Site-scale estimation of Ozone in Northern Bavaria using Gradient Boosting Machines, Deterministic Regional Air Quality Models and a Hybrid Model

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funded by
Bavarian State Ministry of the Environment and Consumer Protection
and by
Bavarian State Ministry of Health and Care

➢ Research motivation

- ‘Mitigating Urban Climate and Ozone Risks’ (MiSKOR) aims to investigate the negative effects of the urban heat island effect and resulting ozone pollution in northern Bavaria (NB).
- Six (out of 13) stations in NB does not monitor ozone but nitrogen oxides (NOx). There is a similar data availability in 707 out of 5068 stations involved in the European air quality database (Airbase).

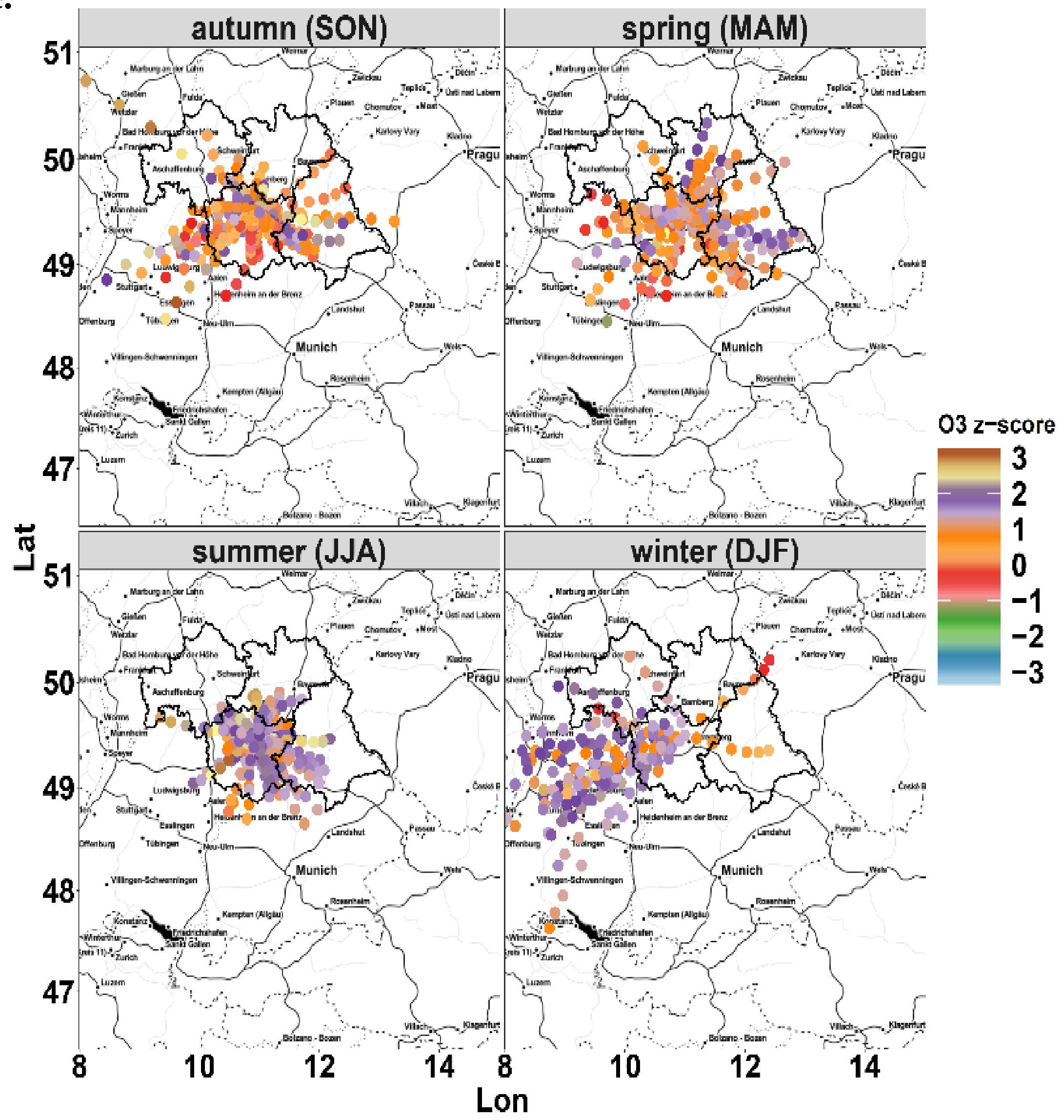
➢ Research outline

