Centro de Investigação em Matemática e Aplicações
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Programa de Doutoramento em Matemática

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DeepParticle: deep-learning invariant measure by minimizing Wasserstein distance on data generated from an interacting particle method

Jack Xin

Department of Mathematics, University of California, Irvine, CA 92697, USA

High dimensional partial differential equations (PDE) are challenging to compute by traditional mesh based methods especially when their solutions have large gradients or concentrations at unknown locations. Mesh free methods are more appealing, however they remain slow and expensive when a long time and resolved computation is necessary.

We present DeepParticle, an integrated deep learning (DL), optimal transport (OT), and interacting particle (IP) approach through a case study of Fisher-Kolmogorov-Petrovsky-Piskunov front speeds in incompressible flows.

PDE analysis reduces the problem to a computation of principal eigenvalue of an advection-diffusion operator. Stochastic representation via Feynman-Kac formula makes possible a genetic interacting particle algorithm that evolves particle distribution to a large time invariant measure from which the front speed is extracted. The invariant measure is parameterized by a physical parameter (the Peclet number). We learn this family of invariant measures by training a physically parameterized deep neural network on affordable data from IP computation at moderate Peclet numbers, then predict at a larger Peclet number when IP computation is expensive.

The network is trained by minimizing a discrete Wasserstein distance from OT theory. The DL prediction serves as a warm start to accelerate IP computation especially for a 3-dimensional time dependent Kolmogorov flow with chaotic streamlines.

Our methodology extends to a more general context of deep-learning stochastic particle dynamics.

This is joint work with Zhongjian Wang (University of Chicago) and Zhiwen Zhang (University of Hong Kong).