Learning inter-particle interactions and active forces from particle trajectories

Miguel Ruiz-Garcia[1], Miguel Barriuso Gutierrez[2], Lachlan Alexander[3], Dirk Aarts[3], Luca Ghiringhelli[4], and Chantal Valeriani[2]
[1]Universidad Carlos III de Madrid
[2]Universidad Complutense de Madrid
[3]Oxford University
[4]NOMAD Laboratory at the Fritz Haber Institute and Humboldt University

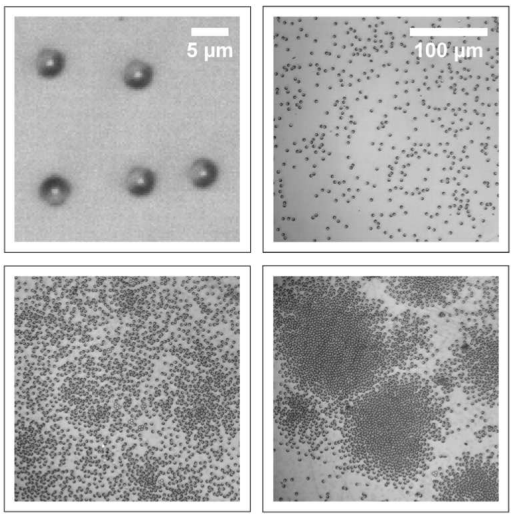

Fig. 1. Motility-induced phase separation in experiment. Panel (a) shows electrophoretic Janus particles when an electric field (E) is applied. They rise to maximise the magnitude of their induced dipoles. Panels (b), (c) and (d) display snapshots of systems in different conditions. Panel (b) shows a system which is too dilute to phase separate ($\phi = 0.10$, $E = 727$). Panel (c) shows a system with an activity that is too low to phase separate ($\phi = 0.29$, $E = 181$). Panel (c) shows a system which phase separates ($\phi = 0.29$, , $E = 363$).

Active particles exhibit complex collective phenomena that emerges from their local interactions.To model such systems, one would usually propose some inter-particle interactions and active forces, simulate the dynamics of a system with many individual elements and finally compare the results with experiments via, for instance, an order parameter. However, not only choosing one order parameter might introduce a bias, but also it is difficult to assess how well the model describes the experimental system. In our work we suggest a completely different approach. What if we could learn the inter-particle interactions and the active forces directly from the data? We propose a machine learning scheme that optimizes the interactions between particles and the active forces to predict the correct particle dynamics. After training the network, one can extract both passive and active interactions between particles and use them (analytically or numerically) to make new predictions or unravel dynamical features of experiments of active particles.

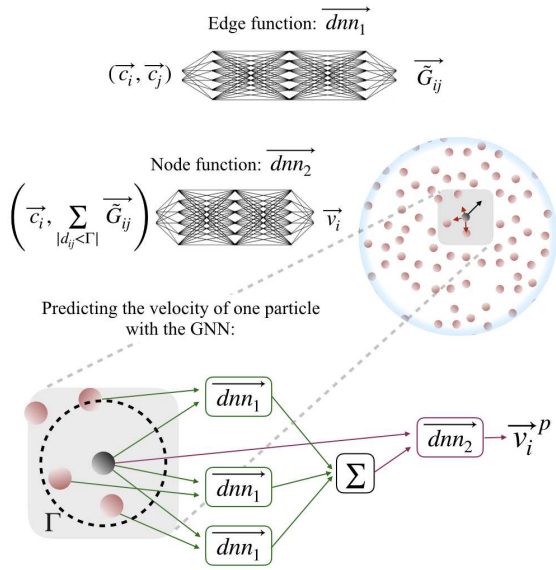

Fig. 2. Predicting the dynamics of active particles with a Graph Neural Network (GNN) while learning the functional form of the inter-particle interactions and the active forces. Our GNN is formed by a node function $\vec{dnn}_1$ and an edge function $\vec{dnn}_2$. Both, $\vec{dnn}_1$ and $\vec{dnn}_2$, are deep neural networks that take the particle coordinates $\vec{c_i}$, the diagrams shown in the figure are just for visualization. After training, the output of $\vec{dnn}_2$, $\vec{v_i}^p$, will be the predicted velocity for particle i. The bottom diagram shows how the GNN is applied to one particle. Applying the GNN to all particles in the system (the graph) provides all the predicted velocities. During the learning process the internal parameters of $\vec{dnn}_1$ and $\vec{dnn}_2$ are optimized so that all the $\vec{v_i}^p$ resemble the real velocities and we can extract the forces present in the system.