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METEOROLOGISKA INSTITUTET
FINNISH METEOROLOGICAL INSTITUTE

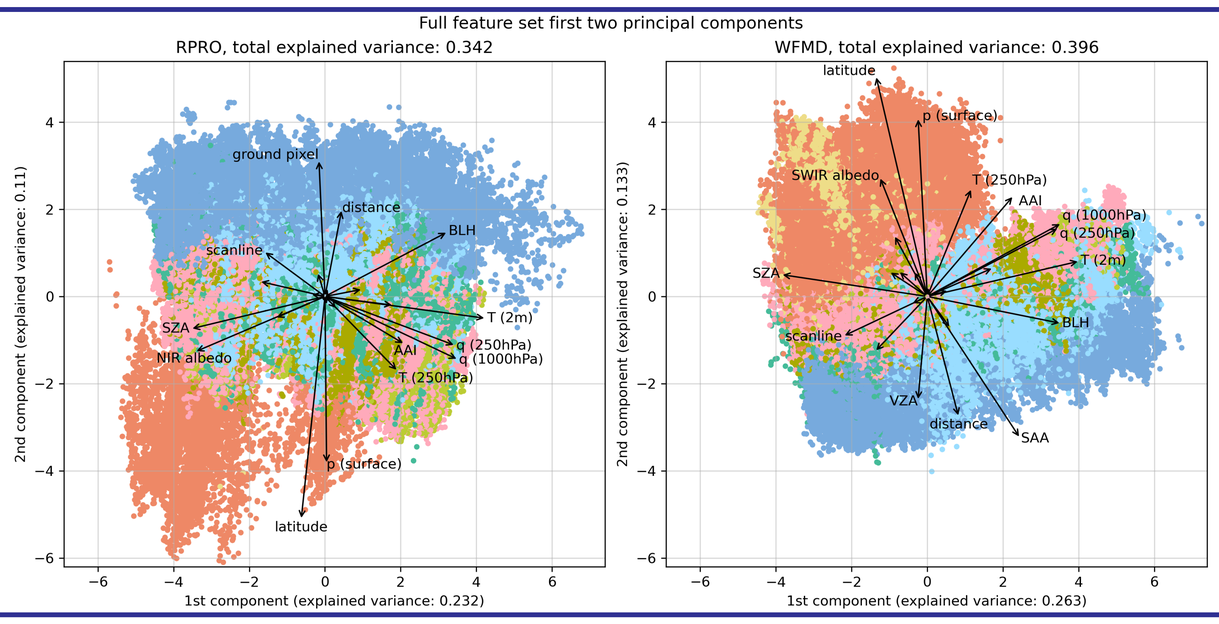
Quantifying environmental impacts on bias in Arctic TROPOMI methane retrievals using machine learning

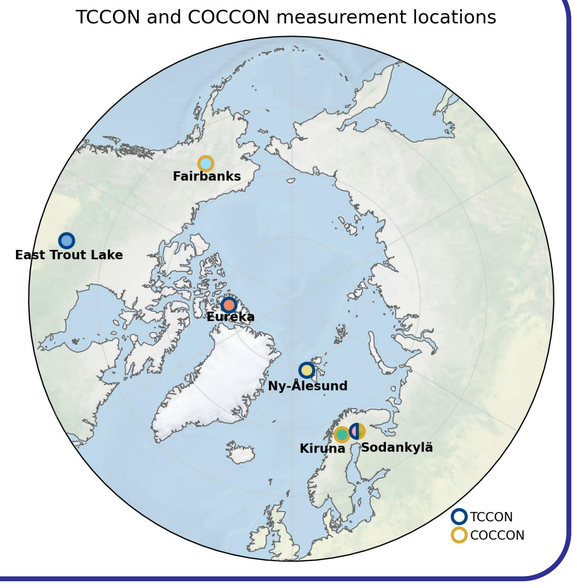
Tuomas Häkkilä[1] (*tuomas.hakkila@fmi.fi*), **Hannakaisa Lindqvist**[1], **Ella Kivimäki**[1], **Tomi Karppinen**[1], **Rigel Kivi**[1], **Johanna Tamminen**[1]

