Review Article

Machine Learning for Condensed Matter Physics

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Abstract. Condensed Matter Physics (CMP) seeks to understand the microscopic interactions of matter at the quantum and atomistic levels, and describes how these interactions result in both mesoscopic and macroscopic properties. CMP overlaps with many other important branches of science, such as Chemistry, Materials Science, Statistical Physics, and High-Performance Computing. With the advancements in modern Machine Learning (ML) technology, a keen interest in applying these algorithms to further CMP research has created a compelling new area of research at the intersection of both fields. In this review, we aim to explore the main areas within CMP, which have successfully applied ML techniques to further research, such as the description and use of ML schemes for potential energy surfaces, the characterization of topological phases of matter in lattice systems, the prediction of phase transitions in off-lattice and atomistic simulations, the interpretation of ML theories with physics-inspired frameworks and the enhancement of simulation methods with ML algorithms. We also discuss the main challenges and outlooks for future developments.

Keywords: machine learning, condensed matter physics, artificial intelligence

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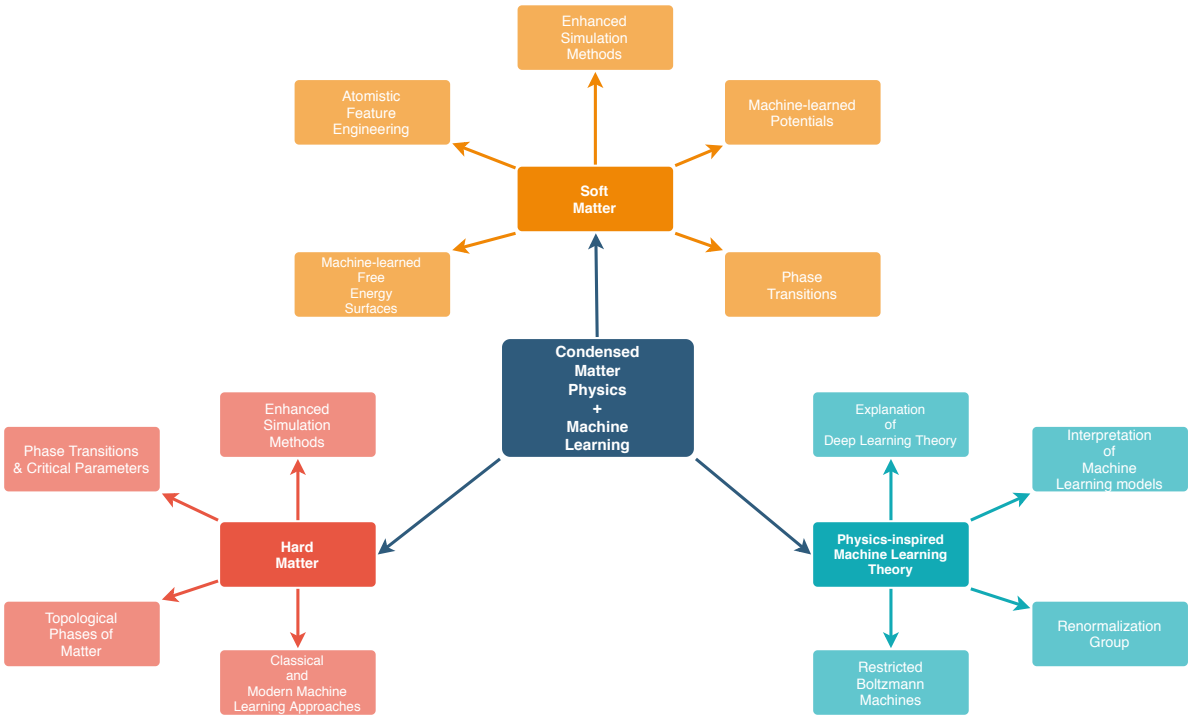

Figure 1. Schematic representation of the potential applications of ML to CMP discussed in this review.

1. Introduction

Currently, machine learning (ML) technology constitutes the backbone of modern society: automatic language translation, movie recommendations, face recognition in social media, fraud detection, and more everyday life activities [1] are all powered by a diverse range of ML methods. Tasks like human-like image classification performed by machines [2]; the effectiveness of understanding what a person means when writing a sentence within a context [3]; the ability to distinguish a face from a car in a picture [4]; and automated medical image analysis [5] are some of the most outstanding advancements that stem from the mainstream use of modern ML technology [6]. Inspired by these notable applications, scientists have thrivingly applied ML technology to scientific fields, such as matter engineering [7], drug discovery [8] and protein structure predictions [9].

