HIGH SCHOOL EDITION
Journal of Student Research
Volume 12 Issue 1 (2023)

The Applications of Machine Learning in the Study of Liquid Crystals: A Review

Dmitri Kalinin[1] and Jason Abercrombie[1#]

[1]Webb School of Knoxville
[#]Advisor

ABSTRACT

Discovered in the 19th century, liquid crystals have only grown more prominent in the last thirty to forty years as a result of electric fields being able to influence their nematic directors. Since these nematic directors can polarize light, liquid crystals have found extensive uses in the field of optoelectronics, including being in many of the devices (such as computers, phones, and tablets) that we have today. With the continued desire to improve these optoelectronic devices comes the desire to improve the liquid crystal systems that help to compose them. The growth of machine learning technologies has been near the forefront of these efforts to improve the efficiency and effectiveness of the development of these systems. In an effort to recognize this prominence, this article presents a review of machine learning's presence and use in the study of liquid crystals, as well as a comparison of machine learning techniques and more traditional experimental methods.

Introduction

Overview of Liquid Crystals

Liquid crystals (LCs) are a type of soft matter whose physical and structural properties bridge the flow properties of a liquid and the symmetrical properties of a crystal. Because of the bridging between solid and liquid properties, liquid crystals have a variety of phases, with some phases having more properties of a liquid and some phases having more properties of a solid. There are two common types of liquid crystals: thermotropic, whose phases change with temperature, and lyotropic, whose phases change with concentration of the mesogen, the main compound of the liquid crystal, in the solution. The main phases of thermotropic LCs are depicted in Figure 1. The nematic phase, the phase that is more like a liquid, has molecules that can be aligned nonuniformly and whose alignments can be influenced by external electric or magnetic fields (like a liquid), and these can act as polarizers for light (like a solid crystal). Its molecules only possess orientational ordering and no positional ordering. This makes nematic liquid crystals extremely prevalent in devices such as optical displays and sensors due to these properties, making them very useful materials (de Gennes and Prost, 1995). The local orientation of liquid crystal molecules can be represented via directors on the mesoscopic level, and many studies of LC implement this concept when analyzing LCs. The smectic phase is the phase that is more like a solid than a liquid, retaining some positional ordering as well as having orientational ordering. To explain the positional ordering more in depth, smectic LCs are constrained to a set of parallel planes, and every director points the same direction relative to these planes, which is where the differentiation in smectic phases comes in. In the smectic A phase, the smectic directors point perpendicular to the plane, whereas in smectic C phase it is some other direction relative to the plane. This enables films to be made out of smectic phases, which are examined extensively due to being a platform to study 2-dimensional fluid dynamics (Oswald and Pieranski, 2005), in studies such as the OASIS studies (Klopp et al., 2019). When heated too much, the LCs will become conventional liquids,

called the isotropic phase as it is characterized by isotropic motion, losing all its molecular ordering. Some LCs also exhibit phases with anisotropic ordering.

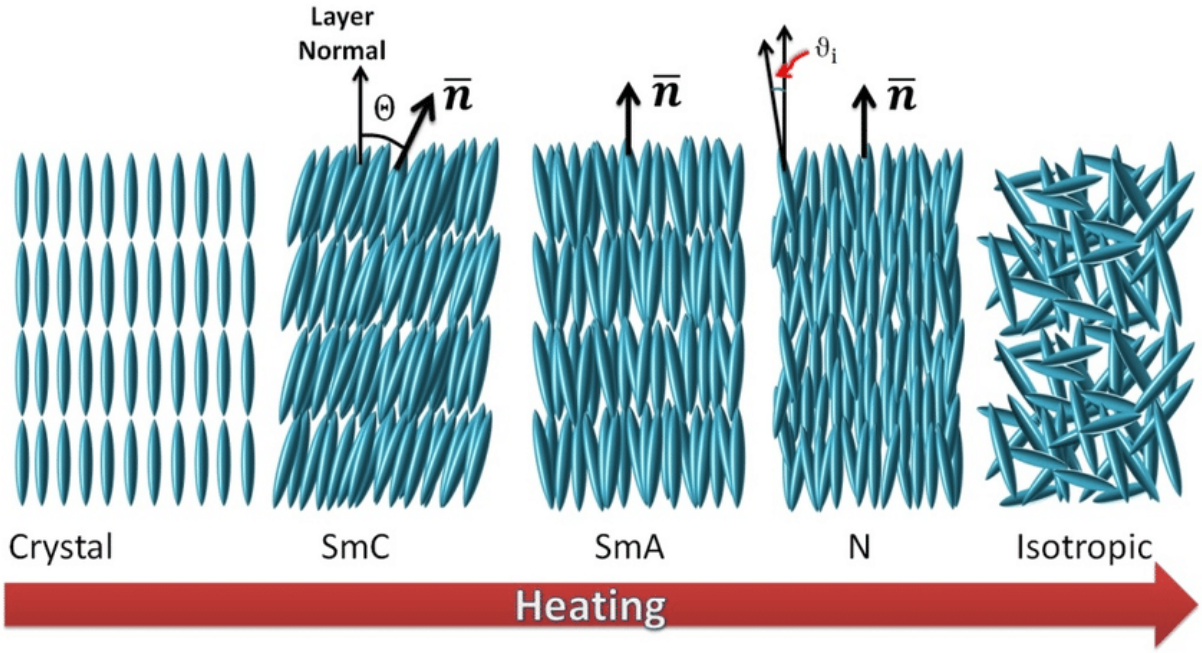

Figure 1. A figure depicting the different phases of thermotropic liquid crystals and their occurrence with increasing temperature, from a solid crystal to an isotropic liquid. As the material gets more heated, it goes from solid crystal to smectic C phase to smectic A phase to nematic and then to isotropic, gradually losing molecular ordering during each phase. In the transition between the solid and smectic phase, the material loses some positional ordering, making the positional ordering only in one direction. In the transition from smectic to nematic, the material loses all positional ordering, only possessing translational ordering. In the transition from nematic to isotropic, the material loses all molecular ordering. Figure used with permission from Dierking and Al-Zangana, 2017.

