Optimization of Copolymerization Conditions for Novel Copolymers Using Existing Polymerization Data and Physical Information

Hiromu Yamada
Nara Intitute of Science and Technology

Polymer properties depend on polymer characteristics such as molecular weight and monomer composition ratios. We have previously developed machine learning approaches to optimize polymerization conditions for desired polymer characteristics. However, these methods require individual data collection and model construction for each copolymer, limiting practical applications for novel copolymer development.

This study aims to construct a machine learning model that enables optimization of polymerization conditions for novel copolymers for which polymerization data have not been accumulated. The model is a DKL-VAE model that integrates the dimensionality reduction capability of Variational Autoencoder (VAE) with the predictive capability of Gaussian Process Regression (GPR).

This model used 88-dimensional features comprising 22 quantum chemical descriptors for four reaction patterns in the initial copolymerization stage. These features were reduced to 7-dimensional latent variables via VAE. The GPR model was constructed using these latent variables and experimental conditions (initiator concentration, solvent/monomer ratio, monomer proportion, reaction temperature, residence time) as inputs to predict number-average molecular weight.

Through iterative learning to minimize GPR prediction errors, we optimized the VAE transformation process for molecular weight prediction. The predictive accuracy of the DKL-VAE model was evaluated using Leave-One-Monomer-Out cross-validation across five copolymer systems (GMA-co-MMA, St-co-MMA, CHMA-co-MMA, THFMA-co-MMA, PACS-co-MMA).