[1]Space and Earth Observation Centre, Finnish Meteorological Institute

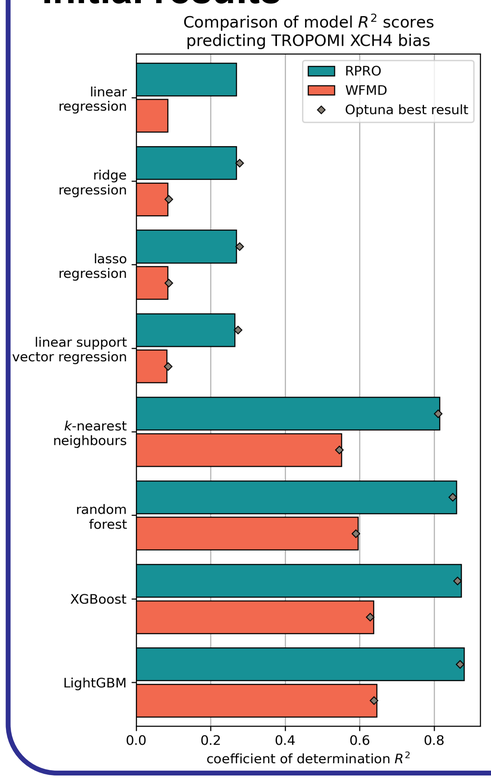
Introduction

- We explore the environmental factors affecting the bias in Arctic TROPOMI XCH_4 observations against ground-based TCCON and COCCON measurements.
- Two TROPOMI XCH_4 products, the operational reprocessed (RPRO) and the WFM-DOAS v2.0 (WFMD), are analysed, using a dataset with a total of 99 893 (RPRO) and 121 339 (WFMD) individual observations co-located near 8 ground-based instruments.