Influenced by the overwhelming effectiveness of ML technology in other scientific fields, physicists have also applied such methods to specific subfields within Physics, with the main objective of making progress in the most challenging research questions. The motivating reasons for this surge of interest at the intersection between Condensed Matter Physics (CMP) and ML are vast. For instance, images, language and music exhibit power-law decaying correlations equivalent to those seen in classical or quantum many-body systems at their critical points [10]; very large data sets, with high-dimensional inputs found in materials science [11] are the quintessential problem that

modern ML methods are tailored to deal with; and the encoding into a latent space of features that represent the atomistic structure found in soft matter and physical chemistry molecular systems [12] is a challenge already solved by modern natural language processing and object detection techniques. It seems as though ML is well-suited to be applied to CMP research problems given all these deep connections between both.

In this work, we review the contributions of ML methods to Physics with the aim of providing a starting point for both computer scientists and physicists interested in getting a better understanding of the interaction between these two research fields. For easier navigation of the topics covered in this review, the diagram shown in Fig 1 displays a schematic representation of the outline, but we shall summarize them briefly here.

We start the review with a very brief overview of both CMP and ML for the sake of self-containment, to help reduce the gap between both areas. We then continue by exploring some of the research inquiries within *hard condensed matter physics.* **Hard Matter** has seen most of the applications, mainly in phase transition detection for lattice models. We continue with the review by analyzing how both classical ML and Deep Learning (DL) techniques have been applied to obtain detailed descriptions of strongly correlated, frustrated and out-of-equilibrium systems. We investigate how standard simulation methods, like Monte Carlo, have also seen enhancements from using ML models. Moving forward, we examine a new research area dubbed **physics-inspired ML theory**, an area where the most rigorous and fundamental physics frameworks have been applied to ML to uncover a true understanding of the learning mechanisms of ML models. We discuss how in this engaging research area a thorough understanding of the learning mechanism behind Restricted Boltzmann Machines has been obtained. We move on to reviewing how common theoretical physics frameworks, such as the Renormalization Group, have been used with interesting results to give insights into the learning mechanisms of the most common models in DL. The review continues with the exploration of **Soft Matter**, which recently has seen a strong surge of ML applications, mainly in the subfields of materials science and colloidal systems, e.g., proteins and complex molecular structures. The identification of a phase transition and the determination of the phases of matter have been the primary topics of research, with enhanced intelligent modeling, atomistic feature engineering, ML potential and free energy surfaces being a close second. The review is closed with some perspectives and outlooks about current challenges.

2. Overview of Machine Learning

In this section, the main ML concepts used in this review are described, following a specific hierarchy composed of problem, model, method, and component. These basic definitions are given to smooth the learning curve for those unfamiliar with the ML terminology, and useful references are included for readers interested in obtaining a deeper insight.

Machine Learning is a research field within Artificial Intelligence aimed to construct a program that fits the given data with a model (either predictive or descriptive); this model adjust its own parameters by optimizing a performance criterion defined on the given data [13]. The parameter adjustment process and the model employed are commonly referred to as *learning from data* and *learning model*, respectively.

Artificial Neural Networks (ANNs) are arguably the most representative models of ML. ANNs attempt to simulate the decision process of neurons of biological central nervous systems [14]. ANNs are graphs where nodes compute activation functions (sigmoidal, radial basis, and any other Tauber-Wiener function [15]) according to the input data provided by the connecting edges. The learning process consists in assigning weights to the edges and updating them according to an optimization algorithm—such as backpropagation, Levenberg-Marquardt, Stochastic Gradient Descent, etc. [16]—. The tasks that ANNs can solve depend on the architecture that specifies how data is processed and stored. The number of current ANNs architectures is immeasurable, but a project trying to track them can be consulted in [17].

Multilayer feed-forward Neural Networks (FFNNs) are one of the essential ANN architectures, where neurons are commonly distributed using input, hidden and output layers [18], all conected with each other. Two examples of these networks are the Multilayer Perceptrons and Radial Basis Function Networks. The learning process in FFNNs is supervised, that is, in addition to the training data—$X \subset \Re^d$—, provided to the input layer, expected output data—$Y \subset \Re$—, labeling each input vector is required to verify the performance of the network. A learning algorithm is then employed based on the network output until the best approximation to an underlying decision function, $f : X \to Y$, is achieved. FFNNs networks have been proved to be universal approximators to any Borel measurable function [19]. In addition to the function approximation, supervised FFNNs may be used for classification, prediction, and control tasks [20]. Autoencoders (AEs) constitute a different type of NN architecture, considered a special case of FFNNs, and designed to learn a latent representation of the training data in order to perform data compression or dimensionality reduction [21, 22]. AEs consist of two parts: an encoder function—$g(\boldsymbol{x}), \boldsymbol{x} \in X$—, and a decoder that produces a reconstruction, $\boldsymbol{r} = f(g(\boldsymbol{x}))$. The main purpose of AEs is to generate an efficient encoding of the input data instead of learning to copy this data perfectly. Despite the success of ANNs to solve a vast number of applications in both science and engineering [23, 24], this model has been criticized due to the lack of providing explicit representations of the learned solutions.

