

Gaussian Processes for Category Models White Paper

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In this article Olga describes how we extend the application of Gaussian Processes technique to classification 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 blood-brain barrier penetration and hERG inhibition. We also compare performance of Gaussian Processes for classification to other known computational methods, namely decision trees, bagging and probit PLS.

This white paper is available as a [PDF](#) file.