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Unraveling heterogeneous diffusion in single particle trajectories

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We propose a machine learning method to characterize heterogeneous diffusion processes at a single-step level. The machine learning model takes a trajectory of arbitrary length as input and outputs the prediction of a property of interest, such as the diffusion coefficient or the anomalous exponent, at every time step. This way, changes in the diffusive properties along the trajectory emerge naturally in the prediction, allowing us to characterize both homogeneous and heterogeneous processes without any prior knowledge or assumption about the system. In this work, we showcase the power of the method in various scenarios. We illustrate its capacity to characterize trajectories with zero to ten discrete changes in the diffusion coefficient of the diffusing particle, considering different segment lengths and localization noise levels. Additionally, we show how to use the same method to study continuous changes, such as the aging of the diffusion coefficient, as well as changes in the anomalous exponent. Finally, we provide results studying an experimental system of Integrin α5β1 diffusing in the membrane of HeLa cells. We find two diffusive states with changes in both the diffusion coefficient and the anomalous exponent, and we show that one of these can be related to trapping events.

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