Like most other types of soft matter, the physics of liquid crystal systems still need to be studied further. The main theoretical models used to describe liquid crystals were developed for other physical phenomena that are extended to liquid crystals. The Onsager model is a theoretical model that has been used to describe liquid crystal systems in equilibrium through dipole-dipole interactions (Onsager, 1931), but it has been generalized to deal with nonequilibrium active matter systems (Yang et al., 2016), finding much use in theoretical liquid crystal study. Another important theoretical model was the Ising model, a statistical mechanical model that details interactions between different molecular spins whose planar form has been applied to computational and theoretical approximations of some liquid crystal systems, especially pertaining to phase transitions and quantitative ordering (Yurke et al., 1997). The XY model is another statistical model developed for liquid crystal systems that has been developed for understanding more complex systems and phase transitions, but, unlike the Ising model, matter following the Ising model cannot have an ordered phase at low temperature, giving use for the Ising model in that case as well (Rojas and Rutenberg, 1999).

However, as the technologies using liquid crystals become more developed, liquid crystals with more specific physical and structural properties are to be desired, such as the procedure to find the nematic order parameter (de Gennes and Prost, 1995). Many traditional experimental techniques to try and optimize and analyze these properties of liquid crystals for these novel technologies are very time consuming, and the time spent performing these techniques to find liquid crystals with specific optimized properties will only increase as time passes. Thus, machine learning has been introduced as an alternative to these time-consuming experimental techniques.

Overview of Machine Learning

Machine learning has grown rapidly over the past 30 years, and has been implemented in many scientific fields to help aid in classification, recognition, and analysis of many phenomena, especially with imaging. Liquid crystals have been particularly popular to study with imaging techniques, as the material is birefringent, so most of its physical properties can be derived using an optical microscope. Additionally, the advent of databases such as LiqCryst, an online compilation of vast amounts of properties of liquid crystals, has made machine learning with liquid crystals easier due to the increased availability of big datasets (Vill, 1995).

Overview of Common Types of Machine Learning Algorithms

A hierarchy of machine learning methods is presented in Table 1. Machine learning can be split into two different categories: supervised learning and unsupervised learning. In supervised learning, both the input and output data is labeled for model training. However, in unsupervised learning, only the input data is labeled.

Table 1. Categorizing machine learning algorithms based on type of learning, tasks used for, and computational complexity.

Machine Learning Method	Type of Learning	Tasks used for	Computational Complexity
Multi Linear Regression	Supervised	Regression	Very low
K-nearest neighbors	Unsupervised	Classification	Low
Support Vector Machine	Supervised	Classification, Regression	Medium
Decision Tree	Supervised	Classification, Regression	Medium
Random Forest	Supervised	Classification, Regression	Medium High
Genetic Algorithm	Reinforcement	Decision Making	Medium
Feedforward Neural Network	Supervised	Classification, Regression	High
Recurrent Neural Network	Supervised	Time-series classification, regression, decision-making	High
Convolutional Neural Network	Supervised	Classification, Regression, Detection	High

.

The simplest machine learning algorithm is Multi Linear Regression (MLR), where the output is linearly related to all of its inputs. Some studies in this review use k-nearest neighbors' classification, where the function is evaluated with the help of already known local functions (it's k nearest neighbors) to separate data into groups based on similarity measure (Peterson, 2009). Another type of machine learning model used is the Support Vector Machine (SVM). This model relies on the construction of a hyperplane, which is how it can be used to differentiate between two classes (Noble, 2006). This construction of a hyperplane can also be used for regression models via finding a

hyperplane that closely approximates all the data (Trafalis and Ince, 2000). Another algorithm that can be used for both classification and regression is a decision tree, which splits sets of data based on rules until every data point in a subset has the same output (Song and Lu, 2015). An algorithm that extends on the concept of decision trees is a Random Forest (RF), which combines randomized decision trees and averages the prediction (Biau and Scornet, 2016). Another type of machine learning model used in this area of research is Genetic Algorithms (GAs), where initial populations of networks are chosen and the ones that are the best are chosen to reproduce their attributes, including some mutations to keep introducing random noise to the model doesn't converge to a solely local optimum (Sutton and Boyden, 1994).

Many of the machine learning models used in the studies that will be discussed are types of neural networks (NNs). Neural Networks consist of input layers, hidden layers, and output layers, all with neurons that have a weight and a bias. At each layer, the input array for that layer will be multiplied by the weights array of the hidden layer and then summed with the bias array for that layer, which is how the input layer can change its shape to match that of the output layer (Abiodun et al., 2018). The weights and biases are optimized via gradient descent, a technique that uses backpropagation and a learning rate to adjust the weights and biases so they can minimize a loss. The first, and simplest, of the machine learning networks that will be discussed is the feedforward neural network (FNN). It takes a 1-dimensional array as input, and returns a one-dimensional array as output after a series of hidden layers with an arbitrary amount of neurons called perceptrons (Abiodun et al., 2018). The second type of neural network used in these studies is a Convolutional Neural Network (CNN). These types of networks take 2-dimensional, 3-dimensional, or 4-dimensional inputs (depending on if 1-dimensional convolution, 2-dimensional convolution, or 3-dimensional convolution is used). The convolution then occurs, taking a section of the image (a kernel) and performing a convolution operation on that matrix, turning it into an array that is multiplied by the weights and biases of a normal neural network layer. This is repeated for every possible kernel in an array (Gu et al., 2017). The third type of neural network that is used very often is Recurrent Neural Networks (RNNs). These networks perform on sequential data, and turn the sequential data into a single array of numbers (Elman, 1990). Other types of networks that only show up in one source will be explained when that source is elaborated on.

Overview of Scope of Review Article

This review article will be discussing three different areas of liquid crystals study which machine learning has had a massive impact on: analyzing physical properties of liquid crystals, analyzing the structural and dynamical properties of liquid crystals, and designing liquid crystal systems with the desired properties. This article will also be comparing the results of studies that use machine learning to similar studies that don't use machine learning wherever it is applicable to put these studies into more perspective, and comparing different machine learning methods used in similar studies to compare the effectiveness of each method, when applicable.

Using Machine Learning to Find Quantitative/Binary Correlations in LCs

One of the many uses of machine learning is to test if a correlation exists between certain input variables and an output variable, as a basic machine learning model will learn if there is a correlation and won't if there isn't. Thus, machine learning has found uses in correlating physical properties of LCs and, in some cases, providing further insight into the physics of LCs.

