Adaptive neural sequence-to-sequence model to predict reaction pathway

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Finding organic synthesis pathways for new molecules has a lot of scientific significance, but it is very difficult because it requires a lot of experimentation that requires too much manpower, time, and resources. Therefore retrosynthetic analysis, which is a method to design a synthetic pathway to target molecules from starting molecules has been studied. Many algorithms have been developed in many studies, but most have been finding new paths based on reaction rules extracted from organic chemical information. Recently, however, an end-to-end training model has been proposed as a data-driven approach that does not require organic chemical information, one of which is the seq2seq model. This model, consisting of an encoder-decoder structure, has been widely used in machine translation studies. Recent studies have used the seq2seq model for reaction pathway prediction. In this study, in order to improve learning performance over existing models, we use a separate network for each reaction class. As a result, it showed higher performance than the previously announced work.