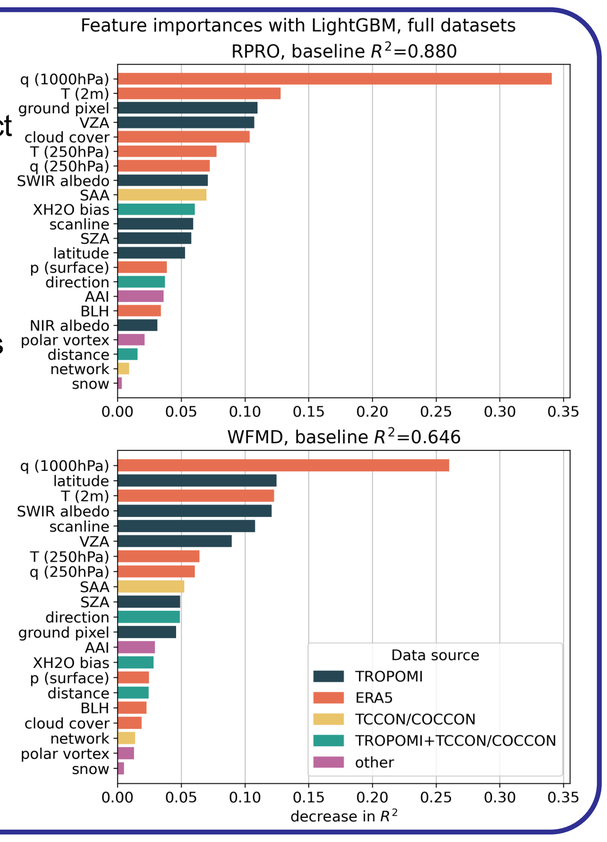


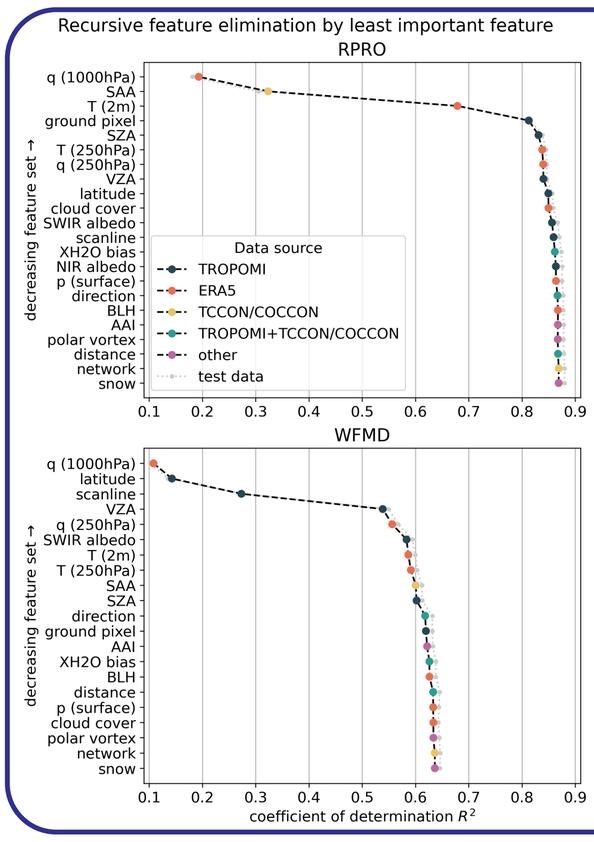


Initial results



- After an initial comparison of ML estimators, we select LightGBM as the best model in predicting the XCH_4 bias for further analysis.
- LightGBM R^2 scores are around 0.88 for RPRO and 0.64 for WFMD.
- Importances are assessed based on permutation feature importance (PFI), showing surface specific humidity dominates in importance for both RPRO and WFMD.



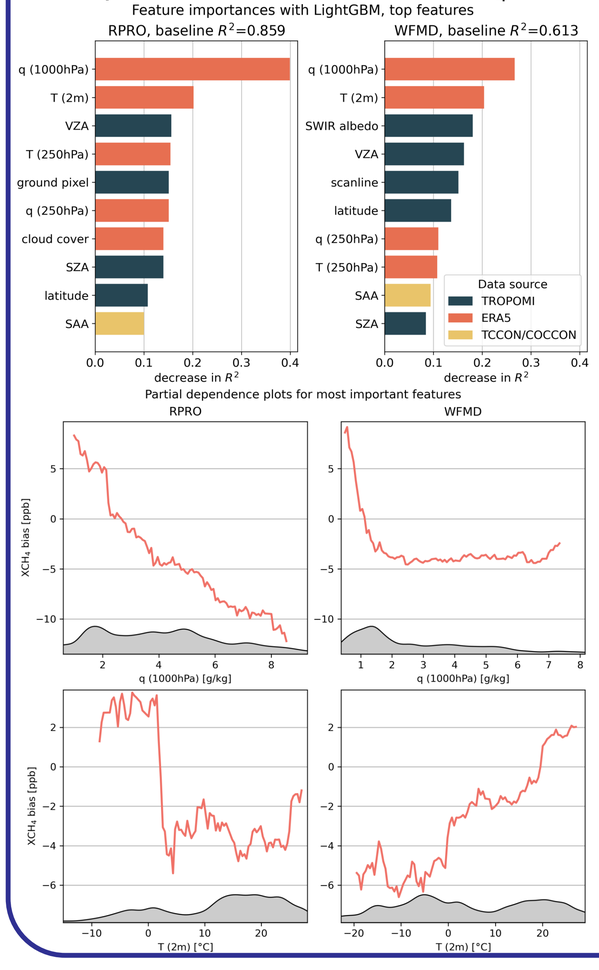


Limiting the dataset

- After calculating PFIs on the full feature set, feature selection is performed to limit the number of features.
- Recursive feature elimination (RFE) is used based on the least important feature to select the 10 top features for further analysis.
- To minimise the effect of coincidental correlation due to similar seasonal cycles, the full analysis is also performed separately on three "seasonal" datasets.