Classifying Between LCs and Non-LCs

An application of machine learning to find correlations is first seen in identifying a compound as a LC or not, primarily through determining if the compounds would exhibit LC behavior. A feedforward neural network that was optimized

via a genetic algorithm was able to classify between liquid crystals and not liquid crystals with similarly structured organic compounds based on length of the rigid core, length of flexible core, molecular diameter, and total weight with 99% accuracy for the training dataset and 83.33% accuracy for the testing dataset (Lisa and Curteanu, 2007). A machine learning algorithm was able to classify between liquid crystals and not liquid crystals given numerous molecular descriptors, numbers that could be derived from a mathematical operation from the raw LC structure, from the LiqCryst database with training set accuracy just under 100% and testing set accuracy in the high 80s percent. Multiple types of machine learning frameworks were tested, including the Support Vector Machine (SVM), k-nearest neighbors (KNN), the Random Forest, Adaboost (a framework that takes the accurate parts of generally poorly trained classifiers to theoretically form the ideal classifier through some weight adjustment), and three Decision Trees with varying depths, but the Random Forest and SVM models performed the best. Descriptor sets from the DRAGON and RDKit software, including adding extra inputs of molecular fingerprinting, were used to see which set would perform better on the dataset, (Chen et al., 2018).

Finding Quantitative Physical Properties of LCs

Another application of machine learning to find correlations is using known physical properties, derived physical properties or images to find other quantitative physical properties of LCs. Specific properties of interest in many of these studies include sample temperature, phase transition temperature, and order parameter for nematic LCs, and pitch length for cholesteric LCs, as these are properties that cannot be observed easily or quickly using traditional experimental methods. Multiple input features of ML models have been used to tackle this problem, and here three are discussed: Quantitative Structure Property Relationships (QSPRs), Ordinal Methods derived from the image, and directly using the image for the machine learning model.

Using QSPRs for ML of Physical Properties of LCs

A more common input feature to use for these simple ML models to predict LC properties are QSPRs, certain quantitative properties calculated using the structure of the LC using theoretical methods, such as Density Functional Theory (DFT) or the AM1 quantum chemical method. Using two-ring and three-ring LC compounds, a feedforward neural network was able to predict the clearing temperature of the set of LCs with a pairwise correlation coefficient of 0.983 for the testing set (Johnson and Jurs, 1999). A MLR model was able to determine nematic transition temperature of LCs with two aromatic rings linked to an ester group with varying terminal chains using nine descriptors calculated using the PM3 theory with an R-squared value of 0.9217 for all 42 LC data points (Villanueva-Garcia et al., 2005). A Multi-linear regression model was able to calculate the nematic transition temperatures of LCs with two aromatic rings linked to an ester group with varying terminal chains using six descriptors calculated using DFT, which proved to be comparable to other MLR models using descriptors calculated by different methods (Al-Fahmi, 2014). Based on eight different descriptors of molecules that all shared a COO- chain linking two terminal hydrocarbon chain, a Radial-based function neural network, a feedforward neural network with only one hidden layer and a radial-based function (whose value at any point is solely dependent from the distance from the input to some other point) for an activation function in the hidden layer (Karayiannis and Mi, 1997), was able to predict the phase transition temperature for these types of molecules with an R-squared value of 0.953, performing better on validation data than the Support Vector Machine model trained on the exact same data (Gong et al., 2008). Using six descriptors of LCs with the exact same specifications as Al-Fahmi's study, both MLR and feedforward neural networks were tested to predict the nematic-isotropic transition temperature, with the neural network performing better on both training and validation sets than the MLR model (Fatemi and Ghorbanzand'e, 2009). The superior performance of nonlinear models compared to linear models was further supported in a study one year later (Xu et al, 2010). Machine learning models were able to use 5 descriptors of LCs containing pyridine to find the nematic-isotropic transition temperature with high accuracy. Although MLR models performed well (with an R-squared value of 0.976), the nonlinear regression models, the SVM

and the projected-persuit regression models, had higher R-squared values for both training and validation sets. (Ren et al., 2017). On a broader dataset of LCs, consisting of 243 five-ring aromatic compounds with varying terminal chains, linkage groups, and substituents on central and outer rings, a Multi-Automated Regression Splines model was able to achieve an R-squared value of 0.900 using 2-dimensional and 3-dimensional descriptors, performing better than the Support Vector Machine (Antanasijevic et al., 2016). From 15 input features describing the structure of an array of LC beads, a random forest regression model was able to find the phase transition temperature with a coefficient of determination of 0.943, and from those 15-input feature plus the phase transition temperature, was able to predict the order parameter with a coefficient of determination of 0.894 (Inokuchi et al., 2019).

The Use of Ordinal Methods as Input Features

One particular method that has grown in popularity for the use as input features for machine learning models is the use of ordinal methods, which consist of estimating a probability distribution of the occurrence of ordinal patterns in an image. A fast and scalable k-nearest neighbors' algorithm has proved to be viable in measuring properties of liquid crystals, such as the temperature and the order parameter, based on the statistical complexity and the permutation entropy which is derived directly from the optical image using ordinal methods, 99% when trained on Monte Carlo simulation training data and 93% on experimental data of nematic textures of E7 liquid crystals. (Sigaki et al., 2019). The algorithm was also able to accurately predict the pitch of a cholesteric LC given the same inputs. When only using either the statistical complexity or the permutation entropy as input features for a machine learning algorithm to determine the order parameter of a LC, the accuracy of the model decreased by 6% (Sigaki et al., 2019). The same type of algorithm was able to classify between first and second order nematic phase transitions very accurately, building off the ordinal methods that were used to approximate both the permutation entropy and statistical complexity in (Sigaki et al., 2019) by introducing ordinal networks, which also analyze transitions among ordinal patterns in an image, analyzing the change of ordinal patterns of liquid crystal textures. (Pessa et al., 2022).

