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Adaptive matrix metrics for molecular descriptor assessment in QSPR classification

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QSPR methods represent a useful approach in the drug discovery process, since they allow predicting in advance biological or physicochemical properties of a candidate drug. For this goal, it is necessary that the QSPR method be as accurate as possible to provide reliable predictions. Moreover, the selection of the molecular descriptors is an important task to create QSPR prediction models of low complexity which, at the same time, provide accurate predictions.

In this work, a matrix-based method [1] is used to transform the original data space of chemical compounds into an alternative space where compounds with different target properties can be better separated. For using this approach, QSPR is considered as a classification problem. The advantage of using adaptive matrix metrics is twofold: it can be used to identify important molecular descriptors and at the same time it allows improving the classification accuracy.

A recently proposed method making use of this concept [2] is extended to multi-class data. The new method is related to linear discriminant analysis and shows better results at yet higher computational costs. An application for relating chemical descriptors to hydrophobicity property [3] shows promising results.

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