Learning to Learn, Learning to Forget

The ability to rapidly learn from high-dimensional data to make reliable predictions about the future of a given system is crucial in many contexts. This could be a fly avoiding predators, or the retina processing terabytes of data almost instantaneously to guide complex human actions. In this work we draw parallels between such tasks, and the efficient sampling of complex molecules with hundreds of thousands of atoms. Such sampling is critical for predictive computer simulations in condensed matter physics and biophysics, including but not limited to problems such as crystal nucleation and drug unbinding. For this we use the Predictive Information Bottleneck (PIB) framework developed and used for the first two classes of problems, and re-formulate it for the sampling of biomolecular structure and dynamics, especially when plagued with rare events. Our method considers a given biomolecular trajectory expressed in terms of order parameters or basis functions, and uses a deep neural network to learn the minimally complex yet most predictive aspects of this trajectory, viz the PIB. This information is used to perform iterative rounds of biased simulations that enhance the sampling along the PIB to gradually improve its accuracy, directly obtaining associated thermodynamic and kinetic information. We demonstrate the method on two test-pieces, including benzene dissociation from the protein lysozyme, where we calculate the dissociation pathway and timescales slower than milliseconds.

Department of Physics
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Theoretical and Applied Physics

Fall 2019

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University of Maryland
Dept. of Chemistry & Biochemistry & Institute for Physical Science and Technology

Wednesday, November 13th

4:00 PM

Innovation Hall

Room E430

Refreshments will be available at 3:30 PM.

In E217

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Biography:

Pratyush Tiwary is an Assistant Professor just starting his 3rd year at the University of Maryland, College Park, with a joint position in the Department of Chemistry and Biochemistry and the Institute for Physical Science and Technology. He is also an affiliated faculty member of the Chemical Physics program and the Biophysics programs. He received his PhD and MS in Materials Science from Caltech, working with Axel van de Walle, and finished his undergraduate degree in Metallurgical Engineering at the Indian Institute of Technology, Varanasi. Prior to starting his tenure-track position, he has been a postdoc at Columbia University, where he worked with Bruce Berne, and at ETH Zurich, where he worked with Michele Parrinello. His interdisciplinary research themed around statistical physics has been recognized through Doctoral New Investigator Award from ACS Petroleum Research Fund, Future of Biochemistry award from the journal Biochemistry, and is being highlighted in the Emerging Investigator special collection by the Journal of Chemical Physics.