Using Images as Input Features

Another popular method for machine learning of physical properties of LCs is using the optical image as the input to the model (with some preprocessing). This method can predict it directly from the image, reducing computational time, and it shows the power of machine learning through the models not knowing any of the physics of the systems. From extracting the RGB values of blocks of an image, a feedforward neural network was able to predict the temperature of a thermotropic LC with extremely high accuracy. In fact, it performed better than the previous method of classifying temperature as a function of LC hue (Grewal et al., 2006), showing the promise of machine learning in these studies. More recently, the use of Convolutional Neural Networks in these types of studies has allowed for easier and more accurate prediction of these physical properties. A study used Convolutional Neural networks to find the order parameter of nematic LCs and the pitch length of cholesteric LCs directly from the optical image. For the network finding the order parameter of nematic LCs, the coefficient of determination on the testing set was 0.997 with four Convolutional layers, outperforming an earlier study that used a k-nearest neighbors' algorithm that used permutation entropy and statistical complexity. For predicting the pitch length of cholesteric liquid crystal, the network became 100% accurate at 3 and 4 convolution blocks, showing the promise for an extremely direct method to predict cholesteric pitch length in experimental configurations when the helical axis of the LC is perpendicular to the viewing direction of the optical microscope (Sigaki et al., 2020).

Machine Learning for Structure and Dynamics of LCs

More complex machine learning networks and/or data preprocessing techniques have shown usefulness in studies of structural and dynamical properties of liquid crystals. Problems of great interest in this field include studying LC phases and phase transitions, prediction of structural dynamics, predicting external stimuli from LC response, studying defects, and studying active nematics.

Studying LC Phases and Phase Transitions

A more specific application of ML to LC structure involves predicting LC phases and phase transitions. One such use has been in distinguishing between nematic and smectic-like structures in liquid crystal polymers, with the use of a random forest model that took order parameters (such as the local McMillan order parameter and the local Onsager order parameter) as input features. Using Sequential Forward Selection, which selects a number of input features from a set of input features that will yield the highest accuracy for the model (Mani and Kalpana, 2016), the most useful order parameters for the analysis of prediction between phases was selected. This provided a better alternative to manually selecting the order parameter(s) that are best suited for classifying that LC system (Doi et al., 2019). Using the machine learning framework by Doi et al. to find the order parameters needed, a machine learning network was able to ease the analysis of multistep phase transitions in anisotropic liquid crystal system, as the order parameter was needed for a complete analysis of the system (Takashi et al., 2021). Using multiple different combinations of a set of 13 input features describing molecular composition and environmental conditions of different liquid crystalline molecules (including temperature), machine learning models were able to predict the existence of a mesophase for that material in those conditions. They found that the ANN performed better than the MLR model for all different sets of descriptors used (Le and Tran, 2019). Another study used a different dimensionality reduction algorithm with a random forest regression to help correlate structural parameters with the occurrence of a ferroelectric nematic phase, which assisted greatly in the design and research of these ferroelectric nematics for eventual use for LC systems with very high dielectric constants (Li et al., 2021). Using infrared spectral data of the liquid crystal 12BBAA (4-bromobenzylidene-4′-dodecyloxyaniline), a k-means clustering algorithm was able to determine the phase of that liquid crystal based on temperature. However, with a window clustering algorithm, that splits the spectral data into wavenumber ranges (the “windows”) and performs k-means clustering analysis on each window to determine the phase in each spectral subset, the study was able to further analyze the melting of the alkyloxy chains within the compound, extracting even more useful information from the complex infrared spectra (Oscieka-Drewniak et al., 2021).

Predicting Structural Dynamics of LCs

Another use of machine learning in studying structure and dynamics has been the prediction of certain structures and dynamics that will arise in certain situations. Through the use of genetic algorithms, a study was able to compute LC director configurations by computing which configuration had the least free energy for a variety of LC systems, such as hybrid cells, 90-degree twist cells, and twisted nematic cells, making the process less time-consuming then the manual methods used beforehand, especially due to how many LC systems the model can be applied to (Yang and Collins, 2020).

Through the use of a diffusion map, a dimensionality reducing algorithm to find the input features that yield high accuracy for the model (Coifman and Lafon, 2006), similar to Sequential Forward Selection, a study used machine learning to correlate the pitch and radius of helicoidal trajectories of chiral twist-bend nematic phase LCs with the pitch and conical angle of the twist-bend nematic phase (Chiappini et al., 2019).

Machine Learning Dynamics of LC Response to External Stimuli

Machine learning has also been used to determine certain external stimulants based on a liquid crystal's optical response to them, either mechanical or chemical. This has a very direct application in improving the potential for liquid crystals as both chemical (Shah and Abbott, 2001) and mechanical (Ireland and Jones, 2000) sensors. A study used a SVM algorithm to classify what environment a LC was in with 99% accuracy, significantly higher than the 60% accuracy of the sensor achieved via traditional means (Cao et al., 2018). To do this, it used Alexnet (Krizhevsky et al., 2012) to extract features from the optical image of the LC under the microscope, using those extracted features as input features for the SVM classifier. Building off this study, another study used an SVM to predict using features extracted from the newer pretrained VGG16 network (Simonyan and Zisserman, 2014) for image analysis as opposed to Alexnet. The classifier performed as accurately, but less features were required to make it perform up to the level of the SVM produced by Cao et al., increasing computational efficiency of this extremely accurate method (Smith et al., 2020).

In the field of analyzing mechanical stimuli to liquid crystals, a study was able to accurately predict the shear and stress on LCs for sensing the shear stress vector for shear sensitive liquid crystal coating images (Zhao et al., 2022). Although not really improving on the accuracy using traditional methods, the learning method is both more computationally efficient (enabling almost real time prediction) than the original Gaussian curve fitting method and is able to be used in more experimental settings than traditional methods.

