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Single-Particle Diffusion Characterization by Deep Learning

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Diffusion plays a crucial role in many biological processes including signaling, cellular organization, transport mechanisms, and more. Direct observation of molecular movement by single-particle-tracking experiments has contributed to a growing body of evidence that many cellular systems do not exhibit classical Brownian motion but rather anomalous diffusion. Despite this evidence, characterization of the physical process underlying anomalous diffusion remains a challenging problem for several reasons. First, different physical processes can exist simultaneously in a system. Second, commonly used tools for distinguishing between these processes are based on asymptotic behavior, which is experimentally inaccessible in most cases.

Finally, an accurate analysis of the diffusion model requires the calculation of many observables because different transport modes can result in the same diffusion power-law a, which is typically obtained from the mean-square displacements (MSDs). The outstanding challenge in the field is to develop a method to extract an accurate assessment of the diffusion process using many short trajectories with a simple scheme that is applicable at the nonexpert level. Here, we use deep learning to infer the underlying process resulting in anomalous diffusion. We implement a neural network to classify single-particle trajectories by diffusion type: Brownian motion, fractional Brownian motion and continuous time random walk. Further, we demonstrate the applicability of our network architecture for estimating the Hurst exponent for fractional Brownian motion and the diffusion coefficient for Brownian motion on both simulated and experimental data. These networks achieve greater accuracy than time-averaged MSD analysis on simulated trajectories while only requiring as few as 25 steps. When tested on experimental data, both net and ensemble MSD analysis converge to similar values; however, the net needs only half the number of trajectories required for ensemble MSD to achieve the same confidence interval. Finally, we extract diffusion parameters from multiple extremely short trajectories (10 steps) using our approach.