CompBioMed Conference 2019

Deep Learning in Cancer Drug Response Prediction

Rick Stevens
Argonne National Laboratory
University of Chicago

Artificial intelligence and machine learning (ML) specifically is having an increasing significant impact on our lives. Since the early wins in computer vision from deep learning (DL) in the 2010's, deep neural networks have increasingly been applied to hard problems that have defied previous modeling efforts. This is particularly true in chemistry and drug development where there are dozens of efforts to replace the traditional drug development computational pipelines with machine learning based alternatives. In Cancer drug development and predictive oncology there are several cases where DL is beginning to show significant successes. In our work we are applying deep learning to the problem of predicting tumor drug response for both single drugs and drug combinations. We have developed drug response models for cell lines, patient derived xenograft (PDX) models and organdies that are used in preclinical drug development. Due to the limited scale of available PDX data we have focused on transfer learning approaches to generalize response prediction across biological model types. We incorporate uncertainty quantification into our models to enable us to determine the confidence interval of predictions. Our current approaches leverage work on attention, weight sharing between closely related runs for accelerated training and active learning for prioritization of experiments. Our goal is a broad set of models that can be used to screen drugs during early stage drug development as well as predicting tumor response for pre-clinical study design. Results to date include response classifications that achieve >92% balanced classification accuracy on a pan-cancer collection of tumor models and broad collection of drugs. Our work is part of joint program of investment from the NCI and DOE and is supported in part by the US Exascale Computing Project via the CANDLE project.