Support Vector Machines (SVMs) are explicit ML models that emerged as an alternative to ANNs [25]. Both ANNs and SVMs have the ability to generalize and may be designed to solve practically the same tasks (classification, regression, density estimations, clustering, among others) [26, 27]. However, while ANNs were inspired by the biological analogy to the brain, SVMs were inspired by statistical learning theory [28]. Because of their solid theoretical basis SVMs can provide explicit solutions with measurable generalization capability by conducting structural risk minimization;

by solving a convex quadratic programming problem, the dreaded problem of local minima that permeates ANNs is avoided; and finally, the model can represent the learned solution based on few parameters [29, 30]. However, SVMs are limited in the size of the datasets that can handle.

Deep Learning (DL) is the most recent subfield of ML, outperforms the capabilities of SVM, and is focused on learning complex concepts, e.g. the image of a person, in terms of simpler concepts, such as the corners, contours or textures within the image [6]. The DL approach enhances previous ANNs architectures through the introduction of new activation functions (rectifier, softplus, and softmax) [31], data operators and optimization algorithms. As a result, Deep Neural Networks are able to deal with huge amounts of heterogeneous information, as well as learning directly from raw data without the user-dependent preprocessing step of receiving the main and filtered features of raw data as valid training vectors (feature extraction) required by classical ANNs.

Convolutional Neural Networks (CNNs) are DL architectures specialized for processing data with a grid-like topology (time-series as one-dimensional data or images as two-dimensional grid of pixels) that use convolution in place of general matrix multiplication in at least one of their layers [6]. The simplest CNN includes an input layer that receives the raw data; next, a convolutional layer filters local regions from the input layer's ouput; a pooling layer is then used to down-sample the spatial dimensions; lastly, a fully connected layer computes the class scores, and an output layer provides the final result.

3. Overview of Condensed Matter Physics

Understanding the intricate phenomena of all types of matter and its properties is the driving force of condensed matter physicists. From quantum theory all the way to materials science, CMP encompasses a large diversity of subfields within physics, as it deals with different time and length scales depending on both the molecular details and the type of matter being analyzed. To study such systems, theoretical, computational and experimental physicists collaborate to gain a deeper insight into the behavior of matter. We shall briefly talk about the two main areas within CMP, *hard matter* and *soft matter*, the essential models as well as the central problems these research areas are focused on. More information about these research areas can be found in standard textbooks, see, e.g., [32, 33, 34] and reviews [35, 36].

3.1. Soft Condensed Matter

Fluids, liquid crystals, polymers, colloids, and many more are the principal types of matter that are studied by Soft Condensed Matter, or Soft Matter (SM). SM has the peculiar property that it will easily respond to external forces. SM will change its flow when a small shear force is applied to it, or thermal fluctuations are applied, thus changing its properties as a whole. We are surrounded by these materials in our

everyday life, from glass windows, toothpaste, hair-styling gel, among others. These materials can show diverse properties and when some external force is applied, they will exhibit a different set of properties, but in all cases SM shows the fascinating property of self-organization of its molecules [37]. Proteins and bio-molecules are also good examples of SM, they change their structure when subjected to thermal fluctuations, while also showing a pattern of self-assembly [38, 39], as is the case in most types of SM. All in all, SM is a subfield of CMP that gained a lot of attention when first introduced in the 1970s by Nobel prize laureate Pierre-Gilles de Gennes [40], because it has shown to be of great importance to science in general, with very useful applications, as well as pushing the boundaries in theoretical, experimental and computational Physics.

In order to explore all these properties and changes in a SM system, a model that describes most of these types of matter is needed. Most fluids and colloidal dispersions show a repulsive behavior, which can be modeled very well with the *hard-sphere* model [41]. A system modeled as a hard-sphere dispersion only shows an infinite repulsive interaction when there exists interparticle separations less than the particle's diameter, and zero otherwise. There is no attractive interaction included in this model. The hard-sphere model is a very simple one, which has also exhibited intriguing but unexpected equilibrium and non-equilibrium states [42, 43, 44]. There are some interesting properties that define the hard-sphere model in SM. First of all, the internal energy of any allowed system configuration is always zero. Furthermore, forces between particles and variations in the free energy—defined from classical thermodynamics as $F = E - TS$, with E being the internal energy, T the temperature and S the entropy—are both determined entirely by the entropy. Moreover, the entropy in a hard-sphere system depends directly on the total volume occupied by the hard spheres, commonly defined as the *volume fraction*, ϕ. When ϕ is small then the system shows the properties of an ideal gas, but as ϕ starts to increase, particles interact with each other and their motion is restricted by collisions with other nearby particles. Even more interesting is the fact that the *phase transitions* of hard-sphere systems are completely defined by ϕ [45]. In general, a SM system does not need to be composed only of hard spheres, it can also be built with non-spherical molecules, for example, rods, sphero-cylinders—cylinders with semi-circular caps—, and hard disks, just to mention a few examples. Nevertheless, all these systems experience a large diversity of phase transitions [46, 47, 48].

