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AI for Fast Atmospheric Chemistry

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In coupled global circulation models, chemical interaction between atmospheric trace gases is modelled through dedicated atmospheric chemistry submodels. As these components tend to be computationally expensive, one is often faced with the situation to either run the models with chemistry in relatively coarse resolution, or to ignore atmospheric chemistry altogether. Here an alternative approach is presented in order to overcome the high computational costs while attaining comparable quality of results. A fully connected neural network is used to make predictions of chemical tendencies. As input data of the neural network serve chemical mixing ratios, temperature, pressure, the ozone column and the solar zenith angle, all resulting from the global numerical atmosphere-chemistry model EMAC. The time period considered is 3 month, divided in time steps of consecutive 11 hours. In total, 181 time steps are analysed, from which the first 128 are used as training data, the following 26 as validation data and the last 27 are kept for final testing. The EMAC model produces results of 110 chemicals at a horizontal grid of 160x320 and 90 vertical levels. In our preliminary approach, only 6 of these chemicals - which correspond to the chemicals describing the Chapman mechanism and the nitrogen oxides - are predicted and the analysis area is restricted to the stratosphere. Further, chemicals that are zero at 95% or more of the data points have been deleted from the input data. The results of the neural network represent the spatial patterns of the climate model data very well and are in the same order of magnitude. Spatial correlations depend on the chemical and the vertical level, but are in general >0.95 at levels where the considered variable is present. However, errors are increasing during the validation period, which is probably due to trends in the analysed data. This work presents a proof of concept that neural networks are able to predict atmospheric chemistry tendencies. Left for future work is a detailed hyperparameter tuning in order to optimize the model and the extension to longer time periods to overcome modelling problems due to seasonal trends in the data.