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Dimensionality reduction techniques for simulations of the spectral radiance in the Hartley-Huggins band

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Atmospheric chemistry observations from space have been a concern to the scientific community since they improve our understanding of environmental issues such as climate change or stratospheric ozone depletion. Atmospheric composition sensors continuously measure the reflected spectral radiances in the ultra-violet, visible and infrared ranges. This information is then used to retrieve the trace gas concentrations.

The new generation of atmospheric composition sensors such as the TROPospheric Ozone Monitoring Instrument (TROPOMI) delivers a great amount of data, which is recognized as Big Data. The operational processing of remote sensing Big Data requires high-performance radiative transfer models (RTMs) for simulating spectral radiances (level-1 data). In particular, ozone total column retrieval algorithms use the level-1 data in the Hartley-Huggins band (280-335 nm). Accurate simulation of this absorption band may require several hundreds of monochromatic computations. The optical parameters which are the inputs for RTMs should be given for each spectral point. Consequently, the whole data set can be very large, and the computation of one spectrum is reduced to multiple time-consuming RTM simulations. However, the input dataset contains a redundant information, which can be excluded by using the dimensionality reduction techniques, e.g. the principal component analysis (PCA). In addition, there is a strong correlation between the input optical data for RTMs and output spectral radiances. Such statistical dependency can be taken into account for accelerating level-1 data simulations, thereby providing the performance enhancement for the whole processing chain. Furthermore, PCA can be used to represent the hyperspectral signal with a reduced number of spectral points. This can improve the performance of machine learning algorithms.

The aim of this work is to analyze the efficiency and potential benefits of the optical data dimensionality reduction techniques for simulating the Hartley-Huggins band. In our talk, a general concept of the PCA-based RTMs is presented and two implementations of this approach are discussed. It is shown that by constructing an appropriate orthogonal basis, it is possible to estimate the optimal spectral sampling, i.e. a set of spectral points containing the maximum information content on the whole spectral behavior and the ozone profile shape. The performance enhancement due to PCA-based RTMs is determined by using synthetic spectra.