# High-dimensional QSAR classification modeling based on improving black hole algorithm

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### Abstract

High-dimensionality is one of the major problems which affect the quality of the quantitative structure-activity (property) relationship (QSAR/ QSPR) classification methods in chemometrics. Applying variable selection is essential to improve the performance of the classification task. Variable selection is well-known as an NP-hard optimization problem. Various evolutionary algorithms are dedicated to solving this problem in the literature. Recently, a black hole algorithm was proposed, which has been successfully applied to solve various continuous optimization problems. In this paper, a new time-varying transfer function is proposed to improve the exploration and exploitation capability of the binary black hole algorithm in selecting the most relevant descriptors (variables) in QSAR/ QSPR classification models with high classification accuracy and short computing time. Based on seven benchmark biopharmaceutical datasets, the experimental results reveal the capability of the proposed time-varying transfer function to achieve high classification accuracy with minimizing the number of selected descriptors and reducing the computational time.

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