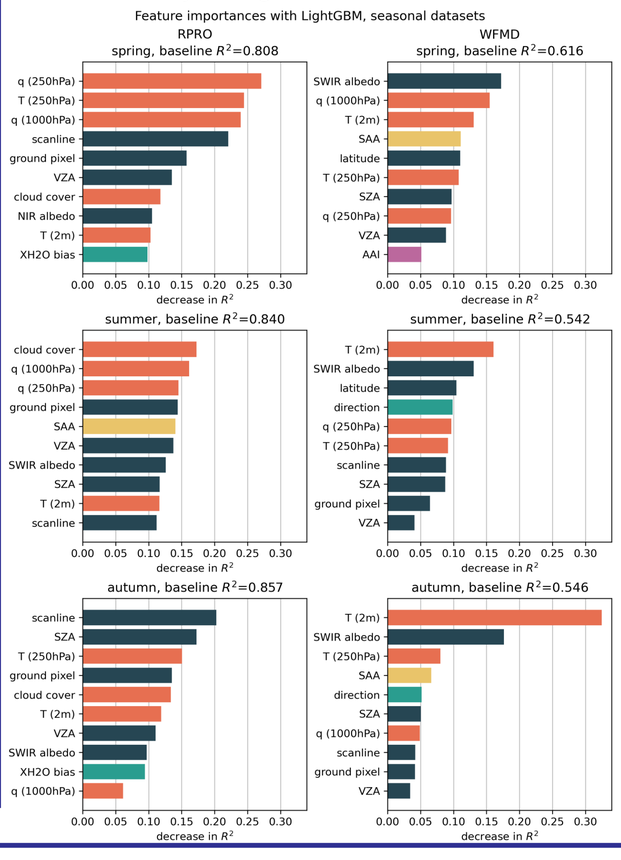
Selected features

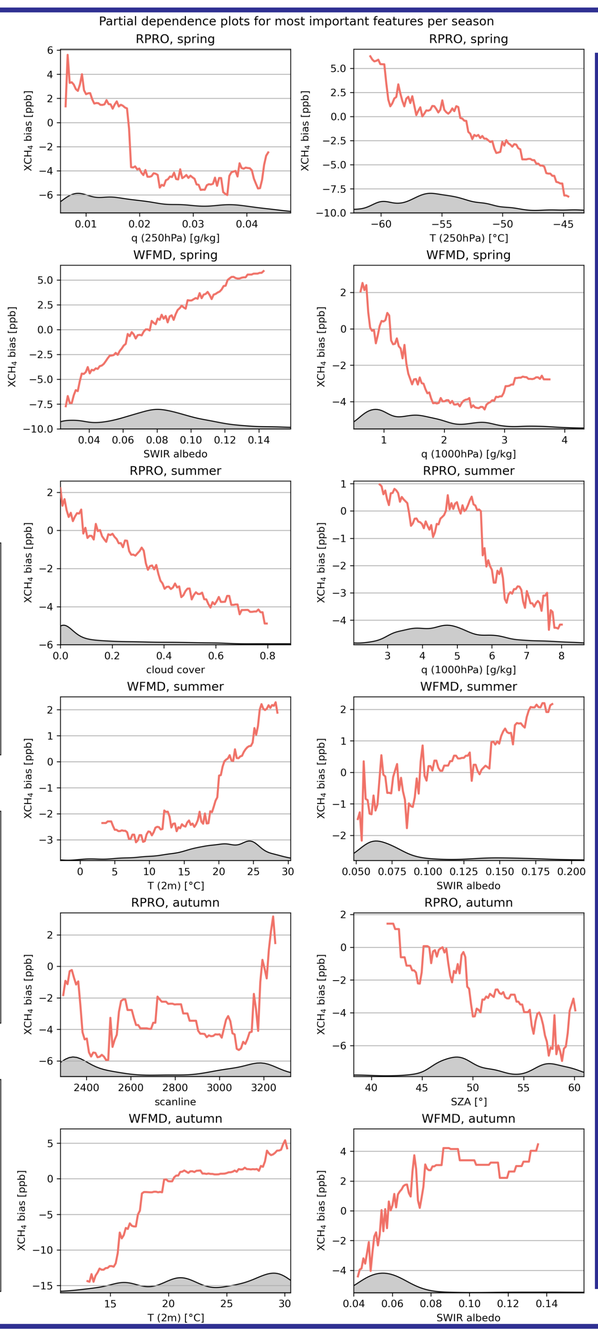
- After RFE, specific humidity at the surface persists as the most important feature, followed by surface temperature, possibly due to seasonality.
- Partial dependence plots show the average relation between the most important features and the XCH_4 bias.



