Monte Carlo Tree Search for Antibody Design

Scope

This project may be instantiated as a Master's project or thesis. Prior knowledge in Reinforcement Learning and Deep Learning is recommended.

Problem setting

Antibodies can be utilized for the treatment of various diseases such as cancer. However, designing antibodies is challenging task due to the combinatorial explosion of potential amino acid sequences that represent antibodies. By focusing on the CDRH3 region of an antibody, which suffices for most antibody specificity, we can reduce the search space to 20^{11} possible sequences. However, this is still an enormous search space requiring efficient exploration.

Method

In recent years Reinforcement Learning methods based on Monte Carlo Tree Search (MCTS) have shown their efficacy in tasks with large search spaces such as the game of Go.
Building upon the insights from [AlphaZero](#) and [MuZero](#) we want to apply such methods to the antibody design task.

As a blackbox for antibody evaluation we use the [Absolut!](#) framework.

Roadmap

We propose the following roadmap for this project:

1. Implement a MCTS algorithm or utilize a public implementation [repository](#).
2. Validate your code on a simple environment (e.g. Lunar Lander).
3. Adapt the algorithm to utilize the Absolut! framework.
4. Evaluate different "Tree Policies" and "Default Policies" for efficient exploration.

Organization

If you are interested in this project, write an email to nrprojects@informatik.uni-freiburg.de with a clear reference to this project proposal or contact vogty@cs.uni-freiburg.de.