

Modern Machine Learning Methods for Drug Design

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Abstract

Drug design has evolved from what used to be a mainly serendipitous process to a multi-billion dollar effort that attempts to develop novel molecules based on scientific reasoning. In this process, industry has adopted computational technologies that enable it to reason the underlying physics and chemistry of molecular processes. Traditional structure and ligand based methods have proved to be very valuable for identification of hit compounds and for lead optimisation. In recent times, deep learning has taken off and shown breakthrough results in technology domains such as computer vision, natural language processing and many other areas. This makes the application of these algorithms very inviting for drug design purposes. In this presentation, a general introduction to the modern machine learning methods will be provided. We will also discuss various ways in which deep learning has started influencing several aspects of drug design during the last few years, and explore select studies rooted in deep learning that try to solve key problems in the drug design pipeline.

Key words: machine learning, deep learning, inverse molecular design, reinforcement learning