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Heterogeneous Transfer Learning for Chemical Process Optimization: A Kinetics Perspective

The IFP group is a leader in research and training in the energy and environmental sector, particularly in the development and commercialization of catalysts. Building accurate predictive models for these catalysts usually requires expensive and time-consuming experiments. To make this process more efficient, it's helpful to leverage existing data from previous generations of catalysts. This is where transfer learning comes, as it allows knowledge gained from modeling older catalysts to be applied to new ones, improving accuracy and reducing the need for large amounts of new data. A first attempt using a Bayesian transfer approach demonstrated promising results: it lowered both development time and cost by transferring data and models from a previously studied fossil-based catalyst (the source) to a new one from the same fossil domain (the target). However, this approach assumes that the models for the source and target catalysts share the exact same structure, which can be a limiting factor. In contrast, this work investigates heterogeneous transfer learning strategies, where the target model includes an extra feature and parameter. Two cases are studied, with and without knowledge of the target model structure. In both settings, the proposed heterogeneous transfer learning techniques achieve good performance on synthetic data sets.

Special/ Invited session

Classification

Both methodology and application

Keywords

Heterogeneous Transfer Learning, Heterogeneous Bayesian Transfer Learning, Deep Heterogeneous Transfer Learning

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Track Classification: Machine Learning