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Predicting Drug Effects

Using Bayesian Artificial Neural Networks for Drug Discovery

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Abstract

Challenges like using predictive modelling of pharmaceutical drug effects can become noticeably more difficult if the model fails to express predictive uncertainty. Taking this into account is of great importance when developing more complex models. In this paper, we cover the theoretical framework of Bayesian Artificial Neural Networks (BANNs). The aim is to be able to apply this class of models in problem domains like drug discovery, where predictive uncertainty is a crucial aspect. In order to compute the intractable posterior distribution for a network model, we use variational inference to approximate the true posterior distribution by a variational posterior distribution. Moreover, our work covers other central areas for using BANN models such as hyperparameter optimisation and pre-processing of the data, e.g. by Principal Component Analysis. Although our empirical results did not suggest satisfactory performance for the explored BANN models, we humbly believe future research oriented more heavily towards model fitting could yield considerably better results.

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