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Machine Learning as a new Approach to Network Medicine

predict safety and side effects of drug combinations

Wednesday, 26th of June 2019, 3pm
HS E1, Lecture Hall Center, 3pm
Auenbruggerplatz 50

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Large datasets are being generated that can transform biology and medicine. Artificial intelligence and machine learning methods are necessary to unlock these data and open doors for scientific discoveries.

In this talk, I will start by describing a new methodology for large-scale predictive modeling of drug combinations. The use of drug combinations, is common to treat patients with complex or co-existing diseases. However, patients are at a high risk of adverse side effects, which emerge because of drug-drug interactions, in which activity of one drug changes if taken with another drug. To tackle this challenge, we captured molecular, drug, and patient data for all drugs prescribed in the U.S. We then developed deep learning methods that allowed us to, for the first time, predict safety and side effects of drug combinations. I will show how we can validate such predictions in the clinic using real patient data.

These new machine learning methods set sights on new frontiers in sciences. In the second part of the talk, I will discuss how the new methods enabled us to predict what diseases a new drug could treat and gave us insights into therapeutic mechanisms of drugs. The methods operationalize insights that diseases are not independent of each other, and that the effects of drugs are not limited to proteins to which they directly bind in the body; instead, these effects spread throughout biological networks in which they act. I will show how the new methods make correct predictions for a large number of recently repurposed drugs, and can operate even on the hardest, yet extremely important, cases when a drug has no indicated disease or when a disease does not yet have any drug treatment. In all studies, we collaborated closely with experimental biologists and clinical scientists to give insights and validate predictions made by our methods.