Machine learning in biological matter: From molecules to extracting equations of motion

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It is difficult to overemphasize the rapid emergence of articial intelligence (AI) and machine learning (ML) methods across almost all walks of life. In this talk, I will discuss some recent advances and problems in using ML in biological matter for studies structure and dynamics. I will focus on a few cases studies to illustrate these matters. The first is using AI/ML with extended structural to determine the phase behaviour of lipid bilayers [1]. Lipid phase behaviour is complex, and even single component bilayers display rich phenomena: The gel and fluid phases of lipid bilayers are planar and conformationally homogeneous, but the ripple phase, which exists at temperatures between the gel and fluid phases, undulates in an asymmetric sawtooth pattern and consists of heterogeneous conformational clusters. The ML approach developed here is used identify the molecular conformations, and changes in their respective proportions that give rise to the changes. Second, I will discuss computationa modeling of cellular systems and data extraction in them [2,3,4]. Finally, the problem of partial wetting of viscous droplets is discussed [5]. Data from multiphase many-body dissipative particle dynamics (mDPD) simulations is analyzed based on the Physics-Informed Neural Network (PINN) framework to predict the ordinary differential equation (ODE) describing the dynamics of the droplet radius. In addition, the error in the discovered parameters is analyzed using Bayesian PINNs (B-PINNs).

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