[BIOINFO 2023]

Multi-Task Aware Learnable Prototypes on Few Shot learning for Molecular Property Prediction

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Molecules have multiple properties, which should be learned as multi-task learning. However, learning a model for multiple tasks is challenging since the model needs to be optimized for multi-tasks simultaneously. This multi-task learning has recently been explored as few-shot learning. The goal of few-shot learning is to learn a model for multiple tasks that can be quickly adapted to related but unseen tasks with a few samples. Despite promising advances in few-shot learning based molecular property prediction, existing methods depend highly on the support set in a specific task, which leads to insufficient information sharing among multiple tasks. Thus, existing methods are limited in reflecting the multiple properties of molecules. To overcome this limitation, we propose Multi-Task aware Learnable Prototypes (MTLP) on few-shot learning for molecular property prediction, which incorporates multi-task information as well as task-specific properties. Specifically, for task-aware embeddings, we design an attention mechanism using Gumbel-softmax with temperature scaling, to measure relationships between molecules and prototypes. For multi-task perspective, we design meta-learning framework with two contrastive losses between support set molecules and learnable prototypes. In extensive experiments on four widely used benchmark datasets for predicting molecular properties, we demonstrate that MTLP outperforms the existing state-of-the-art methods. In addition, the ablation and case studies show the effectiveness of the proposed learnable prototypes in terms of learning molecular embeddings on multiple properties.