Studying LC Defects

One particular phenomenon that is the focus of many studies is defects in liquid crystals, with two main defects of interest being topological defects in nematic LCs and isotropic droplets and pancake layers in smectic LCs. Topological defects are a phenomenon with nematic LCs when the nematic directors lose their order because they want to minimize the stress, rotated by a certain angle around the defect, the angle depending on the topology of the system. The defects are named based on the winding number, which is the number of radians the director rotates around the defects, by 2 pi, with the most common in LCs being +½ and -½ defects (Wenzel et al., 2020). Because of the misalignment of the nematic directors, defects will result in poorer performance of liquid crystals for the optoelectronic applications they are most commonly used for, but the motion of defects can also be an indicator of whether a biological material is extensive or contractive (Kawaguchi et al., 2017). Thus, analyzing the instances and motions of topological defects within liquid crystal systems is of great interest in the field. On the flipside, the alignment of nematic directors is easy to tell from under a microscope (as the different orientation of the directors would polarize incoming light differently), so the use of machine learning has found much potential in the analysis of optical images to classify and detect topological defects in liquid crystals. The use of Convolutional Neural networks and a diverse dataset produced a multi-object detection network for topological defects in smectic phase films that had a maximum mAP score of 0.841. Because of how much data is required to train a multi-object detection network based on the YoloV2 algorithm, the algorithm was trained on simulation data to make it less time consuming as opposed to experimental data. Simulations based on the XY model (specifically the Landau-Ginzberg interpretation) yielded the most accuracy when applying the model to experimental data, which became as accurate as humans while taking much less time, showing improved performance on the machine learning model (Minor et al., 2019). Additionally, FNNs and RNNs have been used to classify the types of defects within LC cells with high accuracy using simulation data of the LC, which gave the model the x-coordinate, the y-coordinate, and the angular orientation of N rod-like molecules ordered by their label. The FNNs required presorting of the data based on position to perform well due to the off-lattice nature of the defect classification, but the RNNs performed well with just the raw data due to their ability to recognize sequential patterns within the data, which invites the further use of RNNs into studies of topological defects of liquid crystal materials. (Walters et al., 2019). From the RGB data of topological defects within a LC produced by a polarized microscope that used phase contrast and polarize functions to color different orientation angles differently, a machine

learning algorithm was able to determine the order parameter of the system and the orientation angle for each pixel of an image, providing a orientation and order map for the study to help in the analysis of the change of molecular ordering in the presence of topological defects (Sakanoue et al., 2021).

Classifying topological defects is also a problem of great interest. From a 10 by 10 kernel of principal directors surrounding a topological defect, with the defect located in the center, an Artificial Neural Network was able to classify whether a defect was a +½ or -½ defect (Wenzel et al., 2020).

Defects can also show up in smectic films in the form of pancake smectic layers or isotropic droplets in the films, and ML has been used for detection of these defects to delve further into the physics of smectic films. A SVM was used to detect droplets in smectic films, outperforming TrackPy (a non-ML computer vision algorithm for blob detection) and serving to be very useful for quick detection of bubbles in smectic films, even if they are obscured somewhat (Hedlund et al., 2021).

Active Nematic Dynamics

Another interesting phenomenon that ML has been applied to is for predicting the dynamics of active nematics, which are nematic phases that are out of thermodynamic equilibrium. In these systems, the defects exhibit dynamics and the whole system is under chaotic flow, and many methods have been developed to stabilize defect trajectories (Doostmohammadi et al., 2018). Although it is known that the dynamics of active nematics depend on the symmetries of the system (Marenduzzo et al., 2007), the physics of active nematic flows not thoroughly explored due to the chaotic dynamics of those types of systems (Tan et al., 2019), making it perfect for machine learning. Since much of the emphasis of the study of active nematics is on defect dynamics, studies initially used non-machine learning particle tracking algorithms to analyze defect dynamics (Wenzel et al., 2020). With the increased usage of the Recurrent Neural Network and the Convolutional Neural Network in scientific studies, machine learning has been employed to forecast the dynamics of active nematic systems. A variant of an autoencoder algorithm that encodes each image in a sequence into feature vectors, then applies a RNN layer to that time series to then encode it into the image of the nematic director dynamics that is going to happen. This was able to do so only using the spatiotemporal data of the image without any other theoretical assumptions, and it proved to be accurate both before and after the Lyapunov time, the time when a nonlinear dynamic system becomes chaotic. Additionally, this performed well on both experimental and simulational data, showing the applicability of the model that doesn't have information about the physics behind the system to predict dynamics. (Colen et al., 2020). In fact, it performed better on experimental data than the Lattice-Boltzmann simulations, which have knowledge of the underlying physics. A network with Convolutional LSTM layers was also able to predict the behavior of nematic liquid crystal systems in both experimental and simulation settings (Zhou et al., 2020). Due to the experimental data in this study not containing all of the active nematics in the system, the studies cannot be compared on experimental data to see which architecture performed better in forecasting active nematic dynamics.

The Future of ML in LC Research

With the use of machine learning in LC research only becoming more widespread as the years progress, there is no doubt that there is still much in store for new ML techniques applied to LC research and new applications of ML to LC research.

For one, reinforcement learning, a subset of machine learning where an agent learns by maximizing its reward given the state of the environment it is used (Sutton and Barto, 1998) that has often been used for algorithms to play video games (Mnih et al., 2013), has found uses in the field of soft matter, such as in the production of circular-shaped colloidal crystals (Zhang et al., 2020), showing that reinforcement learning can be used for liquid crystal study as well, such as through accurate structural modeling. Additionally, reinforcement learning has shown the ability to exploit

interactions to produce desirable dynamics in systems (Liu et al., 2021), which shows its promise in the field of active nematics.

Another type of algorithm that could be used in the future of LC Research is a Generative Adversarial Network (or GAN), which consists of two networks: a generator and a discriminator. The discriminator is trained to discern AI-generated data from real data, and the generator is trained on fooling the discriminator (Goodfellow et al., 2014). It has already been applied to modeling particle showers in electromagnetic calorimeters in high energy physics (Paganini et al., 2018), as well as in constructing 3D electrode microstructures (Gayon-Lombardo et al., 2020), showing promise for its application in modeling both active and passive liquid crystal structures.

With the GAN and reinforcement learning algorithms gaining more popularity in the scientific community, this invites a new use for machine learning in LC research: to design LCs for certain purposes. Li et al. (2021) used a machine learning framework to help find parameters that would lead to the occurrence of a ferroelectric nematic phase, but the design of liquid crystals was not done using ML. However, with the increased popularity of GANs and reinforcement learning in the scientific community, including works using machine learning and GANs to model and produce desirable properties of a system of materials, it is a logical next step for ML to be used directly in the design of LCs and LC systems with desirable properties.

At the moment that this paper was written, ML techniques are only applied for one component of the experimental pipeline. With machine learning's already proven potential as an alternative to time-consuming experimental and by-hand techniques for measuring properties, it is only a matter of time before ML is incorporated into more autonomous experiments. Machine learning was able to extract valuable kinetic parameters from multiple polymerization reactions combined with semi-autonomous experimentation, enabling for mostly autonomous experimentation of polymerization catalysts. This increased autonomy in the experiment reduced both the time for catalytic discovery to occur and the chemical waste produced by a matter of hours (Rizkin et al., 2020), which shows not only the potential for autonomous experimentation in the study of LCs but also underscores the merits of doing so.

