

Simons Machine Learning Center at the New York Structural Biology Center

The Simons Machine Learning Center (SMLC) is a new Simons Foundation funded initiative that is part of the Simons Electron Microscopy Center at the New York Structural Biology Center in New York, NY. Machine learning is transforming structural biology from data collection and structure determination to structure and function prediction. At the SMLC, our mission is to develop machine learning algorithms and software for understanding the structures of biological molecules. We are building a team of machine learning, computer vision, and computational biology experts to push the boundaries of machine learning and structural biology. As part of NYSBC, we have unprecedented access to state-of-the-art instruments (including electron microscopes, NMR, and X-ray), technologists, and structural biologists. We are well-funded and growing quickly.

Project Overview

New computational methods are needed to accelerate cryo-EM and cryo-ET and to extract biological insights from cryo-electron micrographs and tomograms. We are developing machine learning approaches for automating cryo-EM data collection, analyzing micrographs and tomograms, and inferring protein structures from this data. Machine learning methods will enable automatic data acquisition and incorporate on-the-fly feedback during collection to drive increased collection throughput and reduce instrument downtime. The ability to annotate biological structures within massive microscopy and tomography datasets remains a major bottleneck to extracting biological insights from this data. Within this domain, we are especially interested in un-/self-supervised and pose-invariant methods for learning representations of biomolecules that can power new ways to automatically identify and categorize biomolecules in these images. Furthermore, there remain massive gaps in our ability to understand protein function from structural data. New structural determination methods incorporating strong prior knowledge over protein structures will allow us to solve challenging structures with less data. Proteins are also flexible machines and the ability to model proteins as continuous distributions over structures is critical to better understanding their functions.

Job Description

We are looking for Postdocs and Research Scientists to join SMLC to develop machine learning and computer vision methods for analyzing cryo-EM and cryo-ET data. Candidates interested in other aspects of structural biology, particularly protein structure prediction and generative modeling, will also be considered. Applicants should have a strong quantitative background with coding experience, be interested in structural biology applications, and be motivated to learn. Good communication skills and the ability to work independently are musts.

Candidates should expect to:

- Invent and implement new machine learning algorithms for addressing diverse problems in computer vision with application to structural biology
- Conduct experiments and analyses
- Collaborate with experimentalists and hardware technologists
- Publish and present findings at machine learning, computational biology, and/or structural biology venues

Requirements

- PhD in computer science, computational biology/bioinformatics, statistics, physics, or other similar quantitative fields
- Strong coding ability. Experience with machine learning and linear algebra libraries (e.g. numpy, pytorch, tensorflow) is a plus
- Experience working with biological structure data is a plus
- Experience with high performance computing/GPU computing is a plus
- Research experience in machine learning, computer vision, natural language processing, bioinformatics, or other related fields
- Ability to work independently, motivated to learn
- Strong communication skills

Benefits at NYSBC

- Access to significant compute resources and state-of-the-art instruments including 7 Titan Krios microscopes
- Located in NYC, remote work is optional
- Competitive salary
- Generous retirement package
- Medical and dental coverage

Start date: ASAP.

Contact: For more information, please reach out to Tristan Bepler (tbepler@nysbc.org). To apply, please include your CV, a brief cover letter, and contact information for 3 references.