Phase transitions are one of the main challenges in all CMP. When a thermodynamic system changes its uniform physical properties to another set of properties, then the system encounters a phase transition. In SM, phase transitions are one of the most bewildering phenomena that can be analyzed because of the diversity of phases that appear in unexpected circumstances [49, 50]. In particular, a gas-liquid phase transition is defined by a temperature—, known as the *critical temperature*, T_c—, and a density—, called the *critical density*, ρ_c—. These quantities are also known as the *critical point* of the system, meaning that two phases can coexist when the system is held to these special values. When neither of these thermodynamical quantities can be employed, an *order*

parameter is more than sufficient to determine the phase transitions of a system. Order parameters are special quantities that can measure the degree of order between a phase transition; they range between several values for the different phases in the system [51]. For instance, when studying the liquid-gas transition in a system, a specified order parameter can take the value of zero in the gaseous phase, but it will take a non-zero value in the liquid state. In this scenario, the density difference between both phases $(\rho_l - \rho_g)$—where ρ_l is the density in the liquid state and ρ_g in the gas state—can be a useful order parameter.

When traversing the phase diagram of a SM system, one might encounter the so-called *topological defects* [52]. A topological defect in ordered systems is a special type of phase in which the system is stuck in-between two phases, and there is no continuous distortion or movement from the particles that can return the system to an ordered phase. One such example is that of nematic liquid crystals [53]. The nematic phase is observed in a hard-rod system, when all the rods align in a certain direction. Hard rods are allowed to move and to rotate freely. Furthermore, the neighboring hard rods tend to align in the same direction. But if it so happens that some hard rods are aligned in one direction and the rest in another direction, then the system contains topological defects [54]. These defects depend on the symmetry of the order parameter of the phases, as well as the topological properties of the space in which the transformation is happening. Topological defects are of the utmost importance in a large variety of systems in SM, e.g., they determine the strength of the liquid crystal mentioned before.

But these types of systems and problems are not so easily solved. How can we tell when a system will be prone to topological defects? Is it possible to determine the phases that a system will come across given its configuration? Even more challenging questions are always originating when these types of exotic matter appear. But theoretical, experimental or even computational frameworks are not enough to tackle these problems. Physicists are always open to new ways to approach such challenges, and ML is the current best candidate to do so. Current ML technology is slowly starting to become a very powerful tool to deal with these complex systems, and in this review we shall discuss some of the ways ML has been applied to such problems.

3.2. Hard Condensed Matter

When physicists deal with materials that show structural rigidity, such as solids, metals, insulators or semiconductors, their interest in the properties of these materials are the main focus of Hard Condensed Matter, or Hard Matter (HM). Furthermore, in contrast to SM systems, HM deals with systems on smaller scales, i.e., matter that is governed by atomic and quantum-mechanical interactions. Entropy no longer determines the free energy of a HM system, it is now up to the internal energy. One particular example of interest in HM is the phenomenon of *superconductivity*. A material is considered a superconductor if all electrical resistance is absent and it is a perfect diamagnet [55] —i.e., all magnetic flux fields are excluded from the system—. This phenomenon is

described by both quantum and statistical mechanical interactions. This means that superconductivity can be seen as a macroscopic manifestation of the laws of quantum mechanics. As was the case with SM, we are also surrounded by HM materials, for instance, semiconductors are the principal components in microelectronics [56], which in turn are the components of every digital device we use, ranging from computers to smart cellphones. The applications that stem from HM are too great to enumerate in this short review, and the theoretical, experimental and computational frameworks that have derived from HM are nothing short of revolutionary.

In HM, we also need to study a simple model that can help explain most of the investigated materials. Such is the case of lattice systems, and in particular, the Ising model [57]. The Ising Model is the simplest model that can explain ferromagnetic properties as well as accounting for quantum interactions. It is defined in a lattice, much like if it were a crystalline solid. In each site of the lattice, there is a discrete variable σ_k that takes one of either two values, such that $\sigma_k \in \{-1, +1\}$. The energy for a lattice is given by the following Hamiltonian

$$H(\sigma) = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j\sigma_j \tag{1}$$

where J_{ij} is a pairwise interaction between lattice sites; the notation $\langle i, j \rangle$ indicates that i and j are lattice site neighbors; μ is the magnetic moment and h_j is an external magnetic field. As originally solved by Ising in 1924 [58], when the system lies in a one-dimensional lattice, the system shows no phase transition. Later, Lars Onsager proved in 1944 [59] that when the Ising Model lies in a two-dimensional lattice, a continuous phase transition is observed. For dimensions larger that two, different theoretical [60, 61] and computational [62] frameworks have been proposed.