Acknowledgements

I would like to thank my mentor, Jason Abercrombie, for guiding me through the research process. My research process was made much easier by his great guidance of how I should conduct my research, his recommendations for how to convey the information I want to tell for a research paper, and his constant support.

References

Abiodun, O. I., Jantan, A., Omolara, A. E., Victoria, K., Mohamed, N. A., & Arshad, H. (2018). State-of-the-art in artificial neural network applications: a survey. Heliyon, 4(11), e00938. https://doi.org/10.1016/j.heliyon.2018.e00938

Al-Fahemi, J. H. (2014). QSPR study on nematic transition temperatures of thermotropic liquid crystals based on DFT-calculated descriptors. Liquid Crystals, 41(11), 1575-1582. https://doi.org/10.1080/02678292.2014.934310

Antanasijevic, J., Pocajt, V., Antanasijevic, D., Trisovic, N., & Fodor-Csorba, K. (2016). Prediction of clearing temperatures of bent-core liquid crystals using decision trees and multivariate adaptive regression splines. Liquid Crystals, 43(8), 1028-1037. https://doi.org/10.1080/02678292.2016.1155769

Biau, G., & Scornet, E. (2016). A random forest guided tour. Test, 25(2), 197-227. https://arxiv.org/pdf/1511.05741.pdf

Cao, Y., Yu, H., Abbott, N. L., & Zavala, V. M. (2018). Machine learning algorithms for liquid crystal-based sensors. ACS sensors, 3(11), 2237-2245. https://doi.org/10.1021/acssensors.8b00100

Chen, C., Tanaka, K., and Funatsu, K. (2018). Random Forest Model with Combined Features: A practical approach to Predict Liquid-Crystalline Property. Molecular Informatics, 38(4), 1800095. https://doi.org/10.1002/minf.201800095

Chiappini, M., Patti, A., and Dijkstra, M. (2019). Helicoidal dynamics of biaxial curved rods in twist-bend nematic phases unveiled by unsupervised machine learning techniques. Physical Review E, 102(4), 040601. https://doi.org/10.1103/PhysRevE.102.040601

Coifman, R. R., & Lafon, S. (2006). Diffusion maps. Applied and computational harmonic analysis, 21(1), 5-30. https://doi.org/10.1016/j.acha.2005.07.004

Colen, J., Han, M., Zhang, R., Redford, S. A., Lemma, L. M., Morgan, L., … Vitelli, V. (2021). Machine learning active nematic hydrodynamics. Proceedings of the National Academy of Sciences, 118(10), e2016708118. https://doi.org/10.1073/pnas.2016708118

De Gennes, P. G., & Prost, J. (1995). The Physics of Liquid Crystals. Oxford University Press. https://doi.org/10.1063/1.2808028

Dierking, I., & Al-Zangana, S. (2017). Lyotropic liquid crystal phases from anisotropic nanomaterials. *Nanomaterials*, *7*(10), 305. https://doi.org/10.3390/nano7100305

Doi, H., Takahasi, K. Z., Tagashira, K., Fukuda, J., and Aoyagi, T. (2019). Machine learning-aided analysis for complex local structure of liquid crystal polymers. Scientific Reports, 9(1), 1-12. https://doi.org/10.1038/s41598-019-51238-1

Doostmohammadi, A., Ignes-Mullol, J., Yeomans, J. M., & Sagues, F. (2018). Active nematics. Nature Communications, 9(1), 1-13. https://doi.org/10.1038/s41467-018-05666-8

Duc, T. L., Leiva, R. G., Casari, P., & Östberg, P. O. (2019). Machine learning methods for reliable resource provisioning in edge-cloud computing: A survey. ACM Computing Surveys (CSUR), 52(5), 1-39. https://doi.org/10.1145/3341145

Elman, J. L. (1990). Finding Structure in Time. Cognitive Science, 14(2), 179-211. https://doi.org/10.1207/s15516709cog1402_1

Fatemi, M. H., and Ghorbandzad'e, M. (2009). In silico prediction of nematic transition temperature for liquid crystals using quantitative structure-property relationships. Molecular Diversity, 13(4), 483-491. https://doi.org/10.1007/s11030-009-9135-y

Gayon-Lombardo, A., Mosser, L., Brandon, N. P., & Cooper, S. J. (2020). Pores for thought: generative adversarial networks for stochastic reconstruction of 3D multiphase electrode microstructures with periodic boundaries. Computational Materials 6(1), 1-11. https://doi.org/10.1038/s41524-020-0340-7

Gong, Z., Zhang, R., Xia, B., Hu, R., Fan, B. (2008). Study of Nematic Transition Temperatures in Thermotropic Liquid Crystal Using Heuristic Method and Radial Basis Function Neural Networks and Support Vector Machine. QSAR & Combinatorial Science, 27(11-12), 1282-1290. https://doi.org/10.1002/qsar.200860027

Goodfellow, I. J., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., … Bengio, Y. (2014). Generative Adversarial Nets. arXiv preprint arXiv:1411.1784. https://doi.org/10.48550/arXiv.1411.1784

Grewal, G. S., Bharara, M., Cobb, J. E., Dubey, V. N., & Claremont, D. J. (2006). A novel approach to thermochromic liquid crystal calibration using neural networks. Measurement Science and Technology, 17(7), 1918. https://doi.org/10.1088/0957-0233/17/7/033

Gu, J., Wang, Z., Kuen, J., Ma, L., Shahroudy, A., Shuai, B., … Chen, T. (2017). Recent Advances in Convolutional Neural Networks. Pattern Recognition, 77, 354-377. https://doi.org/10.1016/j.patcog.2017.10.013

Hedlund, E., Hedlund, K., Green, A., Chowdhury, R., Park, C. S., Maclennan, J. E., & Clark, N. A. (2022). Detection of Islands and Droplets on Smectic Films Using Machine Learning. Physics of Fluids, 34(10), 103608. https://doi.org/10.1063/5.0117358

Inokuchi, T., Okamoto, R., & Arai, N. (2019). Predicting molecular ordering in a binary liquid crystal using machine learning. Liquid Crystals, 47(3), 438-448. https://doi.org/10.1080/02678292.2019.1656293

