Computer Science
Defense

Deep Learning Approaches Towards Computerized Drug Discovery

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Abstract: Proposing a new drug candidate is an essential part of the drug discovery process, consisting of many sub-tasks. Traditionally, these tasks have been tackled by chemistry and pharmaceutical experts and take years to design. Therefore, this thesis aims to accelerate drug discovery by proposing deep-learning models that accomplishes these tasks effectively and quickly. For the target identification problem, we propose new feature selection methods for both disease-related and prognosis-related features. Next, we propose a new drug-target interaction model to perform the drug re-purposing task. In this model, we present a new molecule representation to overcome the limitation of the current models. We also propose a novel drug generation model that can modify an existing drug to meet given molecule properties. For each project, we present an empirical evaluation to show the competency of the proposed approaches. In addition, we also provide analyses or case studies to demonstrate the practicality of our approaches.

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