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Title:
XAI and ML to predict and understand phage-bacteria interactions from genomic data

Abstract:
Phage therapy is a promising alternative to traditional antibiotics for the treatment of bacterial infections. However, there are still several challenges in phage therapy that need to be addressed. In this work, we focus on three needs in phage therapy that can be addressed using genomic information: selecting phages for a given bacterium, improving phage activity, and extracting understanding elements from predictive models.

To deal with the first challenge I present two approaches for predicting phage-bacteria interactions from genomic information: Inphinity and Deep Inphinity. The former extracts informative features from bacterial and phage genomes to then build machine learning-based predictive models. The latter uses deep learning, more specifically, a 1D convolutional neural network, to build a predictive model directly on both genomic sequences. I present its results on two datasets. I also discuss ongoing efforts to use more recent approaches such as transformers.

To deal with the second challenge, I present PERPHECT, a novel architecture for modifying phage genomes to improve their antibacterial activity. The architecture consists of a genome generator that proposes novel or modified phage genomes, coupled with our interaction predictor used to evaluate the generated phage genomes. I present three generative methods we are currently exploring: recurrent neural networks, generative adversarial networks and simulated phage evolution, as well as the results obtained up to now.

Finally, I discuss our next research direction which applies methods from eXplainable artificial intelligence (XAI) to interpret both the predictive and generative models. This will allow us to extract insights into potential mechanisms and biological functions involved in the phage's antibacterial activity.

Overall, our work highlights the potential of combining genomic information and machine learning in addressing key challenges in phage therapy.