COMMENTARY

Learning active nematics one step at a time

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Machine learning, ranging from regression to deep learning by neural networks, is a set of powerful data analysis tools. Deep learning is especially suited for data-rich but model-limited fields of study, where it has indeed proved to be remarkably successful in tasks such as object and speech recognition. In physics, which aims to describe natural phenomena in terms of universal laws, the application of machine learning tools has been slower, but is gaining traction in recent years (1). The study by Colen et al. (2) applies neural networks as an analysis tool for active-nematic systems, illustrating how these new approaches can provide experimental physicists with better tools to analyze their data. This can involve extracting unknown model parameters from data in systems that are sufficiently well understood, as well as entirely data-driven forecasting approaches that can be used even in the absence of a model.

The use of machine learning for the analysis and prediction of high dimensional spatiotemporal dynamics is an exciting prospect (3). This is nicely demonstrated by the application of deep neural networks to the study of active-nematic systems (2, 4). The machine learning-based approach is particularly beneficial in situations where a direct measurement of all the relevant degrees of freedom, or of the underlying parameters, is not possible. In the former case, if the information about other degrees of freedom is contained within the observed dynamics, it can be extracted and encoded by the neural network. For the inference of unknown parameters, neural networks can be thought of as nonlinear approximators, which smoothly map spatiotemporal patterns to the parameters of the model. More generally, neural networks effectively provide a dimensionally reduced approximation to the full dynamical system.

Applying machine learning to data is more subtle than simply running a known algorithm, as the approximations involved are not yet fully understood or controlled. In particular, it is beneficial to incorporate the physics of the problem in the architecture of the network, including conservation laws, knowledge of the underlying symmetries, and an informed choice of relevant variables as input. For example, in Colen et al. (2), such choices include the use of convolutional and recurrent layers for the parameter inference, to account for the space and time translational invariance of the system, and the use of an input representation of the active nematic that respects its invariance to local reflections.

The focus of the paper by Colen et al. are nematic systems driven by internal forces (5). The microscopic constituents of a nematic system are elongated objects that, as in liquid crystals, have long-range orientational order in the nematic phase. In a continuum description, the local microscopic alignment is represented by a mesoscopic director field, which together with the local velocity of the fluid, are the two relevant fields. Unlike liquid crystals, however, active nematics have internal driving, which produces active stresses, locally injecting energy into the system and exciting flows. A widely used realization of active nematics is networks of cytoskeletal filaments with their associated molecular motors (2, 4, 6, 7). The latter generate active forces: Powered by ATP, they "walk" along filaments, constantly attaching and detaching, and promote filament sliding. Apart from their biological relevance, active nematics hold a promise for material design and control, by changing the level of activity and harnessing the resulting flows. On a more fundamental level, active nematics are a basic model system of an intrinsically out-of-equilibrium material, which is experimentally realizable and controllable (5).

Modeling active-nematic systems is challenging since the microscopic building blocks are nontrivial and their interactions are complex, while an effective coarse-grained approach may not capture all the relevant aspects (8). The simplest coarse-grained model uses the hydrodynamic theory of liquid crystals with the addition of an active stress (5). The elastic free

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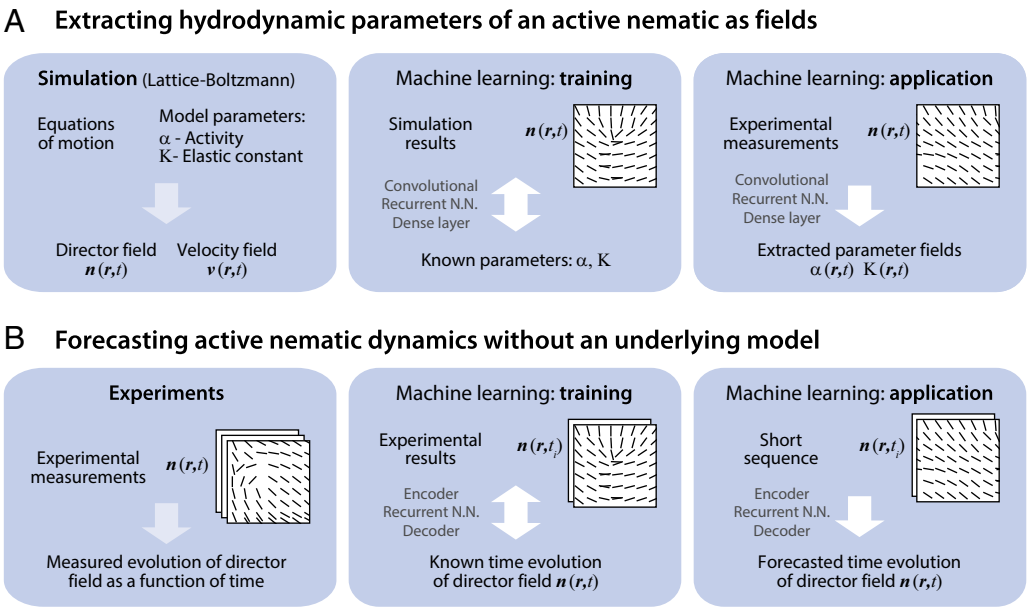

Fig. 1. Machine learning approaches for studying active-nematic systems. (*A*) The workflow for a machine learning approach for extracting hydrodynamic parameters in an active-nematic system characterized by a known model. (*B*) The workflow for a data-driven machine learning approach for forecasting the evolution of an active-nematic system from a short time sequence of nematic fields.

energy of the liquid crystal penalizes gradients of the director field, with an energetic cost proportional to an elastic constant, K. The active stress is modeled to be proportional to the nematic order parameter, with the proportionality constant, α, quantifying the level of activity. At nonzero activity, flows containing energetically costly defects are spontaneously generated, becoming fully chaotic at high enough activity (2, 5, 9).

