SOE 19: Machine Learning in Dynamics and Statistical Physics (joint session DY/SOE)

Time: Friday 10:00–11:15 Location: H19

SOE 19.1 Fri 10:00 H19

Reinforcement learning of optimal active particle navigation — •Mahdi Nasiri and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

In sufficiently complex environments, there is no simple way to determine the fastest route of an active particle that can freely steer towards a given target. In fact, while classical path planning algorithms (e.g. A*, Dijkstra) tend to fail to reach the global optimum, analytical approaches are incapable of handling generic complex environments. To overcome this gap in the literature, in the present work, we develop a policy gradient-based deep reinforcement learning method that employs a hybrid continuum-based representation of the environment and allows, for the first time, to determine the asymptotically optimal path in complex environments. Our results provide a key step forward towards a universal path planner for future intelligent active particles and nanorobots with potential applications in microsurgery as well as in drug and gene delivery.

SOE 19.2 Fri 10:15 H19

Deep reinforcement learning for chemotactic active particles — •Edwin Loran, Mahdi Nasiri, and Benno Liebchen — Institute of Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt, Germany

Throughout evolution, microorganisms have developed efficient strategies for locating nutrients and avoiding toxins in complex environments. Understanding their adaptive policies can provide new key insights for the development of smart artificial active particles. Here, we use a machine learning approach, namely deep reinforcement learning, to develop smart foraging strategies for chemotactic active particles which consume nutrients for their survival. Our method is able to devise efficient chemotactic navigation strategies guaranteeing "survival" inside unknown and complex landscapes while only having access to local sensory data. Our approach is based on deep Q-learning and uses the particle's observation of its surrounding chemical (nutrient) concentration as the input. The presented method highlights the extent of the capabilities of reinforcement learning approaches in mimicking (and going beyond) the evolutionary strategies learned by microorganisms.

SOE 19.3 Fri 10:30 H19

Machine Learning the 2D percolation transition — •Djénabou Bayo[1,2], Andreas Honecker[2], and Rudolf A. Römer[1] — [1]Departement of Physics, University of Warwick, Coventry, CV47AL, United Kingdom — [2]Laboratoire de Physique Théorique et Modélisation (LPTM) (CNRS UMR8089), CY Cergy Paris Université, 95302 Cergy-Pontoise, France

The percolation model is one of the simplest models in statistical physics displaying a phase transition. A classical lattice is occupied randomly with a given probability at each site (or bond). A phase transition from a non-percolating to a percolating state appears around the so-called percolation threshold. Machine Learning (ML) and Deep Learning (DL) techniques are still relatively new methods when applied to physics. Recent work shows that ML/DL techniques seemingly detect the percolation transition from images of percolation clusters. We employ such supervised learning techniques, i.e., classification and regression for 2D site percolation. We find that the identification of spanning clusters provided by such methods does not fully correlate with their existence. Rather, the identification seems to rely on proxy measures such as the site occupation density. Furthermore, constructing challenging cluster distributions show scope for much misclassification when using even highly trained DL networks. Unsupervised ML strategies, such as variational autoencoders, might be able to reconstruct percolation clusters with acceptable spatial resolution, but in many cases struggle to reproduce the geometry of spanning clusters faithfully. Our work uses Python and the ML/DL libraries of PyTorch.

SOE 19.4 Fri 10:45 H19

Exploring structure-property maps with kernel principal covariates regression — •Guillaume Fraux, Benjamin Helfrecht, Rose Cersonsky, and Michele Ceriotti — Institute of Materials, EPFL, Lausanne, Switzerland

Data analyses based on linear methods constitute the simplest, most robust, and transparent approaches to the automatic processing of large amounts of data for building supervised or unsupervised machine learning models. Principal covariates regression (PCovR) is an underappreciated method that interpolates between principal component analysis and linear regression and can be used conveniently to reveal structure-property relations in terms of simple-to-interpret, low-dimensional maps. We introduce a kernel version of PCovR (KPCovR), and demonstrate the performance of this approach in revealing and predicting structure-property relations in chemistry and materials science.

For large datasets, interactive exploration of the resulting map is a great tool to extract understanding. To this end, we introduce chemiscope, an open source software able to display and explore maps with hundred of thousands of points together with the corresponding molecular or crystal structure. Chemiscope is usable as an online tool, or locally through jupyter notebooks.

SOE 19.5 Fri 11:00 H19

Investigation of plasticity in off-resonant delay-coupled reservoir computing — •Jonas Naujoks[1], Felix Köster[1], and Kathy Lüdge[2] — [1]Institute for Theoretical Physics, Technische Universität Berlin, 10559 Berlin, Germany — [2]Institute of Physics, Technische Universität Ilmenau, Weimarer Str. 25, 98693 Ilmenau, Germany

We analyse the effect of neuronal plasticity on the performance of a delay-based reservoir computer modelled by a generic oscillator with self-feedback. The memory capacity and task-specific performance are investigated in the case of non-resonant delay-clock-cycle configurations. By modifying the temporal multiplexing of the input, the responsiveness of the virtual nodes is maximised while promoting individual decorrelation. The training is done in an unsupervised manner. The effect on the task-specific performance is investigated, while we additionally demonstrate that the memory capacity can be tuned.