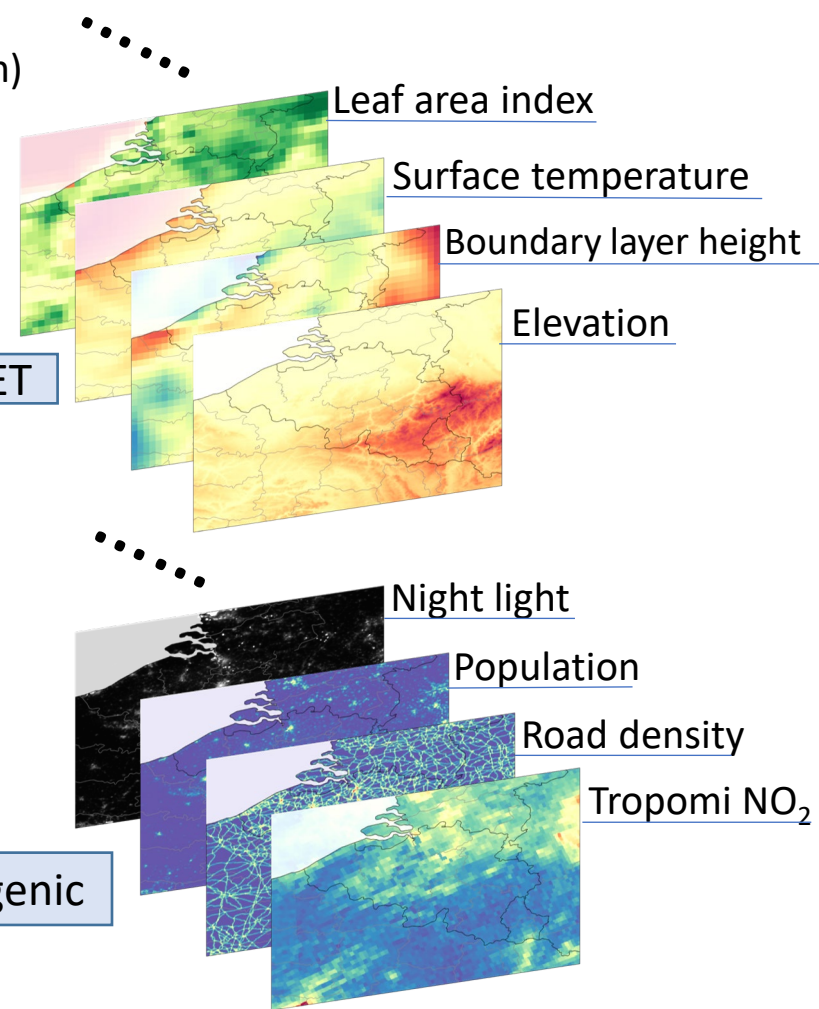


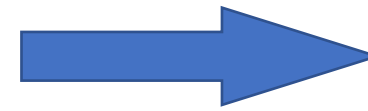
Wei *et al.*, *Environ. Sci. Technol.*, 2022



Surface NO₂ mapping for Belgium by machine learning

Predictor X (23 inputs in total):

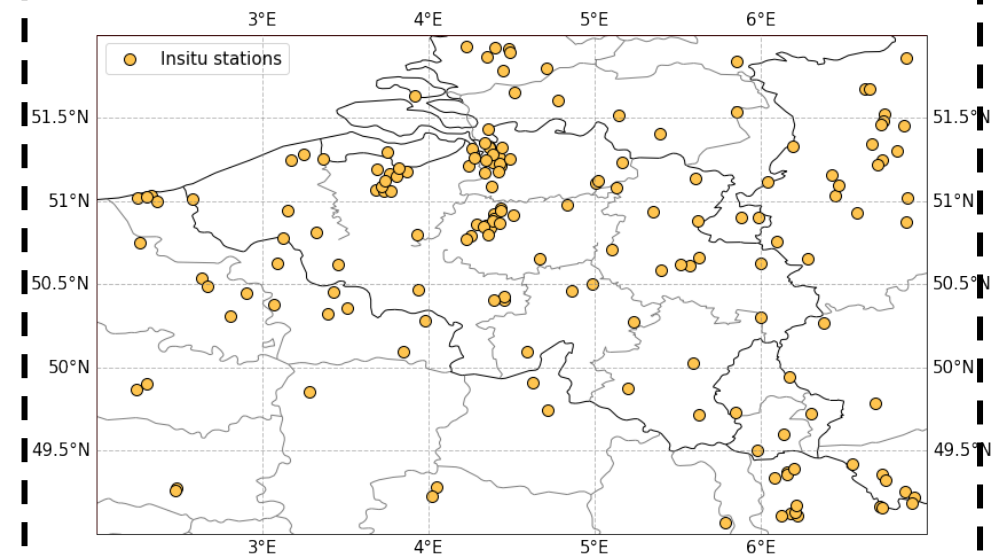
- TROPOMI NO₂ L3 (daily, 1 km)
 - Meteorology:
 - Wind, Temperature, Radiation, Boundary layer height,
 - Leaf area index
 - Land Cover
 - Elevation
 - Emission inventory
 - Road density
 - Population
 - Night light
 - Day of week, Day of year
- MET
- Land
- Anthropogenic
- 