While the Ising Model has seen some very useful applications, it is not the only model that has shaped the research interests within CMP, as it cannot possible contain and explain all of phenomena seen in HM. A generalized model, such as the n-vector model [63] or the Potts model [64] are extensively studied models in HM as well that have been successfully applied to explain even more intricate phenomena [65, 66].

In general, all these models show phase transitions, in the same way as SM systems. This is a very big research area, even more so when the Berezinsky-Kosterlitz-Thouless (BKT) phase transition was discovered [67, 68, 69, 70]. The BKT transition was unveiled on two-dimensional lattice systems, such as the XY model—which is a special case of the n-vector model—. The BKT transition consists of a phase transition that is driven by topological excitations and does not break any symmetries in the system [71]. This type of phase transition was quite abstract in the 1970s when first introduced, but it turned out to be a great theoretical framework that was later discovered in exotic materials [72, 73], which in turn showed puzzling properties. Such was the impact of the BKT transition in CMP that it would later be awarded a Nobel prize in Physics in 2016 [74].

But the BKT transition is a complicated transition to study. Hard condensed matter physicists are always trying to find a better way to look for these kind of unique

aspects in materials. It is an elusive and complicated challenge. In the same spirit as in SM, ML has already been put to the test on this task, if it is possible to re-formulate the problem at hand as a ML problem, it can then be solved by standard ML techniques. We shall examine these applications with more detail in the following sections.

4. Hard Matter and Machine Learning

4.1. Phase transitions and critical parameters

One of the most prominent uses of NNs was on the two-dimensional ferromagnetic Ising Model which has a Hamiltonian similar to 1, with the aim to identify the critical temperature, T_c, at which the system leaves an ordered phase—the *ferromagnetic phase*—and enters a disordered phase—the *paramagnetic phase*. Carrasquilla and Melko [75] introduced a new paradigm by essentially formulating the problem of phase transitions as a *supervised classification* problem, where the ferromagnetic phase constitutes one class and the paramagnetic phase is another one, then a ML algorithm is used to discriminate between both of them under specific conditions. By sampling configurations using standard Monte Carlo simulations for different system sizes, and then feeding this raw data to a FFNN, an estimate of the correlation-length critical exponent ν is obtained directly from the output of the last layer of the trained NN. Finite-size scaling theory [76] is then employed to obtain an estimation of T_c. Even if the geometry of the lattice is modified, the power of abstraction provided by the NN [77] is enough to predict the critical parameters even if it was trained in a completely different geometry; this makes it a very convenient tool to identify critical parameters for systems that do not have a defined order parameter [78].

4.2. Topological phases of matter

Once having shown that ML is able to identify phases of matter in simple models as shown for models that have a similar Hamiltonian to 1, researchers have been interested in trying out these algorithms in more complex systems, and a lot of work has been put into the topic of identifying topological phases of matter using ML algorithms for strongly correlated topological systems [79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89]. For instance, Zhang *et al* [90] have applied FFNNs as well as CNNs to find the BKT phase transition, as well as constructing a complete phase diagram of the XY and generalized XY models, with very promising results. In the case of the FFNN approach, Zhang *et al* found out that a simple NN architecture consisting of one input layer, one hidden layer with four neurons and one output layer is more than enough to obtain the critical exponent ν for the XY model. We can compare this to the results obtained by Kim and Kim [91], where they explain a similar behavior but for the Ising model. In their work, analyzing a tractable model of a NN, they found out that a NN architecture consisting of one input layer, one hidden layer with two neurons and one output layer is sufficient to obtain the critical exponent ν for the Ising model. It is important to keep track of the

model complexity specially for complicated models to avoid overfitting and to reduce the amount of data needed to train the model.

New and interesting methodologies are always arising in order to solve the problem of phase transitions. Kenta *et al* [92] developed a generalized version of the methodology proposed by Carrasquilla and Melko [75] for a variety of models, namely, the Ising model, the q-state Potts model [93] and the q-state clock model. Instead of using the raw data obtained from Monte Carlo simulations as proposed in [75], Kenta *et al* considered the configuration of a specific long-range spatial correlation function for each model, effectively exploiting feature engineering, hence providing meaningful data to the NN, which now contains relevant information from the systems at hand. This strategy has the advantage of generalization for the already trained NN, thus it can be readily applied to similar systems without further manipulation of the physical model or the production of new simulation data. The strategy is also quite general in the sense that it can be readily applied to multi-component systems, with the same precision as standard theoretical methods.

4.3. Classical and modern ML approaches

The amount of success that ML has seen in the area of Lattice Field Theory and Spin Systems has given it a special place in the toolboxes of physicists to make their research effortless and faster. It is specially important to identify those tools as the ones that have seen the most use in this topic, the main one being FFNNs given its generalization and abstraction capabilities for which it has become the workhorse of most of the applications in this field—particularly when the problem can be formulated as a *supervised learning* problem.

