Graph Neural Network-Based Reinforcement Learning for Controlling Biological Networks - the GATTACA framework

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Cellular reprogramming, the artificial transformation of one cell type into another, has been attracting increasing research attention due to its therapeutic potential for complex diseases. However, identifying effective reprogramming strategies through traditional wet-lab experiments is time-consuming and costly.

In this talk, we explore the use of deep reinforcement learning (DRL) to control Boolean network models of complex biological systems, such as gene regulatory and signalling pathway networks. We introduce the Graph-based Attractor-Target Control Algorithm (GATTACA), a framework designed to solve a novel, general target-control problem for BN models of biological networks under the asynchronous update mode, specifically in the context of cellular reprogramming. To facilitate scalability of GATTACA, we consider our previously introduced concept of a pseudo-attractor and we improve our procedure for effective identification of pseudo-attractor states. Then, we incorporate graph neural networks with graph convolution operations into the artificial neural network approximator of the DRL agent's action-value function to leverage the available knowledge on the structure of a biological system and to indirectly, yet effectively, encode the system's modelled dynamics into a latent representation.

Experiments on a number of large-scale, real-world biological networks from literature demonstrate the effectiveness and scalability of our approach.