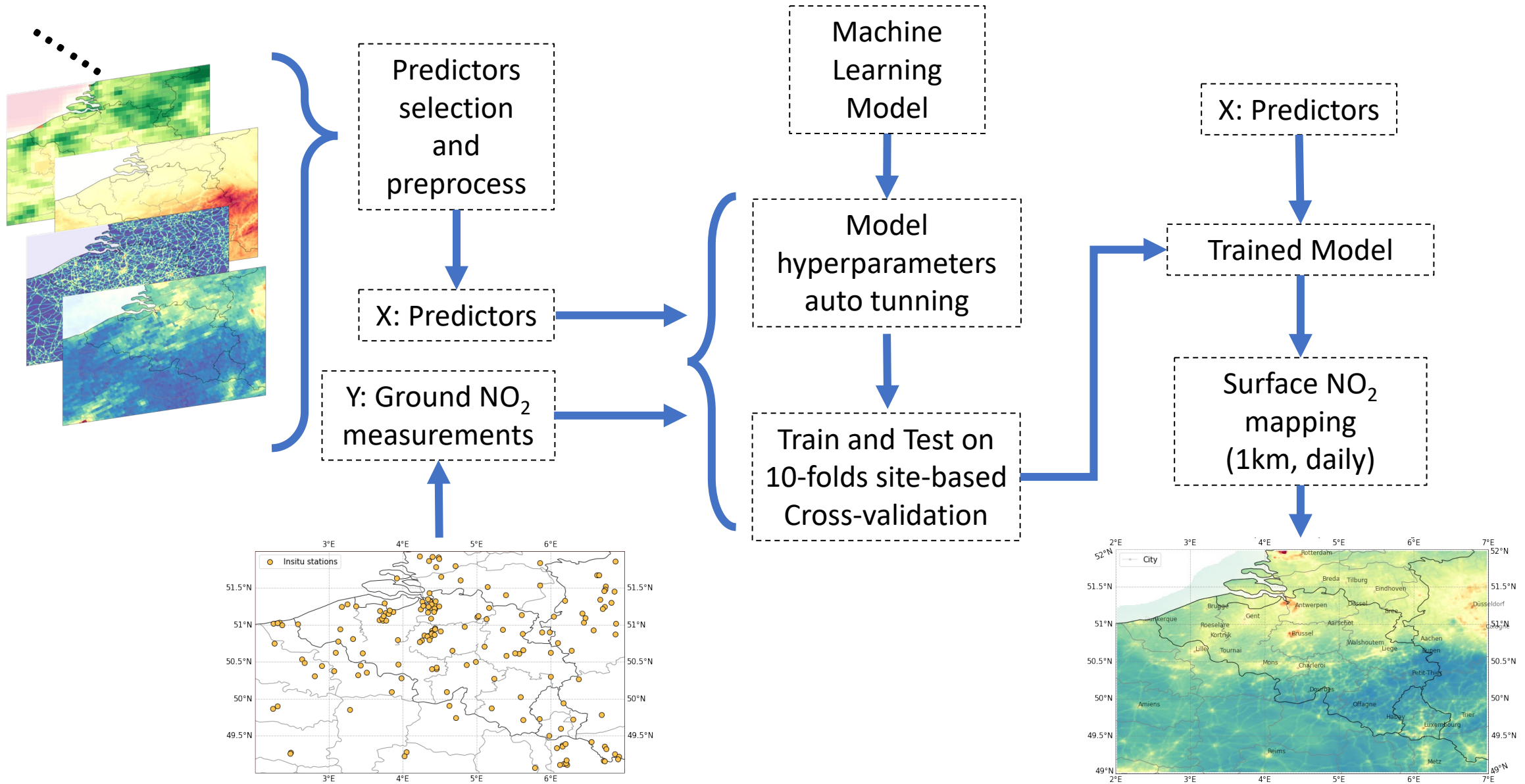
Machine Learning Model

Ground truth Y:

- Ground NO₂ daily measurements (2018-05 ~ 2020-12) (166 stations)

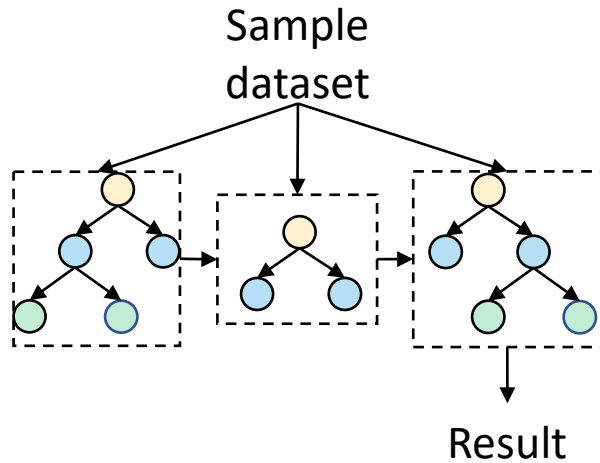


Surface NO₂ mapping for Belgium by machine learning



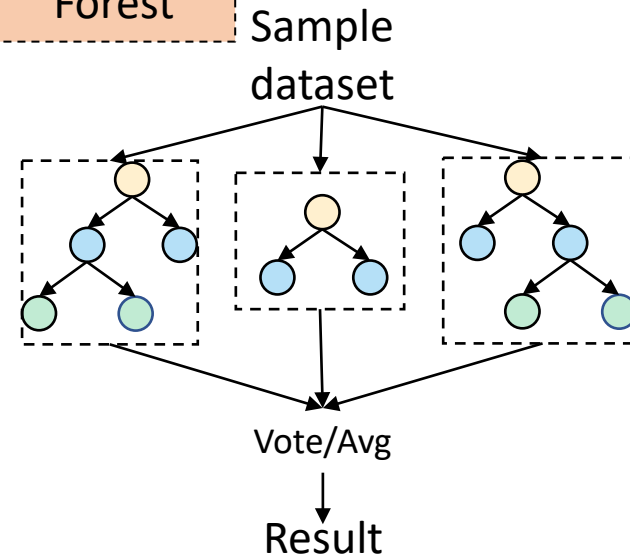
Surface NO₂ mapping for Belgium by machine learning

XGBoost



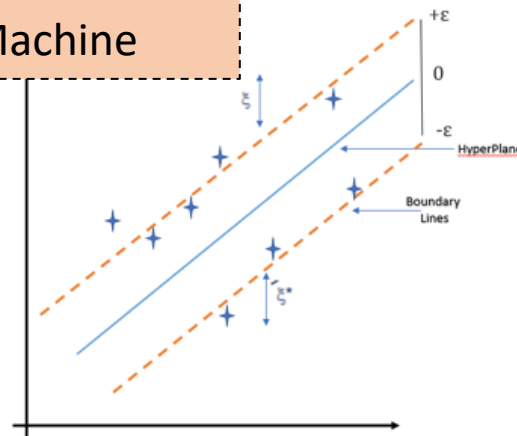
R^2 : 0.74
Pearr: 0.86
RMSE: 5.47
MAE: 4.00

Random Forest



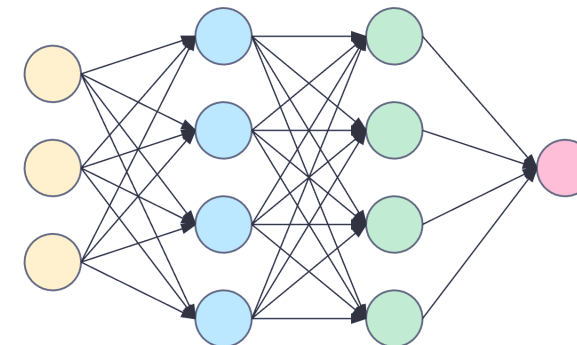
R^2 : 0.59
Pearr: 0.78
RMSE: 6.92
MAE: 5.10