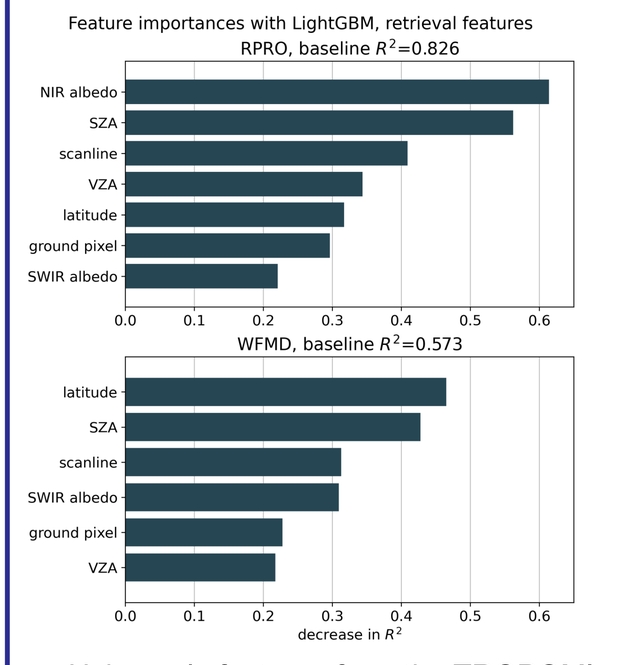
Seasonal datasets

- We select mid-summer data ±25 days of the summer solstice to limit the seasonality in the TROPOMI XCH4 bias, and consider spring and autumn as 50 days before and after this period.
- The reduction in samples results in somewhat worse model scores.
- The seasons show very different PFIs, and there are more differences between RPRO and WFMD compared to the fully merged datasets.

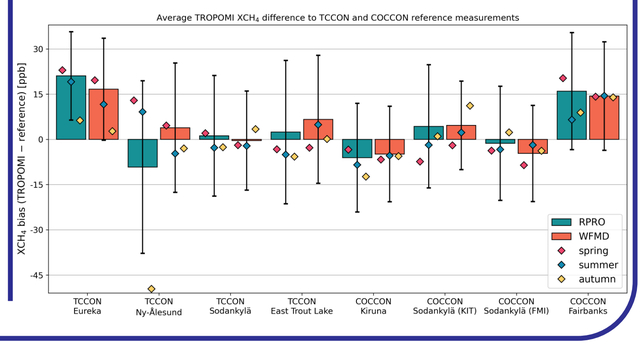




Retrieval features



- Using only features from the TROPOMI XCH_4 retrievals results in only a slight drop in model performance.
- This set of features could be used operationally to correct biases (shown below at each reference station), though further testing is required.



Acknowledgements

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