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Applications of Machine Learning to Soft Matter

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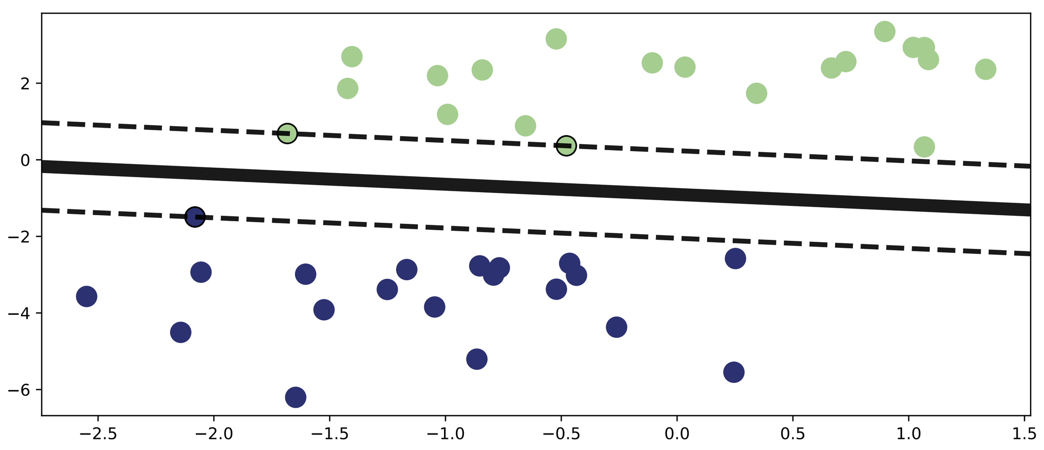
Abstract

With recent developments in Machine Learning (ML) technology, Soft Matter (SM) has been adopting several methodologies to enhance and provide new insights into difficult problems within the field. In this work, we showcase two recent applications of ML to SM systems, namely a data-driven ML model to show how structure is important to glassy dynamics; and a Deep Learning techinique to train ML models in order to detect topological defects in liquid crystals with data from video microscopy experiments. We briefly discuss the advantages and shortcomings of these frameworks, with the hope that future research can adopt some of these ideas and techniques in order to empower problem solving within SM.

Structure and glassy dynamics

In a recent paper [5], Schoenholz *et al.* discovered that structure is an important physical feature to glassy dynamics in three dimensions. By separating particles into two main classes, either *soft* or *hard*, they defined a *softness* parameter using a classifier to accomplish such task.

A particle is determined as soft if it is likely to rearrange, and hard otherwise. These parameters are defined through "structure functions" [6] that preserve the overall isotropic symmetry of the system and include radial density and bond angle information. These functions serve as the feature vectors, and a training set is built with this information. Using a particular classifier called a Support Vector Machine (SVM) [4], the softness of a particle i, S_i, is defined as the shortest distance between its position in the feature space span by the corresponding feature vectors, and the hyperplane that separates both clases, either soft, when $S_i > 0$ or hard, $S_i < 0$.



It is important to note here that SVMs are ML models that do not scale well with large datasets, but the main takeaway of such models is that its formulation is mathematically rigorous and well understood. Here, the important aspect of using a SVM is to give meaning to the classification mechanism of such models in a physical problem.

References

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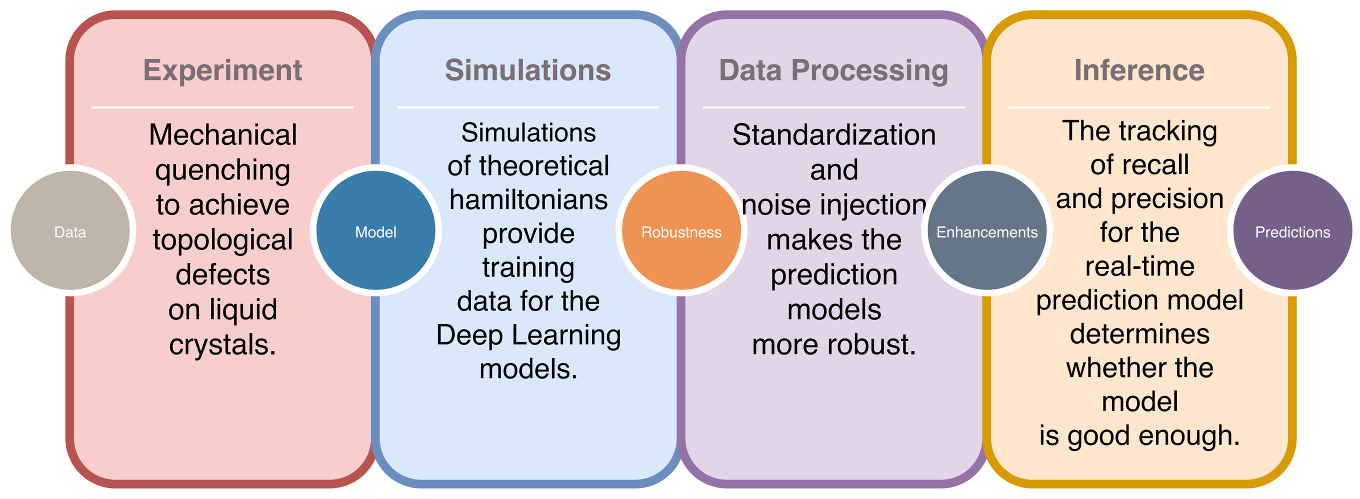
Deep Learning and Video Microscopy



ML technology has also aided the development of robust and fast experimental setups. One such example was developed by Minor *et al.* [7] in a recent work where an end-to-end ML framework, together with simulation data, was created in order to provide an accurate study of topological defect annhilation in liquid crystals.

The complete framework consists of a typical topological defect experiment using a mechanical quencher and video microscopy. In the experiment, the liquid crystal is always ensured to be on the smectic phase. This will provide some of the *testing data*, a dataset that will no be used as input into the ML model. Instead, simulation of the XY model is carried out, with randonmly placed topological defects. With this new dataset, together with a subset of the video microscopy data, will comprise the full traning dataset.

One of the most important outcomes of this methodology is the fact that by having trained a ML model with enough robustness, the same apparatus can be used with different topological defects, with minimal modification of the ML model. This constitutes an important achievement in the sense that modern ML frameworks can be used not only with simulation data, but with experimental data as well.

Discussions

Acknowledgements

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