Support Vector Machine



R^2 : 0.62
Pearr: 0.79
RMSE: 6.62
MAE: 4.82

Vanilla Dense Neural Network

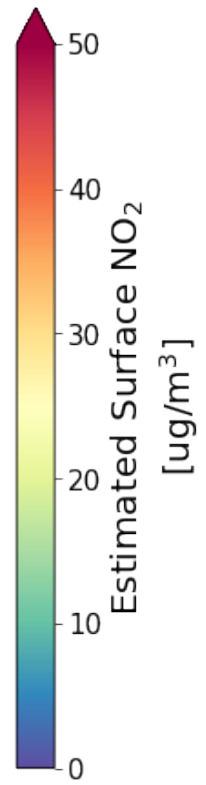
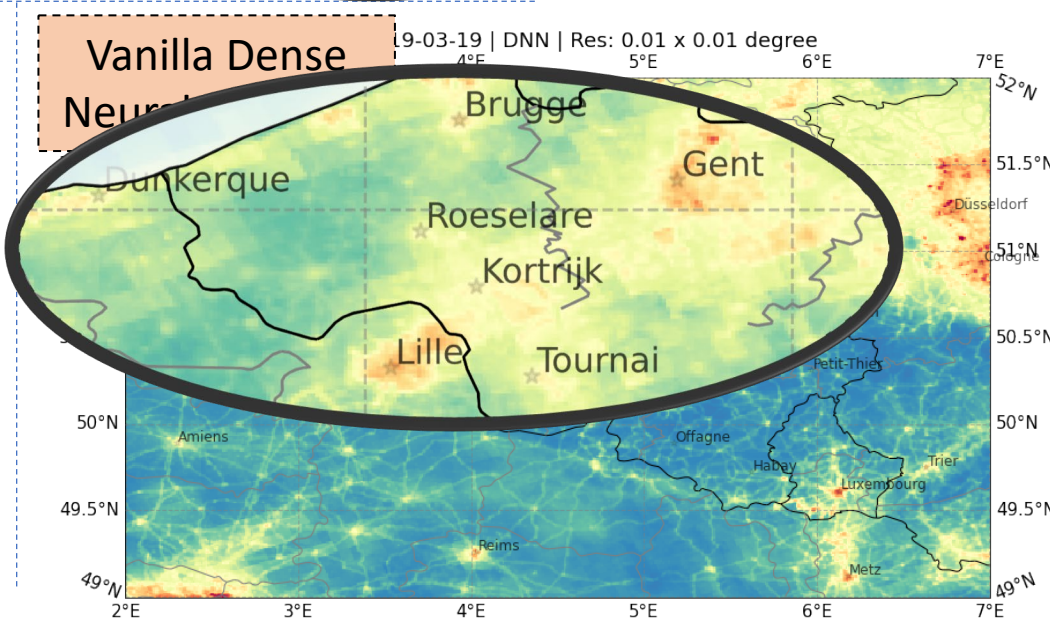
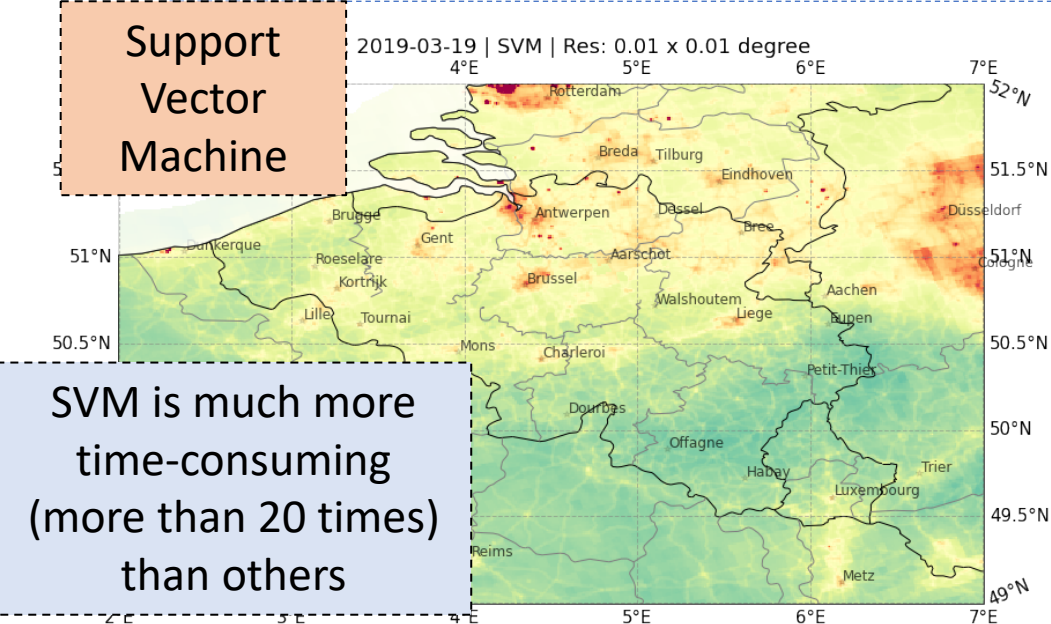
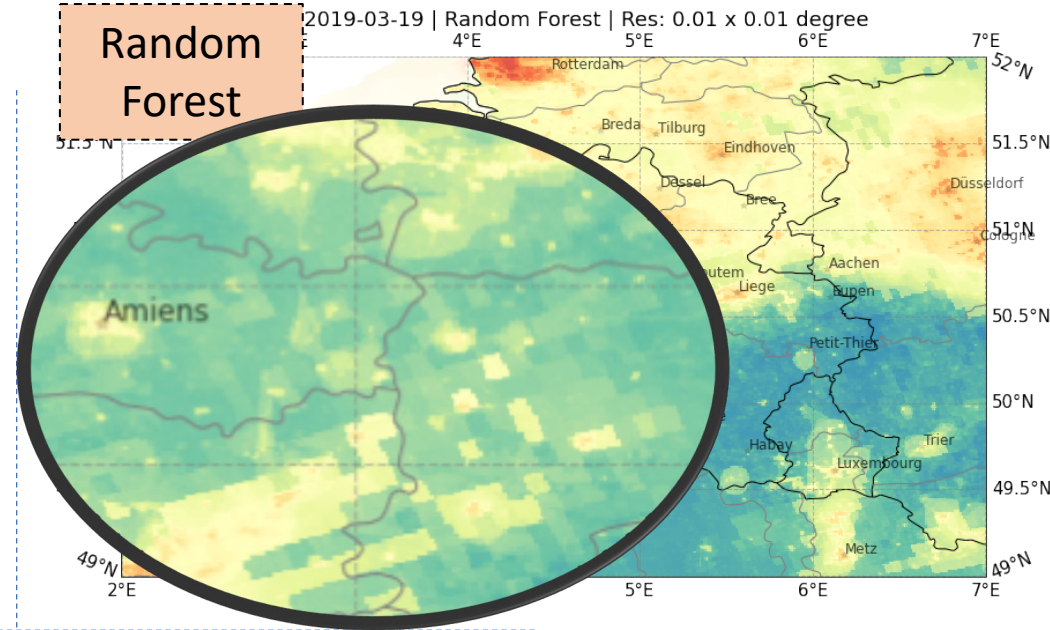
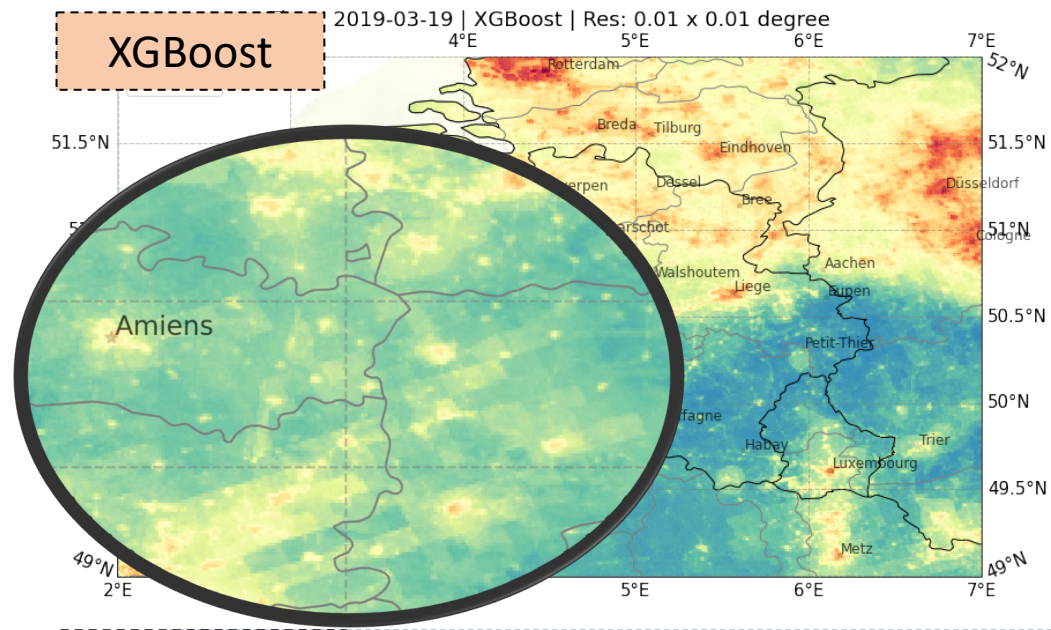


