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Application of deep neural networks for the retrieval of cloud properties for Sentinel-4 and TROPOMI / Sentinel-5 Precursor

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Due to their fast computational performance, neural networks (NN) are nowadays commonly used in the context of remote sensing for solving forward and inverse problems (see [1], [2], [3]). The issue of performance is especially important in the context of operational processing with large amounts of data and strict time requirements. Classical retrieval algorithms often use a radiative transfer model (RTM) as forward model with which an optimization algorithm can then solve the inverse problem of inferring the quantities of interest from the measured spectra. However, these RTMs are usually computationally very expensive and therefore replacing them by a NN is desirable to increase performance. But the application of NNs is not straightforward and there are at least two main approaches:

1. NNs used as forward model, where a NN approximates the radiative transfer model and can thus replace it in the inversion algorithm
2. NNs for solving the inverse problem, where a NN is trained to infer the atmospheric parameters from the measurements directly

The first approach is more straightforward to apply. However, the inversion algorithm still faces many challenges, as the spectral fitting problem is generally ill-posed. Therefore, local minima are possible and the results often depend on the selection of the *a priori* values for the retrieval parameters.

For the second case, some of these issues can be avoided: no *a priori* values are necessary, and as the training of the NN is performed globally, i.e. for many training samples at once, this approach is potentially less affected by local minima. However, due to the black-box nature of a NN, no indication about the quality of the results is available. In order to address this issue, novel methods like Bayesian neural networks (BNNs) [4] or invertible neural networks (INNs) [5] have been presented in recent years. This allows the characterization of the retrieved values by an estimate of uncertainty describing a range of values that are probable to produce the observed measurements. We apply and evaluate these new BNN and INN methods for the retrieval of cloud properties from Sentinel-4 and Sentinel-5 Precursor / TROPOMI in order to demonstrate their potential as operational algorithms.

Keywords: retrieval algorithm, clouds, inversion, machine learning, neural networks, uncertainty quantification

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