Overall, the activity and the elastic constants are the two main parameter sets that control the behavior of an active nematic. However, experimentally, these two types of parameters are often hard to separately control or directly measure: e.g., molecular motors both produce active forces and act as cross-linkers, so changes in motor activity (e.g., by varying ATP concentrations) affect both K and α. In addition, it is often challenging to directly measure both the director and velocity fields, and while the two are coupled, it is difficult to infer the latter from a direct measurement of the former. Instead, Colen et al. (2) developed a machine learning approach to estimate the activity and nematic elasticity of two-dimensional (2D) and 3D active-nematic systems solely from the dynamics of the nematic field (Fig. 1*A*).

Based on direct numerical simulations of the hydrodynamic equations, a neural network is trained to learn the mapping between the dynamics of the director field and the elasticity and activity parameters, K and α (Fig. 1 *A*, *Left*). The measurement algorithm is validated using model simulations, comparing the known model parameters with those inferred by the algorithm (Fig. 1 *A*, *Middle*). This approach is subsequently used to analyze experimental data from different cytoskeletal setups (6, 7, 10) (Fig. 1*A*, *Right*). Previous measurements of the model parameters often relied on quantification of average properties such as the defect density, which can be reliably calculated only if there are enough defects in the system (7, 11). In contrast, the machine learning approach takes into account all local fluctuations of the nematic field. While it is unclear on which features the inference relies, this approach yields more accurate estimates and allows to observe changes in both K and α when varying experimental control parameters such as ATP concentration (2). In addition, the machine learning approach is able to operate well even in the low-activity regime where defects are scarce or in 3D where the common excitations are disclination loops (10).

Experimental developments in active nematics now enable spatiotemporal variation in the activity and elasticity (12). Although Colen et al. use constant parameters in the training of their neural network, they are able to map such variations as demonstrated by the inference of imposed changes in the activity and nematic elasticity. The same type of analysis can also be used to examine the patterns that emerge in experimental systems that are nominally homogeneous. Here, the analysis identified an internally generated temporal variation, primarily in the activity field, suggesting collective dynamics attributed to motor binding and unbinding (2).

While the hydrodynamic theory discussed above seems to capture the qualitative features of experiments quite well, quantitative agreement is more challenging to obtain (7, 11, 13). Apart from the difficulty of matching parameters, the theoretical models themselves might be incomplete. For example, the temporal variations in the activity observed by Colen et al. are unaccounted for in the mesoscopic theory. If predictions of the dynamics are desirable, this motivates the use of model-free techniques, which is the focus of the second part of the work by Colen et al., as well as another recent work (4), which forecast the short time evolution of the nematic director field based on a time series of snapshots (Fig. 1*B*).

Even though a specific physical model is not employed in this approach, incorporating physical insight into the algorithm is important. For example, the use of a residual neural network considering the differences between subsequent frames (rather than the nematic field itself) is particularly suited for the inference in dynamical systems whose evolution is described by partial differential equations (2, 14). In addition, to reduce noise, Colen et al. implement a "sharpening step" in which the predicted nematic field is smoothed after each application of the neural network by minimizing the elastic energy of the nematic in the

regions between defects (while retaining the defects), reflecting the inherent tendency of nematic constituents to locally align.

Remarkably, the machine learning approach is able to predict key defect events, including generation (also called defect unbinding), motility, and annihilation (2, 4). While the ability to forecast the behavior of a chaotic system is inherently limited, the machine learning approach appears to predict the short-time behavior of active-nematic systems well, outperforming the predicted dynamics calculated using a simulated system with fitted parameters (2). Furthermore, the long-term behavior of the nematic field generated by the neural network has similar statistical characteristics to the experimental observations (e.g., with regard to the average defect density) (2). This is a nontrivial feature of the machine learning approach developed by Colen et al., which is not a direct corollary of the ability to provide reasonable short-term predictions (4), but rather suggests that the neural network has managed to encode a faithful representation of key aspects of the dynamical system.

The use of machine learning in physics is growing in different directions, following the exciting developments in other fields such as computer science and engineering. The study by Colen et al. exemplifies how these new approaches can be harnessed to extract model parameters in a chaotic dynamical system, and provide a data-driven, model-independent approach to forecast its spatiotemporal dynamics. The latter can be particularly relevant for living systems, where nematic fields characterizing, e.g., cytoskeletal alignment or cellular orientations can be identified, and their topological defects have recently been shown to be correlated with biological function (15, 16). Given the importance of biological signaling and regulation in living systems, it will be insightful to examine to what extent predictions based solely on the nematic field can forecast their behavior. From a materials engineering perspective, designing active matter provides an attractive avenue for generating "smart materials" that are able to change their properties in response to their environment (12). The ability to predict the complex behavior of such systems can facilitate the realization of closed-loop feedback control, able to steer and direct active-nematic systems to produce, e.g., a desired flow pattern or structure. More generally, the application of machine learning techniques to problems in physics holds much promise, the realization of which will require a deep understanding of both the machine learning algorithms and the physics of the system at hand.

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