R^2 : 0.65
Pearr: 0.81
RMSE: 6.42
MAE: 4.62

Start with models that used in previous works

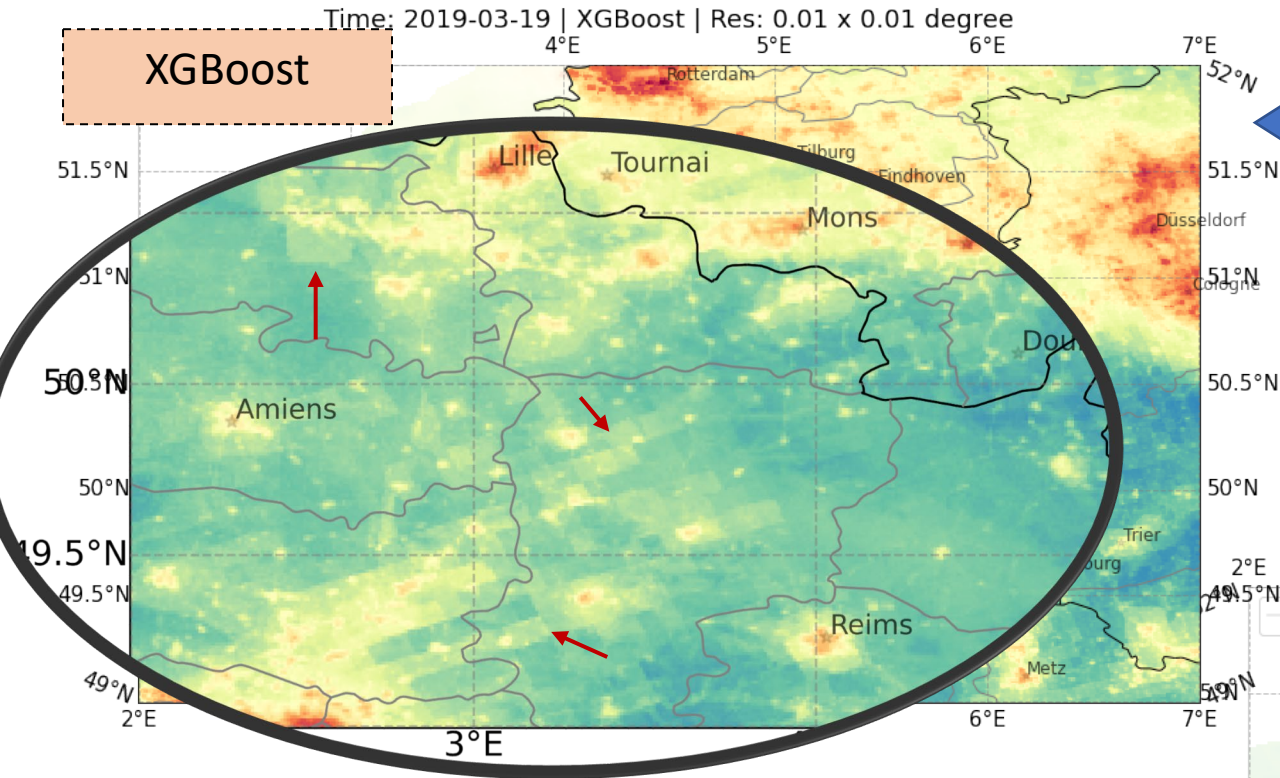
Test models on sites-based 10-folds Cross validation

