



PHYSICS COLLOQUIUM: Prediction of protein-ligand binding affinity from sequencing data with interpretable machine learning

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About The Speaker:

H. Tomas Rube is an Assistant Professor in Applied Mathematics at University of California, Merced. His research focuses on developing machine learning methods for discovering the grammar whereby proteins read genetic sequences, with the goal of designing synthetic regulatory circuits. Previously, Tomas was a Postdoctoral Researcher at Columbia University and University of California, San Francisco. He obtained his Ph.D. in Physics from Stanford University.

Abstract:

Sequence recognition is critical for cellular information processing and allows proteins to physically interact with specific nucleic acid or polypeptide ligands. Such interactions are increasingly profiled at high throughput using affinity selection and massively parallel DNA sequencing. However, these assays do not provide the biophysical parameters that most rigorously quantify molecular interactions. This seminar will discuss how to measure these parameters using a combination of machine learning and upgraded high-throughput experiments. Specifically, we will discuss how predictions of protein-DNA interactions improve when the machine learning is constrained by domain knowledge, and how the absolute strength of these interactions can be predicted based on a new experiment called KD-seq. When coupled with a new experiment screening randomized peptides, these computational methods also can profile the kinetics of kinase-substrate interactions. Altogether, these results illustrate how improved methods for data integration unlock new experiments and provide a more quantitative view of molecular recognition.

Date:

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Time:

10:30 AM - 11:50 AM

Location:

Granite Pass 135

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