Predicting Anti-cancer Drug Combinations with Machine Learning

In her Master’s Thesis titled “Predictive Modeling of Anticancer Efficacy of Drug Combinations”, Heli Julkunen, a student of Life Science Technologies at Aalto University, presents a novel computational approach for predicting anti-cancer effects of drug combinations. The proposed method can perform highly accurate predictions of drug combination efficacies in individual cancer cell lines, having the potential to aid the discovery of novel combination therapeutics.

The fundamental challenge of modern cancer drug development is to design therapies with maximal effectiveness and minimal side effects, tailored for each patient according to the characteristics of the particular type of cancer and the individual genomic background. Anti-cancer drugs are often administered in combination to prevent the emergence of drug resistance, improve the therapeutic efficacy and reduce the side-effects of the treatment. However, as the number of possible drug combinations is essentially limitless, computational methods are required to accelerate the discovery of new drug combinations.

In her Master’s Thesis, Heli Julkunen developed a computational framework for predicting the anticancer effects of drug combinations in individual cancer cell lines. The method uses an efficient machine learning model which utilizes the multidimensional structure of the underlying data. The practical applicability of the method was demonstrated not only in predicting effects among already known drug combinations, but also in extending the predictions to novel drug combinations. The proposed method was shown to perform highly accurate predictions of the anti-cancer efficacies of drug combinations, significantly outperforming simpler approaches.

Given the high cost of experimental screening of drug combinations, this method could provide time- and cost-effective means towards prioritizing the most promising drug combinations for further experimental and clinical validation. This could enhance our understanding of the combined effects of drugs, ultimately having the potential to provide guidance for precision medicine application of these therapeutics and accelerate the development and expansion of drug combination therapeutics in cancer treatment.

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