Surface NO₂ mapping for Belgium by machine learning



SVM is much more time-consuming (more than 20 times) than others

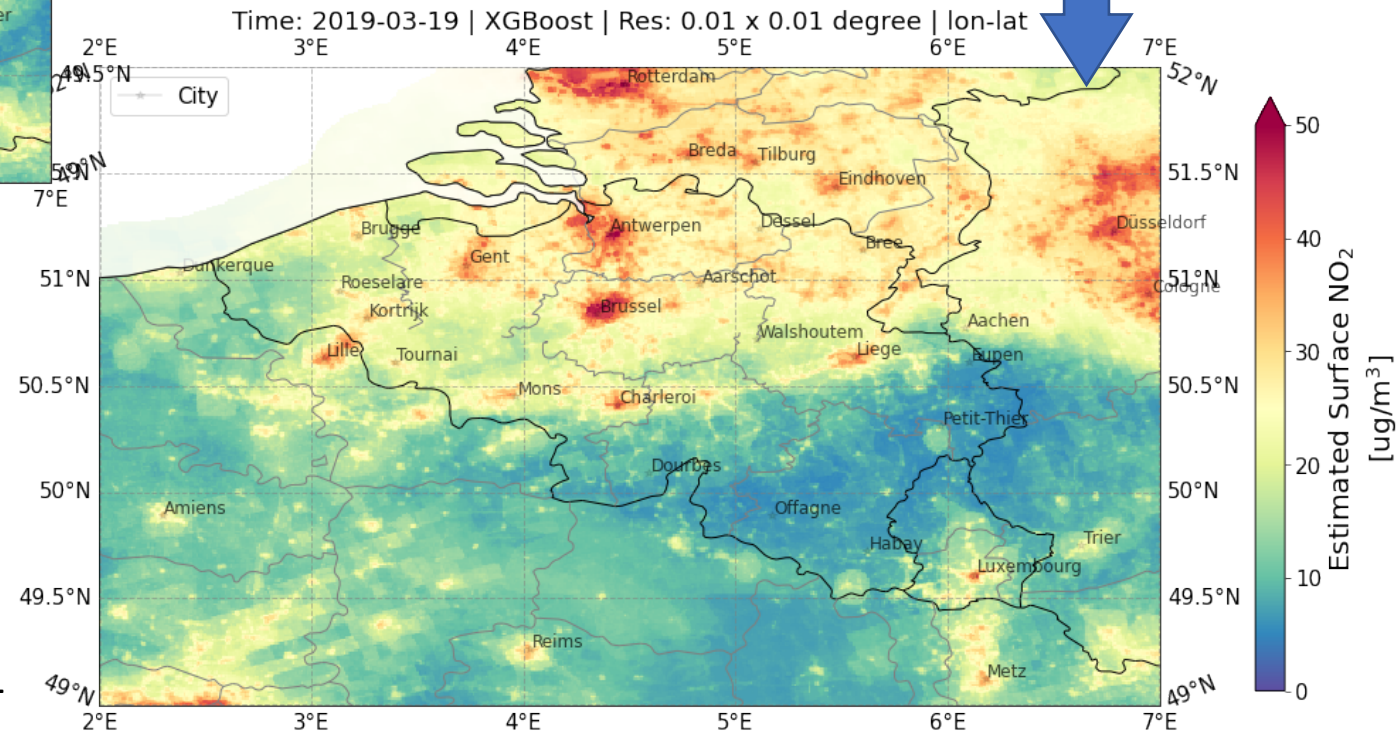
Surface NO₂ mapping by XGBoost



XGBoost achieves superior predictive accuracy but

- Prediction shows some checkerboard pattern of artifacts.

- Incorporating spatial locations (longitude, latitude) as predictors doesn't improve spatial continuity and mitigate artifacts in predictions.



Tree models exhibit **limitations** especially regarding the ability of **producing spatially continuous** maps without step-wise changes. Nevertheless, some **artifacts remained**, which were most pronounced at locations with a complex distribution of emission sources.

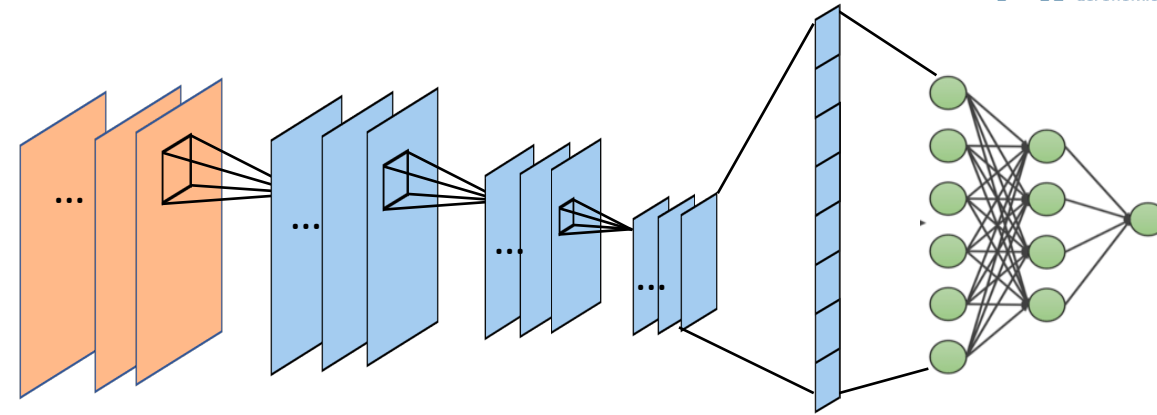
-- Kim et al., *Remote Sens. Environ.*, 2021

Surface NO₂ mapping by 2D-CNN

Sun *et al.*, (2022, in preparation)

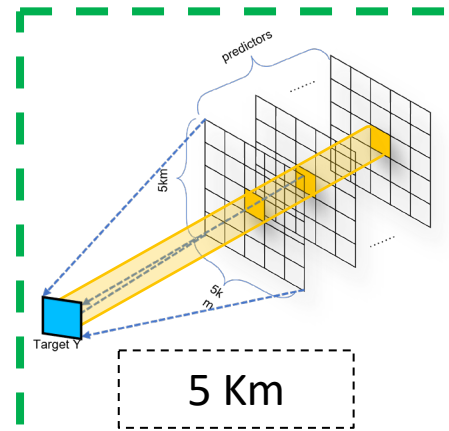
2D-Convolutional Neural Network

- Given NO₂ has a relationship with surrounding environments.
- 2D-CNN considers neighboring pixels of the target grid.

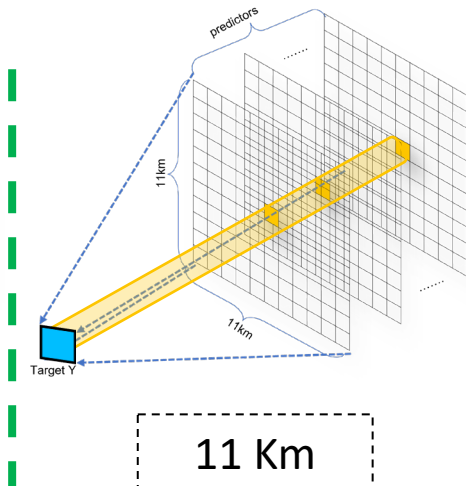


- Receptive field size is essential to model predictive accuracy and pattern continuity.
- A large receptive field will introduce more predictors' variance in the model

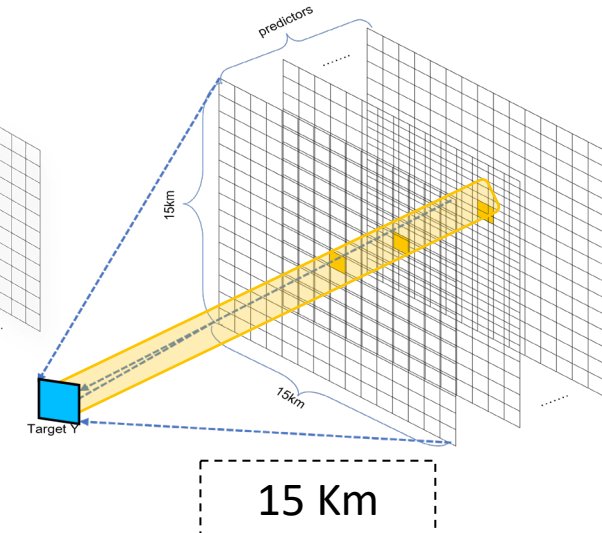
- The model will benefit from fine-resolution predictors.
- The model will become conservative when many predictors are downsampled from coarse resolution as variance doesn't increase significantly.