Ireland, P. T., & Jones, T. V. (2000). Liquid crystal measurements of heat transfer and surface shear stress. Measurement Science and Technology, 11(7), 969. https://doi.org/10.1088/0957-0233/11/7/313

Johnson, S. R., & Jurs, P. C. (1999). Prediction of the Clearing Temperatures in a Series of Liquid Crystals from Molecular Structure. Chemistry of Materials, 11(4), 1007-1023. doi:10.1021/cm980674x

Kawaguchi, K., Kageyama, R., & Sano, M. (2017). Topological defects control collective dynamics in neural progenitor cell cultures. Nature, 545(7654), 327-331. https://doi.org/10.1038/nature22321

Karayiannis, N. B., & Mi, G. W. (1997). Growing radial basis neural networks: Merging supervised and unsupervised learning with network growth techniques. IEEE Transactions on Neural networks, 8(6), 1492-1506. https://doi.org/10.1109/72.641471

Klopp, C. Trittel, T., Eremin, A., Harth, K., Stannarius, R., Park, C. S., … Clark, N. A. (2019). Structure and dynamics of a two-dimensional colloid of liquid droplets. Soft Matter 15(40), 8156-8163. https://doi.org/10.1039/c9sm01433k

Krizhevsky, A., Sutskever, I., & Hinton, G. E. (2012). Imagenet classification with deep convolutional neural networks. Advances in neural information processing systems, 25. https://doi.org/10.1145/3065386

Le, T. C., and Tran, N. (2019). Using Machine Learning to Predict the Self-Assembled Nanostructures of Monoolein and Phytantriol as a Function of Temperature and Fatty Acid Additive for Effective Lipid-Based Delivery Systems. ACS Appl. Nano Mater., 2(3), 1637-1647. https://doi.org/10.1021/acsanm.9b00075

Li, J., Nishikawa, H., Kougo, J., Zhou, J., Dai, S., Tang, W., … Aya, S. (2021). Development of ferroelectric nematic fluids with giant ε dielectricity and nonlinear optical properties. Science Advances, 7(17), eabf5047. https://doi.org/10.1126/sciadv.abf5047

Lisa, C., & Curteanu, S. (2007). Neural Network Based Predictions for the liquid crystal properties of organic compounds. In Computer aided chemical engineering (Vol. 24, pp. 39-44). Elsevier.. https://doi.org/10.1016/S1570-7946(07)80030-7

Liu, Y., Zou, Z., Tsang, A. C. H., Pak, O. S., & Young, Y. N. (2021). Mechanical rotation at low Reynolds number via reinforcement learning. Physics of Fluids, 33(6), 062007. https://doi.org/10.1063/5.0053563

Mani, K., & Kalpana, P. (2016). An Efficient Feature Selection based on Bayes Theorem, Self Information and Sequential Forward Selection. International Journal of Information Engineering & Electronic Business, 8(6). https://doi.org/10.5815/ijieeb.2016.06.06

Marenduzzo, D., Orlandini, E., & Yeomans, J. M. (2007). Hydrodynamics and Rheology of Active Liquid Crystals: A Numerical Investigation. Physical Review Letters, 98(11), 118102. https://doi.org/10.1103/PhysRevLett.98.118102

Mnih, V., Kavukcuoglu, K. Silver, D., Graves, A., Antonoglou, I., Wierstra, D., & Riedmiller, M. (2013). Playing Atari with Deep Reinforcement Learning. arXiv preprint arXiv:1312.5602. https://doi.org/10.48550/arXiv.1312.5602

Minor, E. N., Howard, S. D., Green, A. A. S., Glaser. M. A., Park, C. S., & Clark, N. A. (2019). End-to-End Machine Learning for Experimental Physics: Using Simulated Data to Train a Neural Network for Object Detection in Video Microscopy. Soft Matter, 16(7), 1751-1759. https://doi.org/10.1039/C9SM01979K

Noble, W. S. (2006). What is a support vector machine? Nature Biotechnology, 24(12), 1565-1567. https://doi.org/10.1038/nbt1206-1565

Onsager, L. (1931). Reciprocal relations in irreversible processes. I. Physical Review, 37(4), 405. https://doi.org/10.1103/PhysRev.37.405

Osiecka-Drewniak, N., Czarnecki, M. A., & Galewski, Z. (2021). Investigations of phase transitions in liquid crystal 12BBAA using window clustering of infrared spectra. Journal of Molecular Liquids, 341, 117233. https://doi.org/10.1016/j.molliq.2021.117233

Oswald, P., & Pieranski, P. (2005). Smectic and columnar liquid crystals: concepts and physical properties illustrated by experiments. CRC Press, Boca Raton. https://doi.org/10.1201/9781420036343

Paganini, M., de Oliviera, L, & Nachman, B. (2018). CaloGAN: Simulating 3D high energy particle showers in multilayer electromagnetic calorimeters with generative adversarial networks. Physical Review D, 97(1), 014021. https://doi.org/10.1103/PhysRevD.97.014021

Pessa, A. A. B., Zola, R. S., Perc. M., & Ribiero, H.V. (2022). Determining liquid crystal properties with ordinal networks and machine learning. Chaos, Solitons & Fractals, 154, 111607. https://doi.org/10.1016/j.chaos.2021.111607

Peterson, L. E. (2009). K-nearest neighbor. Scholarpedia, 4(2), 1883. https://doi.org/10.4249/scholarpedia.1883

Ren, Y., Zhang, Y., & Yao, X. (2017). QSPRs for estimating nematic transition temperature of pyridine-containing liquid crystalline compounds. Liquid Crystals, 45(2), 238-249. https://doi.org/10.1080/02678292.2017.1314026

Rizkin, B. A., Shkolnik, A. S., Ferraro, N. J., & Hartman, R. L. (2020). Combining automated microfluidic experimentation with machine learning for efficient polymerization design. Nature Machine Intelligence, *2*(4), 200-209. https://doi.org/10.1038/s42256-020-0166-5

Rojas, F., & Rutenberg, A. D. (1999). Dynamical scaling: The two-dimensional XY model following a quench. Physical Review E, 60(1), 212. https://doi.org/10.1103/PhysRevE.60.212