For more classical approaches, SVMs have also been implemented on the phase transition problem [87, 94] with promising results given their ease of use and physical interpretation of the results, which we shall discuss in detail in section 5.4. Many other classical techniques—specifically the ones that stem from *unsupervised learning* methods —have become very prominent algorithms. For instance, one such technique is the nonlinear dimensionality reduction algorithm t-distributed Stochastic Neighbor Embedding (t-SNE) [95] that Zhang *et al* [90] used to map high-dimensional features onto lower dimensional spaces for the sake of *feature engineering* in the Potts model. Another prime example is Principal Component Analysis (PCA) [96, 97] which has proved to be one of the best feature extraction algorithms that can be used in Spin Systems [98, 99], as it can be readily applied to raw configurations and extract meaningful information like structure factors and order parameters. DL has also been wielded as a powerful technique to understand quantum phase transitions [100] in the form of adversarial NNs [101]; to provide a thorough description of many-body quantum systems [102] by employing Variational Autoencoders [103, 6]; and CNNs [6] have been applied, for instance, to learn quantum topological invariants [104], or to solve frustrated many-body models [105]. One of the main reasons for DL to be such a strong asset is

that it hardly needs some type of human manipulation or modification of the input data, making it so that these algorithms do not demand *feature engineering* of the raw data, therefore enabling the physicist to automate their research workflow and spend less time in difficult and bias-prone *feature engineering* tasks.

4.4. Enhanced Simulation Methods

The standard computer simulation technique in HM is the Monte Carlo (MC) method, an unbiased probabilistic method that enables the sampling of configurations from a classical or quantum many-body system [106, 107, 108, 109]. Throughout the decades, specific modifications have been performed on the MC method to enhance it, creating a better, more rigorous method that could be used in all types of simulations—from observing phase transitions to computing quantum path integrals—. It is in this situation that ML has something to offer in order to improve the original MC method; such is the case of the Self-learning Monte Carlo (SLMC) method developed by Li *et al* [110]. In this novel scheme, the classical MC method is used to obtain configurations from a similar Hamiltonian to 1—these configurations will serve as the training data—then a ML method is employed—linear regression, in this case—to learn the rules that guide the configuration updates in the simulation. This enables the MC method to *learn by itself* under which conditions a given configuration is updated without external manipulation or guidance, efficiently sampling configurations for the most general possible model. Demonstrated on a generalized version of the Hamiltonian 1, the SLMC method is extremely efficient when producing configurations from the system, lowering the autocorrelation time from each of the updates. Li *et al* discuss that, although a ten-fold speedup from the original MC method is obtained, the SLMC still suffers from the quintessential problem of the original MC method—when approaching the thermodynamical limit, the method heavily slows down, rendering it useless—. Almost simultaneously, Huang and Wang [111] developed a similar scheme but using restricted Boltzmann Machines (RBMs). This interesting approach consists of building special types of RBMs that can use the physical properties of the system being studied. The strategy by Huang and Wang lowers autocorrelation time as well as raising the acceptance ratio of sampled configurations. The SLMC method has sparked interesting new research [112, 113, 114, 115, 116]; recently, Nagai, Okumura and Tanaka [117] have shown that the SLMC is even more promising by coupling it with Behler-Parrinello NNs [118], making it more general and less biased towards specific physical systems. It will come as no surprise that in a few years the SLMC will become the standard MC method in most of condensed matter physics sub-fields.

4.5. Outlooks

Current research is geared towards enhancing mainstream methodologies in CMP with ML, and enabling physicists to obtain high-precision results while also providing a complete understanding of the learning mechanisms of the ML algorithms employed.

Another current area of research in Spin Systems is that of figuring out which ML techniques are more suitable to understand out-of-equilibrium systems [119], or even more complex frustrated models [120], just to name a few. It is now a time of prolific and interesting research within two communities of researchers that would not have thought of as having a common ground in their interests, but all these fascinating results have created a bridge to join efforts in pushing the boundaries of what we can learn by ourselves and the things that we can task a computer to learn on our behalf.

5. Physics-inspired Machine Learning Theory

5.1. Explanation of Deep Learning Theory

The gain in knowledge between ML and CMP is not one-sided as one might think. ML has also benefited greatly from CMP with its thorough and rigorous theoretical frameworks that it possesses. Despite their huge success in human-like tasks—e.g., the classification of images [2]—, ML, and more importantly DL are unable to explain why this success is even possible in the first place. In 2016, Zhang et al. [121] took it upon themselves to run detailed experiments that showed the lack of complete understanding of the current learning theory from a theoretical perspective; on the practical side of things, DL is still very prosperous in its results. Since then, physicists have tried to give insights [122] into this topic, creating a fruitful research area with extremely interesting cross-fertilization between both communities. For a more thorough and complete analysis on the explanation and interpretability of DL contributions until now, the reader can refer to the recent review on the topic by Fan, Xiong and Wang [123].

