

Machine Learning with Small Amount of Data

Surrogate Modelling of Thermodynamic Properties with Gaussian Processes

Master Thesis

Thermodynamic property calculations are essential in many engineering and scientific applications, yet conventional reference tools can be computationally demanding. In this thesis, a compact surrogate model that learns the underlying property relationships from a limited set of high-quality reference data points, will be trained. It shall then provide fast predictions with controlled accuracy.

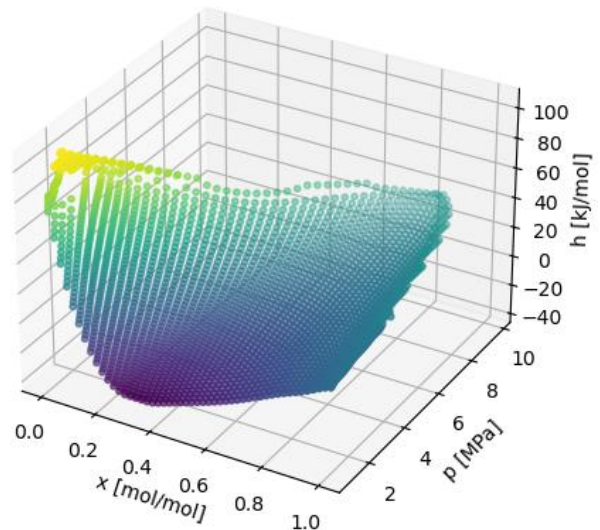
Therefore, Gaussian Processes will be used, as a flexible, non-parametric learning technique, that can be quickly evaluated. By construction, they additionally provide an estimate of the predictive uncertainty which will be used to introduce step-wise adaptive learning.

Requirements:

- basic knowledge in probability theory, preferably Gaussian Process regression
- thermodynamic understanding, especially of mixtures
- programming skills with python

Tasks:

- design and build a property database for an exemplary mixture
- implement the Gaussian Process regression model
- evaluate the model accuracy for different sets of hyperparameters



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