- Multiple linear regression and decision tree-based extreme gradient boosting (MLR- and Tree-XGBM) and logistic regression are used to estimate, classify (if ozone concentration >120 µg/m3 then class = 1, otherwise class = 0) and forecast hourly ozone concentrations in NB on a site scale.
- These machine learning algorithms (MLAs) are compared with two state-of-the-art dynamical models Copernicus CAMS-EU and DLR WRF-Polyphemus.
- The feasibility of using a Hybrid model, which is produced by the combination of estimations MLR-XGBM and CAMS-EU, is also studied .

➢ Ozone transport for MLAs

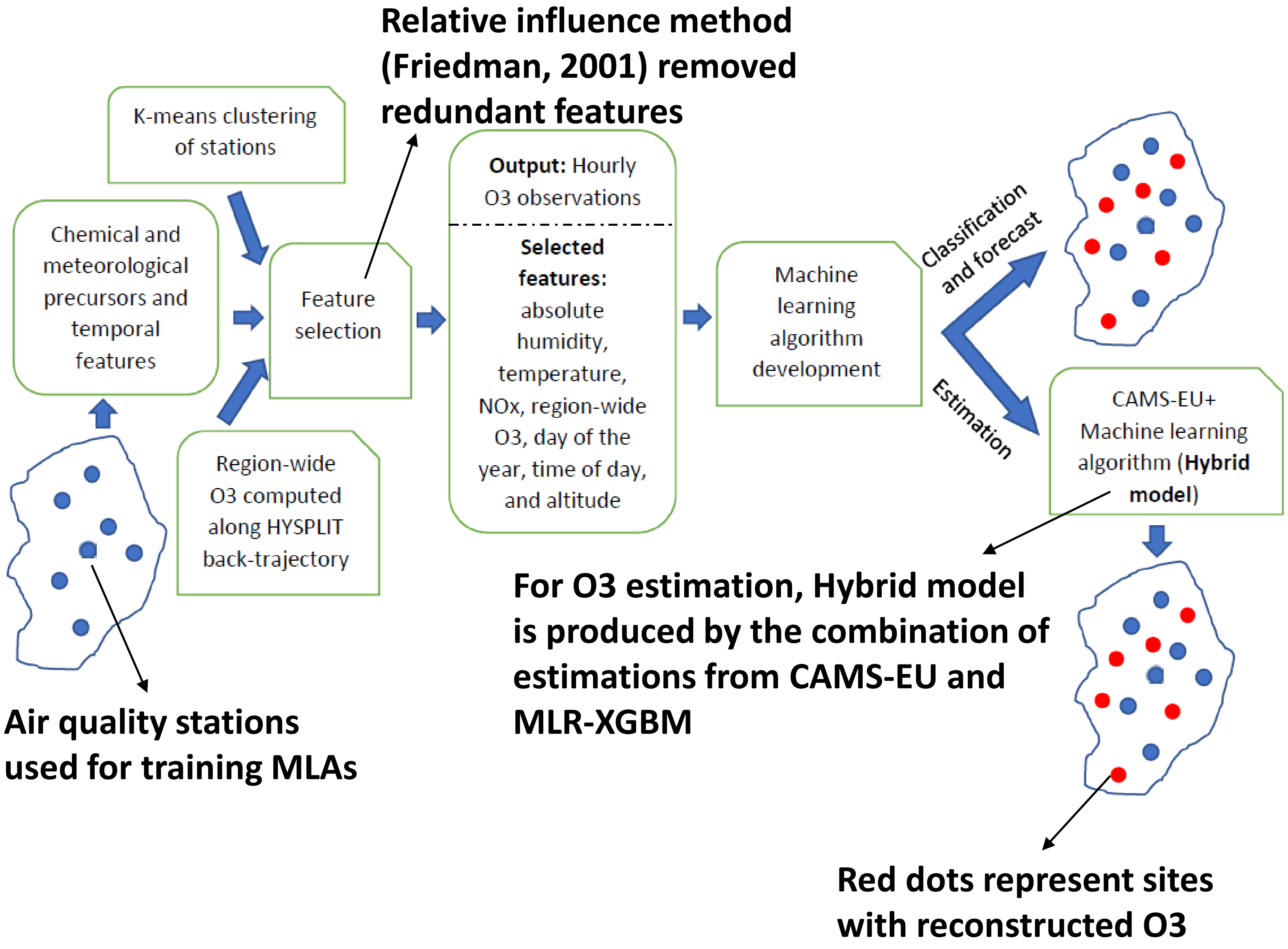
- In order to provide a predictor which represents the regional transport of ozone, a region-wide average of surface ozone concentrations (BT-O3), taken from surface stations along 6-hour back trajectories, is computed over NB.
- During ozone peaks, trajectory interval marks are mostly filled with high seasonal ozone z-scores. This may imply regional transport of ozone to NB during ozone peaks.