5.2. Renormalization Group

The lack of theoretical understanding of the learning theory in most ML algorithms seemed like a good challenge for condensed matter physicists that exerted experienced manipulation in theoretical frameworks, such as the Renormalization Group (RG) [60, 61]. RG consists of a mathematical framework that allows a very rigorous and systematic investigation of a system by working with short-distance fluctuations and building up this information to understand long-distance interactions of the whole system. In 2014, Mehta and Schwab [124] provided such an insight by creating a mapping between the Variational Renormalization Group and the DL workflow that is common nowadays. This turned out to be an interesting take on the problem, resulting in a very rigorous framework by which one could explain the learning theory that Deep NNs follow when data is fed to them. In the same spirit, Li and Wang [125] proposed a new scheme, this time in a more systematic way, by means of hierarchical transformations of the data from an abstract space—the space of features present in the data—to a latent space. It turns out that this approach has an exact and tractable likelihood, facilitating unbiased training with a step-by-step scheme; they proved this through a practical example using Monte Carlo configurations sampled from the one-dimensional and two-

dimensional Ising models. More research regarding a deep link between RG and DL has been carried out since then, for instance Koch-Janusz and Ringel [126] showed that even though the association between RG and DL is strong, most of the practical methodology to achieve good results from this is not so readily available. By using feed-forward NNs, they proved that a RG flow is obtainable without discriminating the important degrees of freedom that are sometimes *integrated out* by following the RG framework. This seems like a promising and enriching area of research as new insights are constantly developed [127, 128, 129].

5.3. Restricted Boltzmann Machines

Instead of giving a complete explanation of a learning theory, CMP has been able to give thorough explanations of ML algorithms; such is the case of the *Restricted Boltzmann Machine* (RBM) [130]. This type of model is a very interesting case of the inspiration drawn from statistical physics onto ML. In the RBM, a NN is trained with a given data set, the intelligent model then learns complex internal representations of the data, after the model has been trained it outputs an approximation of the probability distribution of the input data. The resulting approximate probability distribution is then linked to a certain ML task, be it *classification* [131], *dimensionality reduction* [132], *feature selection/engineering* [133], and many more. The underlying structure of the model is not a conventional FFNN instead it is a type of model that is built using graphs [134]. The principal mechanism by which the RBM learns features is by computing an *energy* function $E(h, v)$ from certain *hidden*—h —and *visible* —v —units that form a *configuration*; after computing this *energy* function $E(h, v)$ one evaluates the Boltzmann factor of the energy to obtain a probability for the given configuration —$P(h, v) = e^{-E(h,v)}/Z$ —. From classical statistical mechanics we know that the *partition function* $Z = e^{-E(h,v)}/\sum_i e^{-E(h,v)}$ is the normalizing constant needed to ensure that $0 \leq P(h, v) \leq 1$. It is this link between the Maxwell-Boltzmann distribution and the energy function from the RBM that makes it an ideal candidate to be analyzed under the statistical mechanics framework.

Interestingly enough, RBMs are extremely versatile, despite the fact that it is a ML method for which the training mechanisms are not as fast as in more modern ML algorithms, thus special technical schemes have been developed for the task [135]. For example, Huang and Toyoizumi [136] introduced a mean-field theory approach to perform the training using a message-passing-based method that evaluates the partition function as well as its gradients without requiring statistical sampling—which is one of the drawback of traditional learning schemes—. Further work on understanding the thermodynamics of the model were carried out [137] with encouraging results, showing that the learning mechanism in general is completely tractable, albeit complex when the model enters a non-linear regime. The RBM can also be seen as the inverse Ising model [138], where instead of obtaining physical quantities like order parameters and critical exponents from system configurations, one has as input the physical observables

and intends to obtain insights on the system itself. With this theoretical framework in mind the first steps to produce rigorous explanations of the algorithm were done by Decelle et al. [139] by studying the linear regime of the training dynamics using spectral analysis.

RBMs are such rich and resourceful models that have been applied to a number of hard tasks; for instance, the modeling of protein families from sequential data [140, 141]. Another such complex task is that of continuous speech recognition, on which a special type of RBM was employed with promising results [142]. Within the realm of CMP, these models have been used to construct accurate ground-state wave functions of strongly interacting and entangled quantum spins, as well as fermionic models on lattices [143]. RBMs are currently finding their way as the favorite ML model in CMP and quantum many-body physics [144], so it might be just a few years more until we can experience widespread use of this exceptional tool.

