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Web Seminar

Bayesian kernel regression for functional data

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Abstract

Material properties obtained by experiment or simulation are often not inherently scalar values, but rather functional values such as spectra or distributions. Even material properties measured as scalar values can be regarded as a function of experimental conditions, since their values vary with experimental conditions such as temperature and pressure. In this study, we propose a functional output regression model based on the kernel method. This model allows the prediction of the functional properties of a given material. Compared to training ordinary supervised learning models separately, which target the prediction of scalar outputs, this model is expected to capture the covariance structure within the function, resulting in improved learning efficiency and prediction accuracy. In addition, this model provides a predictive distribution of functional outputs derived analytically from a Bayesian perspective, allowing quantification of prediction uncertainty and sampling of predicted functions for a given material. In the seminar, I will explain the model in detail along with several applications in materials science.

This model can be regarded as a complete kernelization of the functional output model proposed in previous study [1]. The complete kernelization simplifies the form of the model and allows for the derivation of analytically optimal solutions, Bayesianization, and theoretical consideration of the model. Since this model has a strong theoretical relationship with multi-task learning model based on a separable kernel [2], this point will also be explained if time permits.

References

[1] Iwayama, Megumi, et al. "Functional Output Regression for Machine Learning in Materials Science." Journal of Chemical Information and Modeling 62.20 (2022): 4837-4851.

[2] Ciliberto, Carlo, et al. "Convex learning of multiple tasks and their structure." International Conference on Machine Learning. PMLR, 2015.