Seminar

Learning Optimal Collective Variables for Biophysical Processes via Dimension Reduction

Satyabrata Bandyopadhyay

TCIS, Hyderabad

Computer simulation has now become a very popular method for modelling biologically relevant processes on both spatial and temporal resolution at an atomistic scale. With the advent of GPU-based hardware coupled with modern algorithms over the past several decades, molecular dynamics (MD) simulations are currently sampling bio-molecules at multi-microsecond time scales at a routine basis. Consequently the analysis of these modelled data would be of too large amount to interpret and understand easily. Again these large bio-molecules due to their very subtle inherent complexities are generally associated with a very huge number of dimensions involved in these processes. Hence in order to analyse and interpret these large amounts of high dimensional data we need to have some dimension reduction algorithms to extract the significant and meaningful information to infer nice human interpretation. In my entire work we have performed a series of studies on the learning of some mathematical variables also called Collective Variables to track down such biophysical phenomena. Our analysis revealed that learning the optimal collective variables from dimension reduction is very crucial in order to understand and explain these bio-physical processes. In this talk I will show the works done along this way.

Monday, June 27th 2022

02:30 PM

Auditorium