the seasonal average of z-score of ozone concentration along back trajectories when seasonal area-averaged ozone concentration in NB > seasonal 90th percentile.



➢ Development of machine learning algorithms

Along with BT-O3, simple area-averaged O3 (AA-O3), meteorological and chemical precursors, and spatial and temporal features are fed into MLAs .



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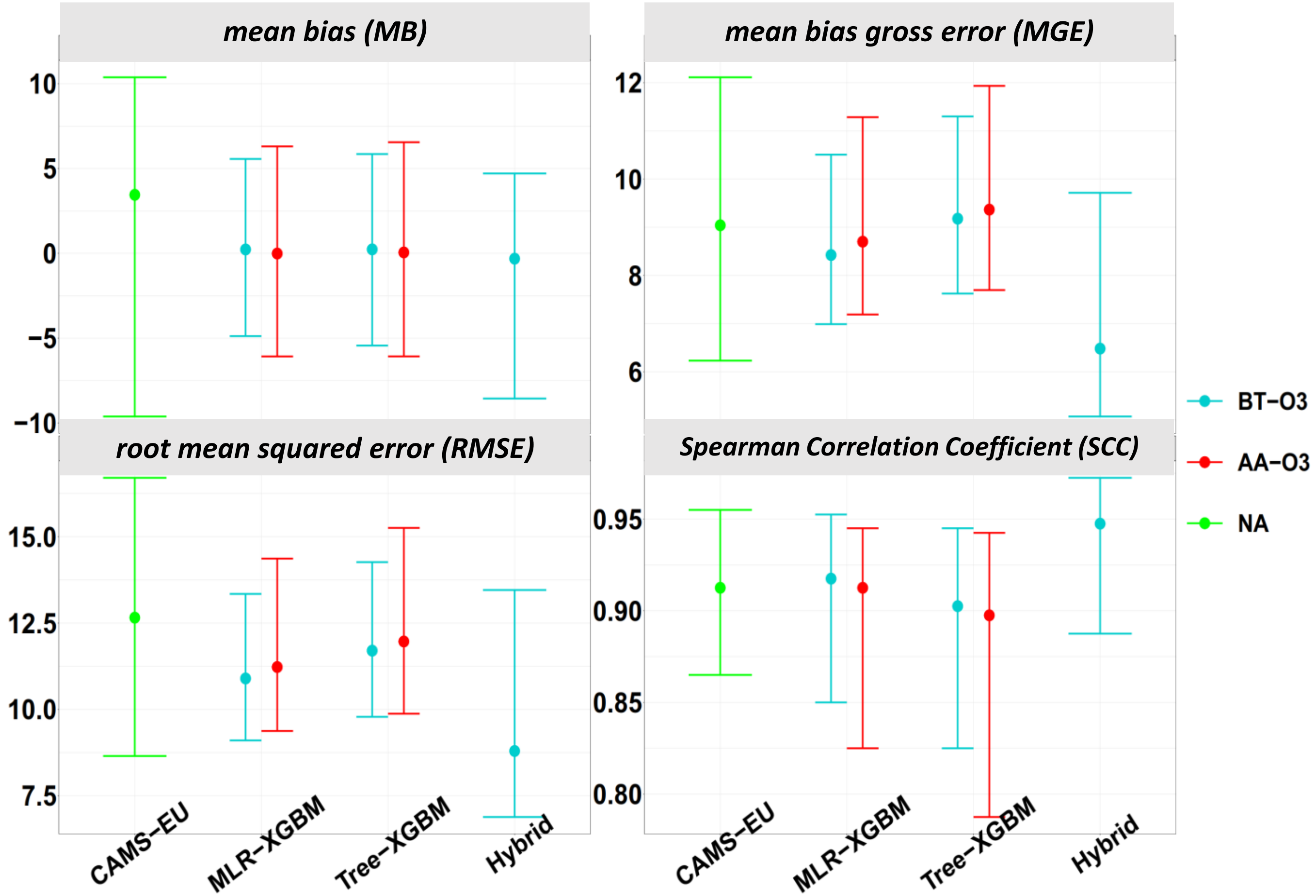
➢ Models performance in O3 estimation