R^2 : 0.68
Pearr: 0.82
RMSE: 6.14
MAE: 4.47

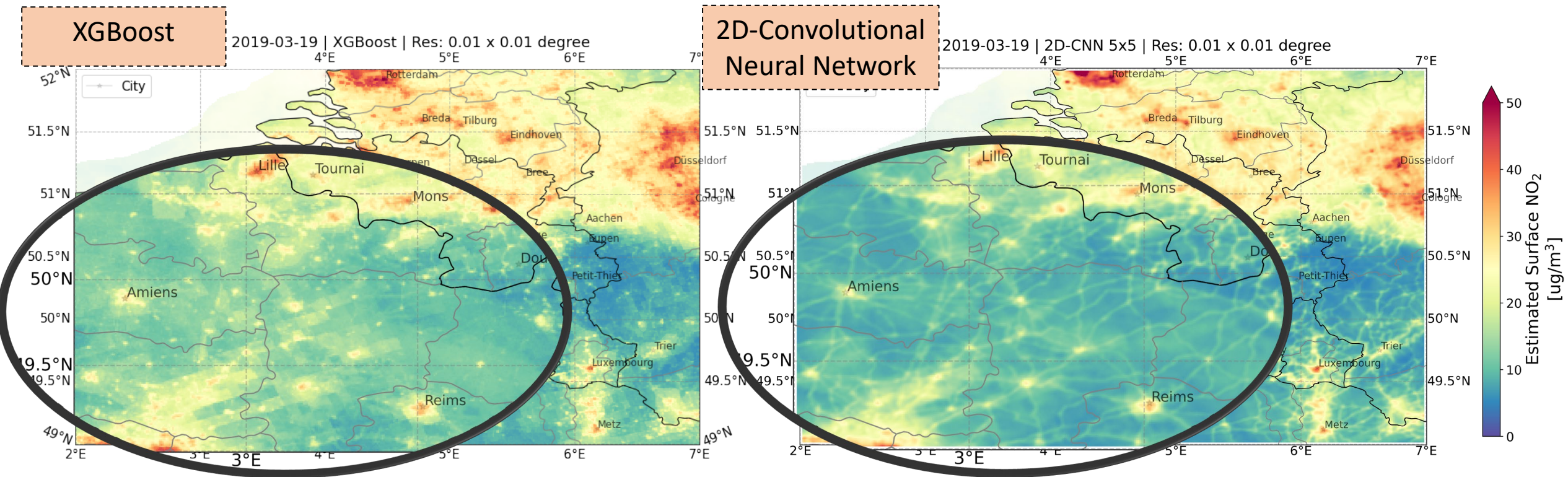


R^2 : 0.66
Pearr: 0.82
RMSE: 6.31
MAE: 4.59



R^2 : 0.61
Pearr: 0.82
RMSE: 6.78
MAE: 4.79

Compare XGBoost and 2D-CNN on spatial mapping



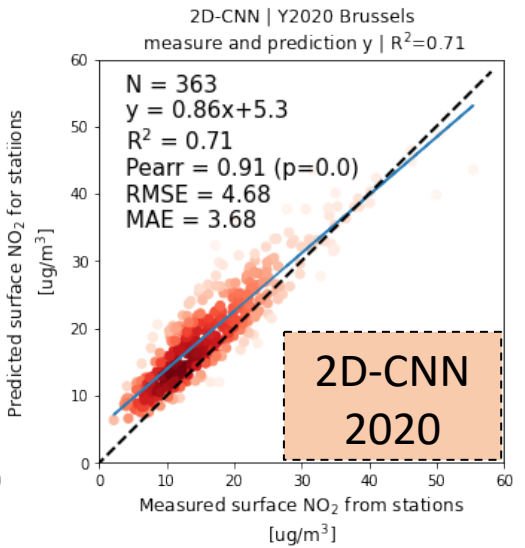
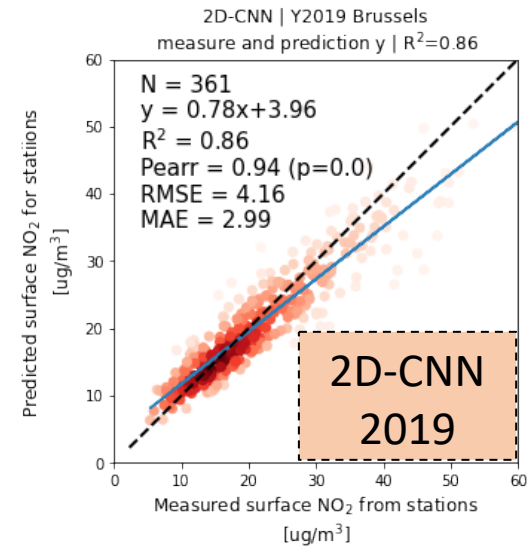
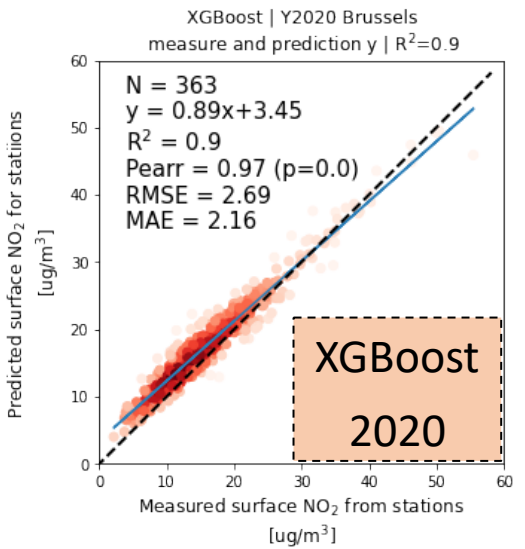
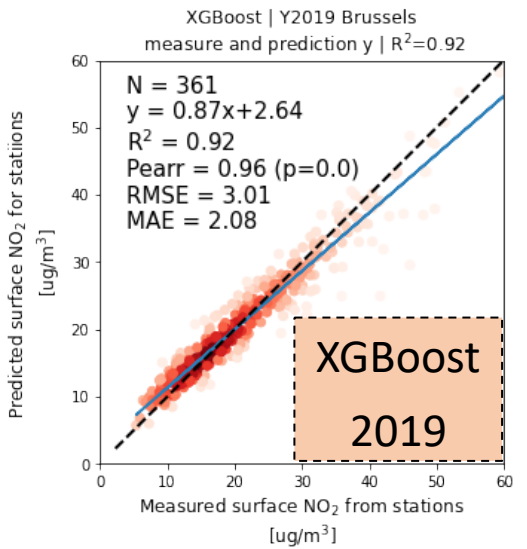
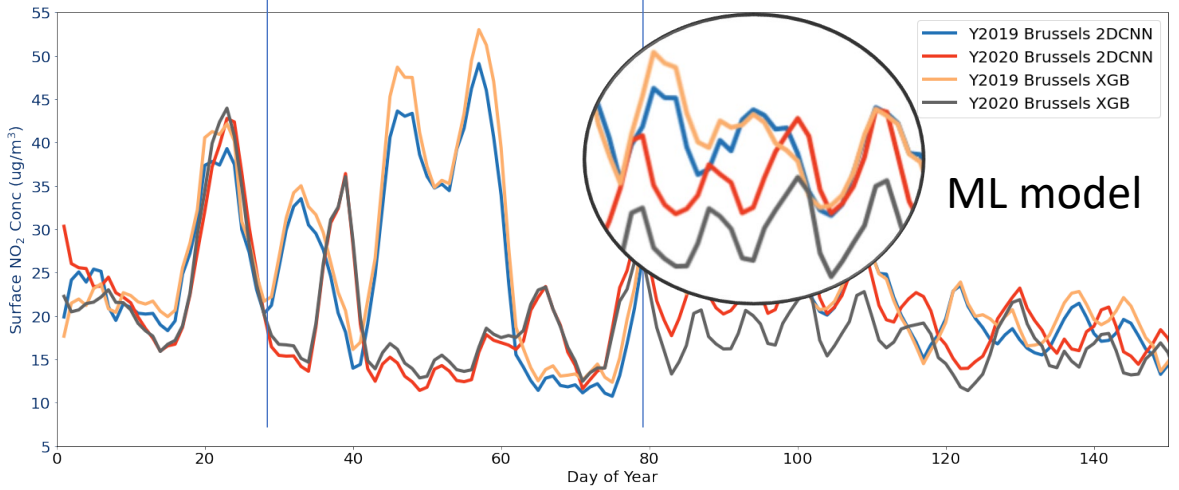
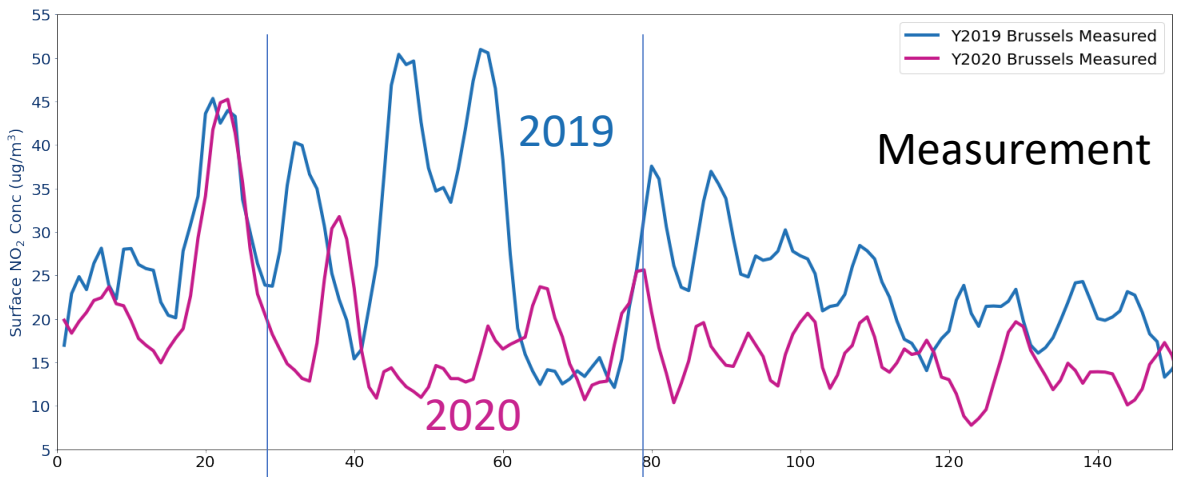
R²: 0.74
Pearr: 0.86
RMSE: 5.47
MAE: 4.00

A tree-based XGBoost performs best in statistical tests, but discrete patterns indicate obvious artifacts, especially in local mapping.

R²: 0.68
Pearr: 0.82
RMSE: 6.14
MAE: 4.47

The 2D-CNN considering neighboring pixels within 5 Km provides a continuous NO₂ pattern and mitigates the artifacts to a large extent, but still sacrifices some accuracy.

Compare XGBoost and 2D-CNN on time-series

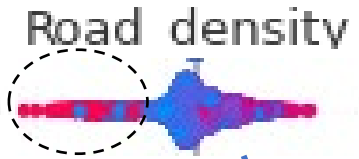


- 2D-CNN and XGBoost can identify the dramatic change in NO₂ during the Covid-outbreak.
- XGBoost performs better in time series since 2D-CNN becomes conservative after Covid and cannot well capture the difference between two years.

