

Improving Normalizing Flows to Sample from Boltzmann Distributions

Wednesday, 13 April 2022 12:00 (30 minutes)

Sampling from Boltzmann distributions through normalizing flows promises to be computationally much cheaper than molecular dynamics (MD) simulations. However, flows struggle to approximate complicated target distributions due to topological constraints and still heavily rely on MD samples to be trained on. Here, we present two lines of research addressing these issues, the former by introducing a more expressive base distribution for normalizing flows and the latter through a novel bootstrapping training procedure using only samples from the flow as well as the density of the target.

Poster title

Poster

Primary authors: STIMPER, Vincent (Max Planck Institute for Intelligent Systems); MIDGLEY, Laurence Illing; SIMM, Gregor; Prof. SCHÖLKOPF, Bernhard (Max Planck Institute for Intelligent Systems); HERNANDEZ-LOBATO, Jose Miguel (University of Cambridge)

Presenter: STIMPER, Vincent (Max Planck Institute for Intelligent Systems)

Session Classification: Session V