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Aerosol Thermodynamics using Machine Learning

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Aerosol chemical composition is an important driver for hygroscopic growth and hence cloud activation. A major fraction of the aerosol consists of inorganic components, for which thermodynamic equilibrium models are commonly used to describe the chemical composition, including total water uptake.
However, these thermodynamics are relatively computationally expensive calculations, minimising the Gibbs free energy of the total system. Consequently, faster computations are desirable, which can be facilitated using machine learning techniques.

In this study, we apply neuronal networks, being trained on the output of an equilibrium thermodynamics model (ISORROPIA 2), to represent both the chemical composition and associated aerosol water uptake. We investigate the quality of the trained network against independent data from the equilibrium model and find a good agreement of the trained network model against the original data. Furthermore, we also test the applicability of the trained model in a parameter space outside of the trained data set to analyse whether the trained network is able to properly represent the physico-chemical system, and hence a suitable replacement of the equilibrium model by a neuronal network is appropriate.

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