



THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

Department of Mathematics

PHD STUDENT SEMINAR

BPNET in kinetic lumping

By

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Abstract

Biological events often occur at microseconds timescale, and while simulation tools and computation resources had a large advancement in the past few decades. Getting a reliable sampling of these long-timescale events is still challenging. By splitting the phase space into “states” and consider the dynamics within microstate to be memoryless, one can extrapolate long timescale dynamics through repeated propagation. However, the splitting of phase space itself is a tricky task.

In this work, we have proposed a new lumping method that is based on an objective function related to projection operator. To efficiently find a good lumping, we have also constructed a neural network and take the use the reverse projection score as the loss, which we called BPnet. We will demonstrate that our proposed scheme indeed perform well from simple numerical system to real biological systems.

Date : 3 May 2021 (Monday)

Time : 4:30pm

Zoom Meeting : <https://hkust.zoom.us/j/95161278698> (Passcode: 386237)

All are Welcome!