Enhanced Group Contribution Method Based on Graph Convolution Neural Network

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Although pure chemical properties are essential for the chemical process, many of them are not reported. The experiment measurement, however, often requires too much effort and resources. To avoid these problems, Group Contribution (GC) method is widely used. GC method provides a quick estimation, but its accuracy is questionable for complex molecules and isomers. Molecular-Graph Convolution Neural Network (M-GCNN) was introduced to overcome this limitation. M-GCNN made a successful prediction by analyzing atoms one by one based on neighbors. But it shows limitation that it requires large amounts of experimental data. In this work, we proposed a new model; Group Contribution-Graph Convolution Neural Network (GC-GCNN); for the pure property prediction. GC-GCNN learns from the GC connection relationship, which effectively reduces the required data. NIST and DIPPR experimental data source were used for training and testing. GC-GCNN prediction results showed better agreement with the properties where relatively small experimental data exist, compared with M-GCNN. Furthermore, we were able to extrapolate suspected data from database by predicting the trained data.