PhD THESIS DEFENSE: Learning particle dynamics: from diffusion to interactions

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10:00

Elements Room and Online (Teams)

Understanding how a complex system works from its components, such as a virus invading a cell or particles aggregating in a liquid, is a fundamental question in the study of nature that provides great biological benefits. To solve this question, it is interesting to observe the path taken by the components of a system, as this contains valuable information that helps us to characterize them and understand how they interact with each other. Advances in the last decade in the field of machine learning offer a promising numerical tool, as they allow the automatic extraction of relevant features and relationships, while also predicting the system's behavior.

In this thesis, we focus on the analysis of particle trajectories observed in complex systems, addressing two fundamental aspects: the random and therefore difficult-to-characterize

individual behavior, as occurs in the lungs, where we inhale air and oxygen diffuses into the capillaries of the alveoli; and behavior due to multiple ways of interacting, in some cases unknown, such as that of a large flock of birds migrating together.
In particular, we consider three problems:
1) the accurate estimation of parameters that characterize the anomalous diffusion observed in biological processes,
2) the identification of significant parameters to describe stochastic processes,
and 3) the extraction of the functional form of the multiple forces present in particle systems.
To tackle each of the problems, we developed a specific machine learning model designed to extract meaningful information from trajectories and rigorously evaluated it on a series of simulated systems with known dynamics.
The first method, KISTEP, predicts anomalous diffusion properties at each time step, for trajectory segments, and for a set of trajectories, allowing for detailed analysis at each level, based on individual trajectories. With this method, we participated in the AnDi Challenge 2, a scientific competition comparing computational methods dedicated to characterizing fractional Brownian motion trajectories that resemble biological phenomena observed in experiments such as cell endocytosis or protein immobilization.
The second method, SPIVAE, helps to identify the minimal representation of stochastic processes thanks to its unsupervised, interpretable, and generative features. Furthermore, it is capable of generating new trajectories that reproduce the learned characteristics of the process. The analysis performed with SPIVAE revealed the expected parameters of BM, fractional BM, and confined BM, while it learned a nonlinear combination in the case of the scaled BM.
The third method, FISGAE, employs a graph neural network to infer in an unsupervised manner the functional form of the forces acting between particles. FISGAE successfully learned the forces between 21 interacting particles with non-reciprocal linear forces, while in the more complex scenario of a Lennard-Jones gas, it learned well the force at short distances.
In conclusion, this research provides methods to facilitate the analysis of particle systems directly from their trajectories, unlocking insights otherwise unavailable. The proposed methods have the potential to benefit experimental and theoretical researchers, and even artificial intelligence developers, by enabling a more comprehensive understanding of complex systems. Furthermore, the developed frameworks are ready for future improvements, which could be achieved through the integration of more sophisticated architectures, thereby paving the way for even more advanced applications and discoveries.

Tuesday October 14, 10:00 h. Elements room
Thesis Director: Prof. Dr. Maciej Lewenstein and Dr. Carlo Manzo

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