Sakanoue, H., Hayashi, Y., & Katayama, K. (2021). Inference of Molecular orientation/ordering change nearby topological defects by the neural network function from the microscopic color information. Scientific Reports, 11(1), 1-10. https://doi.org/10.1038/s41598-021-88535-7

Shah, R. R., & Abbott, N. L. (2001). Principles for measurement of chemical exposure based on recognition-driven anchoring transitions in liquid crystals. Science, 293(5533), 1296-1299. https://doi.org/10.1126/science.1062293

Sigaki, H. Y. D., de Souza, R. F., de Souza, R. T., Zola, R. S., & Ribiero, H. V. (2019). Estimating physical properties from liquid crystal texture via machine learning and complexity-entropy methods. Physical Review E, 99(1), 013311. https://doi.org/10.1103/PhysRevE.99.013311

Sigaki, H. Y. D., Lenzi, E. K., Zola, R. S., Perc, M., and Ribiero, H. V. (2020). Learning physical properties of liquid crystals with deep convolutional neural networks. Scientific Reports, 10(1), 1-10. https://doi.org/10.1038/s41598-020-63662-9

Simonyan, K., & Zisserman, A. (2014). Very deep convolutional networks for large-scale image recognition. arXiv preprint arXiv:1409.1556. https://doi.org/10.48550/arXiv.1409.1556

Smith, A. D., Abbot, N., & Zavala, V. M. (2020). Convolutional Network Analysis of Optical Micrographs for Liquid Crystal Sensors. Journal of Physical Chemistry C, 124(28), 15152-15161. https://doi.org/10.1021/acs.jpcc.0c01942

Song, Y. Y., & Ying, L. U. (2015). Decision tree methods: applications for classification and prediction. Shanghai archives of psychiatry, 27(2), 130. https://doi.org/10.11919%2Fj.issn.1002-0829.215044

Sutton, P., & Boyden, S. (1994). Genetic Algorithms: A general search procedure. American Journal of Physics, 62(6), 549-552. https://doi.org/10.1119/1.17516

Sutton, R. S., & Barto, A. G. (1998). Reinforcement Learning: An Introduction. MIT Press. https://doi.org/10.1017/s0263574799271172

Takashi, K. Z., Aoyagi, T., & Fukuda, J. (2021). Multistep nucleation of anisotropic molecules. Nature Communications, 12(1), 1-9. https://doi.org/10.1038/s41467-021-25586-4

Tan, A. J., Roberts, E., Smith, S. A., Olvera, U. A., Arteaga, J., Fortini, S., … Hirst, L. S. (2019). Topological chaos in active nematics. Nature Physics, 15(10), 1033-1039. https://doi.org/10.1038/s41567-019-0600-y

Trafalis, T. B., & Ince, H. (2000). Support Vector Machine for Regression and Applications to Financial Forecasting. In Proceedings of the IEEE-INNS-ENNS International Joint Conference on Neural Networks. IJCNN 2000. Neural Computing: New Challenges and Perspectives for the New Millennium (Vol. 6, pp. 348-353). IEEE. https://doi.org/10.1109/IJCNN.2000.859420

Vill, V. (1995). Conception and Realization of a Liquid Crystal Database LIQCRYST. Liquid Crystals Today, 5(3), 6-7. https://doi.org/10.1080/13583149508047608

Villanueva-Garcia, M., Gutierrez-Parra, R. N., Martinez-Richa, A., & Robles, J. (2005). Quantitative structure-property relationships to estimate nematic transition temperatures in thermotropic liquid crystals. Journal of Molecular Structure: THEOCHEM, 727(1-3), 63-69. https://doi.org/10.1016/j.theochem.2005.02.033

Walters, M., Wei, Q., & Chen, J. Z. Y. (2019). Machine learning topological defects of confined liquid crystals in two dimensions. Physical Review E, 99(6), 062701. https://doi.org/10.1103/PhysRevE.99.062701

Wenzel, D., Nestler, M., Reuther, S., Simon, M., and Voigt, A. (2020). Defects in active nematics - algorithms for identification and tracking. Computational Methods in Applied Mathematics, 21(3), 683-692. https://doi.org/10.1515/cmam-2020-0021

Xu, J., Wang, L., Zhang, H., Yi, C., & Xu, W. (2010). Accurate quantitative structure-property relationship analysis for prediction of nematic transition temperatures in thermotropic liquid crystals. Molecular Simulation, 36(1), 26-34. https://doi.org/10.1080/08927020903096064

Xu, Y., Rather, A. M., Song, S., Fang, J. C., Dupont, R. L., Kara, U. I., ... & Wang, X. (2020). Ultrasensitive and selective detection of SARS-CoV-2 using thermotropic liquid crystals and image-based machine learning. Cell Reports Physical Science, 1(12), 100276. https://doi.org/10.1016/j.xcrp.2020.100276

Yang, S., & Collings, P. J. (2020). The Genetic Algorithm: Using Biology to Compute Liquid Crystal Director Configurations. Crystals, 10(11), 1041. https://doi.org/10.3390/cryst1011104

Yang, X., Li, J., Forest, M. G., & Wang, Q. (2016). Hydrodynamic theories for flows of active liquid crystals and the generalized onsager principle. Entropy, 18(6), 202. https://doi.org/10.3390/e18060202

Yurke, B., Pargellis, A. N., Majumdar, S. N., & Sire, C. (1997). "Experimental measurement of the persistence exponent of the planar Ising model." Physical Review E, 56(1), R40. https://doi.org/10.1103/PhysRevE.56.R40

Zhang, J., Yang, J., Zhang, Y., & Bevan, M. A. (2020). Controlling colloidal crystals via morphing energy landscapes and machine learning. Science Advances, 6(48), eabd6716. https://doi.org/10.1126/sciadv.abd6716

Zhao, J., Zhang, J., and Wang, B. (2022). A learning-based approach for solving shear-stress vector distribution from shear-sensitive liquid crystal coating images. Chinese Journal of Aeronautics, 35(4), 55-65. https://doi.org/10.1016/j.cja.2021.04.019

Zhou, Z., Joshi, C., Liu, R., Norton, M. M., Lemma, L., Dogic, Z., … Hong, P. (2021). Machine Learning Forecasting of Active Nematics. Soft Matter, 17(3), 738-747. https://doi.org/10.1039/D0SM01316A