

ML Keynote Talk – Generative models, manifolds and symmetries: From QFT to molecules

Wednesday 2 November 2022 11:15 (40 minutes)

The study of symmetries in physics has revolutionized our understanding of the world. Inspired by this, the development of methods to incorporate internal (Gauge) and external (space-time) symmetries into machine learning models is a very active field of research. We will introduce some of the latest work in the field. We will then present our latest work on invariant generative models and its applications to lattice-QCD and molecular dynamics simulations. In the molecular dynamics front, we'll talk about how we constructed permutation and translation-invariant normalizing flows on a torus for free-energy estimation. In lattice-QCD, we'll present our work that introduced the first $U(N)$ and $SU(N)$ Gauge-equivariant normalizing flows for pure Gauge simulations and its extensions to incorporate fermions.

Presenter: REZENDE, Danilo

Session Classification: ML Keynote Talk