Finding Numerical Solutions to Partial Differential Equations With Deep Learning

Molin, Holger (School: Procivitas Privata Gymnasium Helsingborg)

Quasi-stationary distributions underlie a great number of fundamental phenomena and are valuable tools in molecular biology and neuroscience, where they are used to model interactions between molecules. Established methods for approximating them tend to be computationally expensive and scale poorly into high-dimensional cases due to the computational complexity of the meshes used, hindering effective biochemical simulation and the development of future medicines. This paper outlines and evaluates methods for obtaining the density of quasi-stationary distributions belonging to a class of Ornstein-Uhlenbeck processes on a bounded domain. It does so by approximating the solutions to a corresponding class of partial differential equations with the hope of achieving better computational efficiency. The proposed solution attempts to replace the mesh with random point sampling through a physics-informed neural network. To optimize performance, several architectures, hyper-parameters, and algorithms were experimented with. The findings show that changing the hyper-parameter betas could improve convergence five-fold and that methods like learning rate annealing are less successful than previously thought. The final model demonstrates a computational speed-up of 36 times when compared to a Fleming-Viot simulation, a 3% difference in results, and promising scalability into high dimensionalities.

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