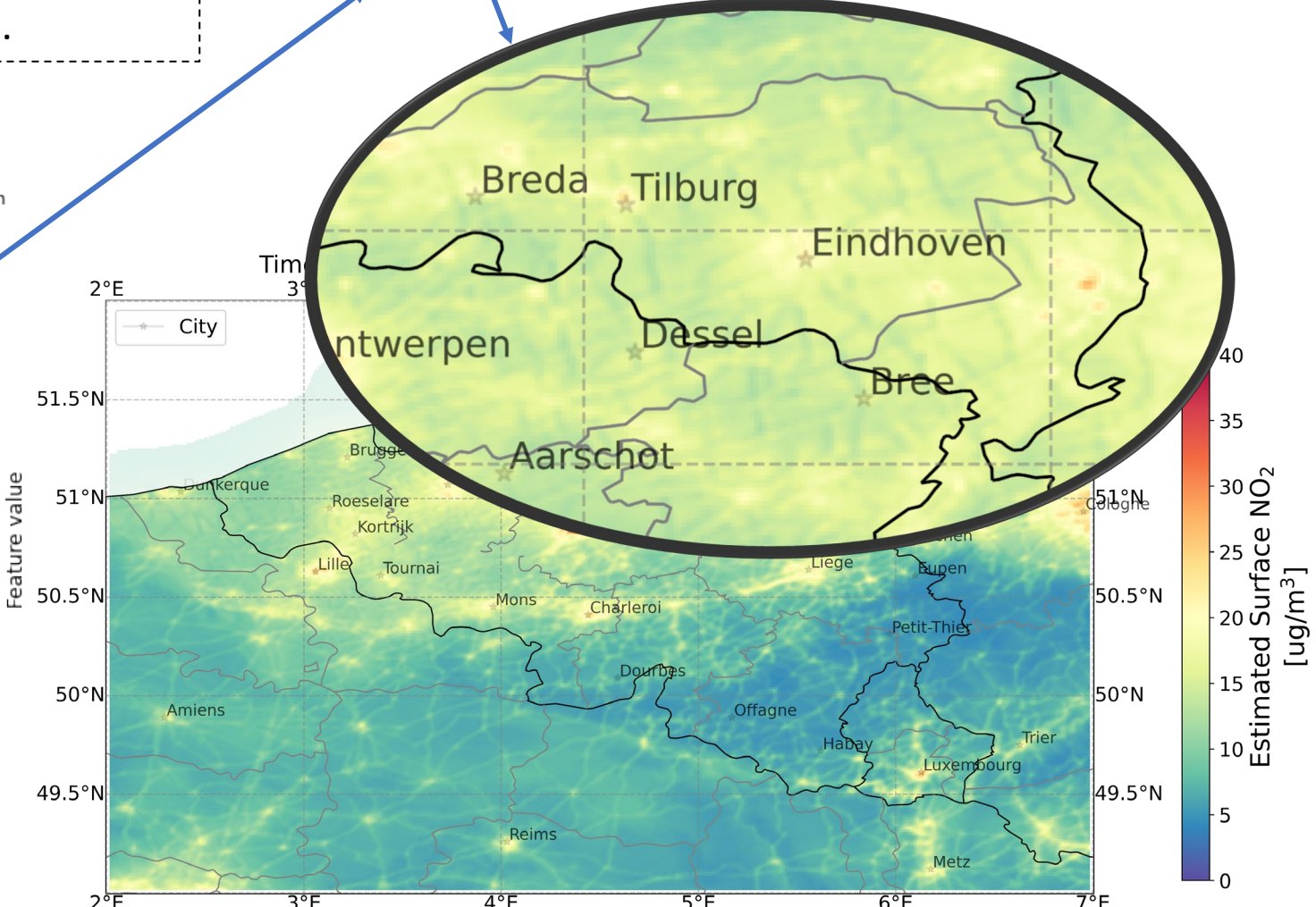
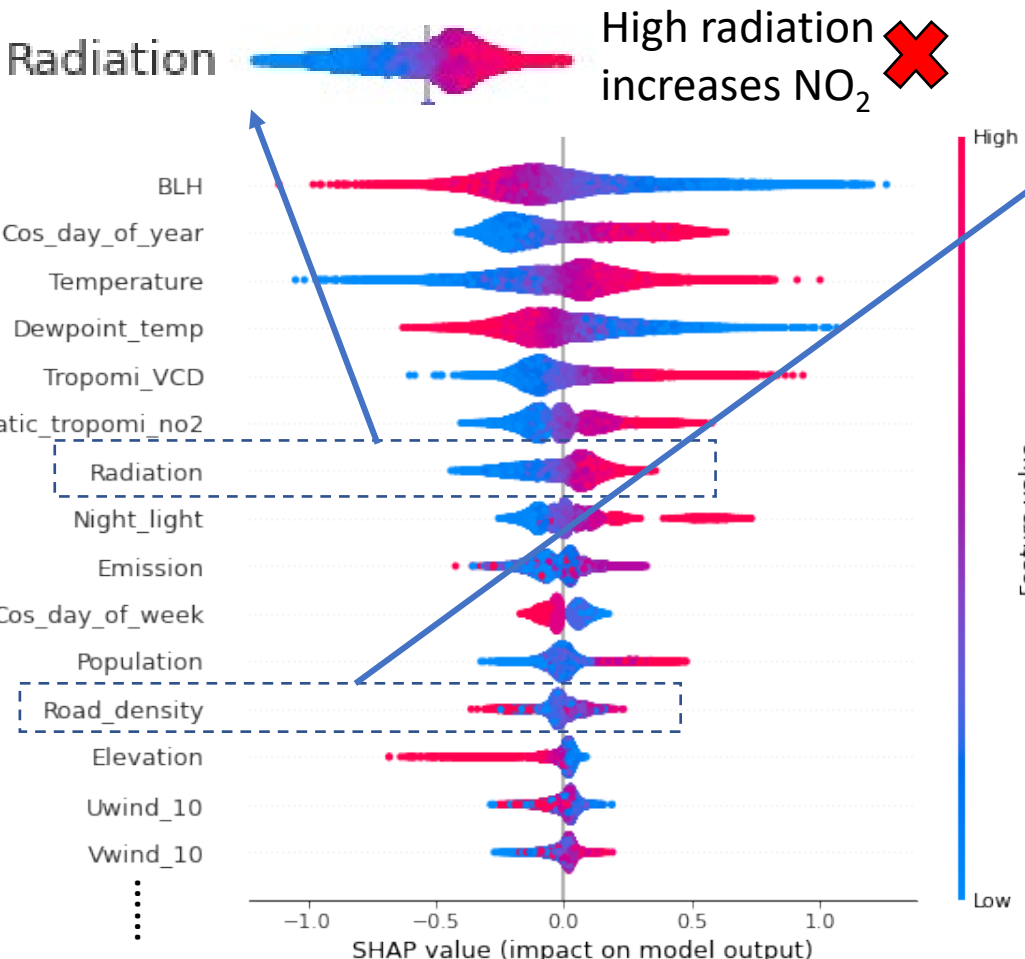
Issue in NO₂ mapping by 2D-CNN

- Involving as many influential predictors as possible can improve the model's accuracy.
- However, the auto-correlation between variables may cause the model to capture a wrong relationship.

Sometimes high road density reduces NO₂ ❌? ✅



Traffic volume might need to be included



Conclusion

- Use machine learning models to map surface NO₂ should consider both accuracy and spatial pattern.
- The 2D-CNN model provides surface NO₂ mapping with continuous patterns and fewer artifacts.
- In comparison to XGBoost, 2D-CNN performs conservatively and loses some accuracy.
- Auto-correlation within variables may cause the model to capture the wrong relationship and manufacture other possible artifacts.
- Given the trade-off between predictive accuracy and plausible spatial pattern, the ensemble of different models could be an option.

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Thank You