Inferring pointwise diffusion properties of single trajectories with deep learning

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In order to characterize the mechanisms governing the diffusion of particles in biological scenarios, it is essential to accurately determine their diffusive properties. To do so, we propose a machine learning method to characterize diffusion processes with time-dependent properties at the experimental time resolution [1]. Our approach operates at the single-trajectory level predicting the properties of interest, such as the diffusion coefficient or the anomalous diffusion exponent, at every time step of the trajectory. In this way, changes in the diffusive properties occurring along the trajectory emerge naturally in the prediction and thus allow the characterization without any prior knowledge or assumption about the system.

First, we benchmark the method on synthetic trajectories simulated under several conditions. We show that our approach can successfully characterize both abrupt and continuous changes in the diffusion coefficient or the anomalous diffusion exponent. Finally, we leverage the method to analyze experiments of single-molecule diffusion of two membrane proteins in living cells: the pathogen-recognition receptor DC-SIGN and the integrin $\alpha5\beta1$. The analysis allows us to characterize physical parameters and diffusive states with unprecedented accuracy, shedding new light on the underlying mechanisms.

We provide a python library with tools to easily reproduce the results, and tutorials to use the proposed method to study other phenomena [2].

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[1] B. Requena et al. *arXiv preprint* arXiv:2302.00410 (2023).

[2] B. Requena and G. Muñoz-Gil. Step python library (github.com/borjarequena/step), December 2022.

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