# A group contribution method based on empirical models

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Today's chemical processes involve many components, and it is necessary to know their basic physical properties for process design and operation. However, it is impossible to find all property information in the literature. In general, there are two ways to evaluate properties of chemical compounds: the experimental measurement and predictive approaches based on empirical models. The latter is called the group contribution method (GCM), and its basic concept is that specific functional groups or fragments of a molecule contribute to the value of its physical property. The advantage of the GCMs is that they reduce the effort and cost compared to experiments. This study proposes a novel GCM method suitable for high-dimensional, sparse data sets. In order to improve its applicability and accuracy, the database is extended and divided into non-ring group compounds and ring group ones. Support vector regression (SVR) is adopted as the regression model, and a derivative-free optimization approach, referred to as particle swarm optimization, is incorporated into the parameter optimization step.