- XGBMs outperformed CAMS-EU.
- MLR-XGBM yielded better performance than Tree-XGBM.
- Compared to AA-O3, MLR-XGBM with BT-O3 has yielded a better performance.
- Hybrid model yielded the highest overall correlation (SCC ≃ 0.95) and the lowest errors (e. g. RMSE ≃ 9.2 ug/m3).



Seasonal performance of CAMS-EU, XGBMs, and a hybrid model estimating hourly ozone concentration. No input sensitivity analysis is implemented on CAMS-EU estimations, shown by "NA" in legend. Dots (Error bars) are showing the mean (maximums and minimums) of performance metrics computed using LOOCV for seven studied stations.

➢ Models performance in O3 classification

- **Estimations previously obtained from CAMS-EU were binarized (CAMS-EU_bin) into two classes of occurrences (ozone concentration > 120 µg/m3) and non-occurrences (ozone concentration ≤ 120 µg/m3).**
- **MLR-XGBM (the more efficient XGBM for the site-scale estimation) as well as logistic regression (LR) are applied for the classification problem using the same features as used for the ozone estimation.**
- **LR and MLR-XGBM with BT-O3 yielded much better performance than CAMS-EU.**

The averaged skill scores of ozone classifiers/binarized estimations obtained at seven studied stations. Skill scores of MLR-XGBM and LR with BT-O3 and AA-O3 are shown outside and inside parenthesis, respectively.

Model	Sensitivity	Specificity	Accuracy
CAMS-EU_bin	0.65	0.99	0.82
LR	**0.94 (0.92)**	**0.95 (0.93)**	**0.95 (0.92)**
MLR-XGBM	0.93 (0.88)	0.95 (0.94)	0.93 (0.91)

➢ Models performance in O3 forecast

- The performance of MLR-XGBM, with BT-O3, for the forecast of hourly O3 was compared with that of CAMS-EU and WRF- Polyphemus.
- MLR-XGBM 24-hour forecast is normally less accurate than 1-hour forecast. Yet it has yielded much lower mean RMSE and higher mean SCC (19.34 and 0.83) than both dynamical models.

The averaged evaluation metrics calculated for the forecast of hourly ozone obtained at seven studied stations.

Model	MB (ug/m3)	MGE (ug/m3)	RMSE (ug/m3)	SCC
CAMS-EU	14.69	23.57	29.61	0.64
WRF-Polyphemus	10.86	22.75	29.15	0.65
MLR-XGBM_1h	**-0.39**	**9.68**	**12.92**	**0.93**
MLR-XGBM_24	**-1.81**	**14.99**	**19.34**	**0.83**

Conclusions

- we used machine learning algorithms (MLAs) to estimate, classify, and forecast hourly ozone concentrations on a site scale in northern Bavaria.
- For ozone estimation, we also investigated the feasibility of combining MLR-XGBM and CAMS-EU estimations. This new model is called Hybrid model. In order to feed ozone transport into MLAs, the daily average of ozone observations, along 6-hour back trajectories (BT-O3), was used as a feature.
- The Hybrid model explained around 90% of ozone variability, with the mean RMSE of around 9.2 (ug/m3), throughout the year when estimating hourly ozone.
- LR and MLR-XGBM performed best in the site-scale classification and forecast, respectively.
- BT-ozone improved the performance of MLAs in all three modelling tasks compared to simple area-averages of ozone.