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NitroNet – A new deep-learning model for the prediction of NO_2 profiles based on TROPOMI satellite observations

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Nitrogen dioxide (NO_2) is an important air pollutant and has been widely recognized for its hazardous impact on human health. Tropospheric NO_2 is routinely monitored using satellites (e.g. TROPOMI onboard Sentinel-5P), in situ instruments, and ground-based spectroscopic measurements (e.g. multi-axis differential optical absorption spectroscopy, MAX-DOAS). However, these measurements do not give the full picture: Satellite instruments can only measure the integrated load (column density), in situ measurements are mostly deployed at the surface, and MAX-DOAS instruments are still very sparse. In consequence, it is currently impossible to obtain sufficiently resolved NO_2 profiles from measurements alone. Regional chemistry and transport (RCT) simulations can be used to simulate NO_2 profiles where no observations are available, but they are computationally expensive and require meticulous parameter calibration to achieve acceptable agreement with observational reference data.

We present **NitroNet**, a new deep-learning model for the prediction of tropospheric NO_2 profiles. The model is based on a feedforward neural network, which was trained on a synthetic dataset from the RCT model WRF-Chem. NitroNet receives vertical NO_2 column densities (VCDs) from TROPOMI and ancillary variables (meteorological, emissions, etc.) as input, from which it predicts tropospheric NO_2 concentration profiles. The NO_2 VCD is descriptive of the profiles' magnitudes, while their shapes are derived from the ancillaries (e.g. the boundary layer height). The ancillaries are taken from the TROPOMI NO_2 data product, ERA5 reanalysis data, and the EDGARv5 emission inventory. By prior filtering of the training data based on their agreement to reference data, NitroNet can achieve better agreement with TROPOMI's NO_2 VCDs and surface in situ measurements than WRF-Chem at a much faster runtime. On the downside, these predictions are available only once per day, when the TROPOMI overpass occurs. We showcase the model's performance against a variety of validation data (satellite, in situ, and MAX-DOAS measurements), and its ability to generalize to different seasons and geographical regions.

What makes NitroNet unique in the field of deep-learning air pollution models is its training on *synthetic* data. This conceptual difference to the many recently developed models, trained on empirical observations alone, unlocks important new possibilities: Due to the paucity of other observations, empirical training sets are practically confined to surface concentrations from in situ measurements. Synthetic data generation, on the other hand, allows for training sets with full NO_2

profiles instead. Moreover, synthetic training examples do not suffer from the cross-sensitivities of in situ measurements to other nitrogen compounds (up to a factor of 2).

The NO_2 profiles produced by NitroNet can be used as high-resolution replacements for the a priori profiles in satellite retrievals, or for studies on surface level air pollution.