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## Abstract

In this article, we extend the application of the Gaussian processes technique to classification quantitative structure–activity relationship modeling problems. We explore two approaches, an intrinsic Gaussian processes classification technique and a probit treatment of the Gaussian processes regression method. Here, we describe the basic concepts of the methods and apply these techniques to building category models of absorption, distribution, metabolism, excretion, toxicity and target activity data. We also compare the performance of Gaussian processes for classification to other known computational methods, namely decision trees, random forest, support vector machines, and probit partial least squares. The results indicate that, while no method consistently generates the best model, the Gaussian processes classifier often produces more predictive models than those of the random forest or support vector machines and was rarely significantly outperformed.

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