5.4. Interpretation of Machine Learning models

Nevertheless the success they have achieved, ML algorithms are prone to a lack of interpretation, resulting in so-called *black box* algorithms that cannot grant a full rigorous explanation of the learning mechanisms and features that result in the outputs obtained from them. For a condensed matter physicist it is more important to understand the core mechanism by which the intelligent model obtained the desired output, so that it can later be linked to a useful physical model. As an example, we can take the a model with Hamiltonian 1 and train a FFNN on simulation data, following the methodology of Carrasquilla and Melko [75]; once the NN has been trained, the critical exponent is obtained and used to compute the critical temperature, but the question remains, what enabled the NN to obtain such information? Is there a mechanism to extract meaningful physical knowledge from the weights and layers from the NN? To answer this type of questions researchers have had to resort to arduous extraction and analysis from the underlying model architectures. For example, Suchsland and Wessel [145] trained a shallow FFNN on two-dimensional configurations from Hamiltonians similar to 1, then proceeded to comprehensively analyze the weight matrices obtained from the training scheme, while also performing a meticulous study of the reasons why activation layers and their respective neurons fire a response when required; they found out that both elements—training weights and activation layers—play a crucial role in the understanding of how the NN is able to output the physical observables that we give a meaning to. They also determined that the learning mechanism corresponds to a domain-specific understanding of the system, i.e., in the case of the Ising model, the NN effectively learned the structure of the surrounding neighbors for a particular spin, with this information it then proceeded to compute the magnetization order parameter as part of the computations involved in the training and predicting strategies.

Another approach is to use classical ML algorithms like SVMs given that these

models provide a rigorous mathematical formulation for the mechanism by which they learn from given features in the data. Ponte and Melko [87], as well as Gianetti et al. [94] exploited these models and used the underlying *decision function* of the SVMs to map the Ising model's order parameters and obtained a robust way to extract the critical exponents from the system. Within this approach, one does not need to provide a meticulous explanation of the learning mechanism for the model, this has already been done in its own theoretical formulation—instead, an adjustment of the physical model with respect to the ML algorithm needs to be performed in order to successfully achieve a link between both frameworks. Nonetheless, this approach has the disadvantage that it can be hard to map the ML method to the physical model, as it requires a deep and experienced understanding of the physical system, while simultaneously needing a comprehensive awareness of the theoretical formulation of the ML algorithm being used.

5.5. Outlooks

The approach of illustrating the training scheme, as well as the loss function landscape of a ML algorithm with CMP has proven to be both intriguing and effective. Baity-Jesi et al. [146] used the theory of glassy dynamics to give an interesting interpretation of the training dynamics in DL models. Similar work was performed by Geiger et al. [147], but this time with the theory of jamming transitions, disclosing why poor minima of the loss function in a FFNN cannot be encountered in an overparametrized regime—i.e., when there exists much more training samples than parameters to fit in a NN —. Dynamical explanations of training schemes have the advantage of providing precise frameworks that have been understood in the physics community for a long time, but it is an intricate solution as it needs a scrupulous analysis of the model, leaving little room for generalization on other ML models. It is true that FFNNs, as well as Deep NNs are the less understood intelligent models, but they are not the only ones that need a carefully detailed framework; maybe in future research we can see how other ML models benefit from all these powerful techniques developed so far by the CMP community.

6. Soft Matter and Machine Learning

6.1. Enhanced Simulation Methods

Molecular dynamics (MD) is a classical simulation technique that integrates Newton's equations of motion at the microscale to simulate the dynamical evolution of atoms and molecules [148]. It is, along with the MC method, a fundamental tool in computer simulations within CMP, specifically in SM. The powerful method of MD enables the scientist to obtain physical observables through a controlled and simulated environment, by-passing limitations that most experimental setups have to deal with. MD has become a cornerstone method to model complex structures, such as proteins [149] and chemical structures [150], just to name a few. But such complex structures have to deal with large number of particles—with their many degrees of freedom—as well as complicated

interactions in order to obtain meaningful results out of the simulations. This creates a difficult challenge to overcome, as efficient exploration of system configurations is a difficult task, even with MD simulation code accelerated with modern hardware. In order to reduce the computational burden of modelling such systems, special enhanced sampling methods have been developed [151], but not even these schemes can alleviate the arduousness of modelling complicated systems. ML is seen as a very promising candidate to surpass modern solutions in MD simulations, as shown primarily by Sidky and Whitmer [152]. In their novel approach, Sidky and Whitmer employed FFNNs to learn the free energies of relevant chemical processes, effectively enhancing MD simulations with ML and creating a very comprehensive method to obtain high-precision information from simulations that were not previously readily available. Another interesting procedure to enhance MD simulations was the automated discovery of features that could be potentially fed into intelligent models, making it possible to create a systematic and automated workflow for materials research. Sultan and Pande [153] developed such techniques by training several classical ML methods —Support Vector Machines, Logistic Regression, and FFNNs —, showing that given a MD framework one could set up a complete, self-adjustable scheme to obtain the system's free energy, entropy, structural information and many more observables.

Although in its early stages, the enhancement of classical methods with ML is an intriguing area of research. When no rigorous foundation is needed, ML models are able to exceed human performance in the modelling of atomistic simulations, making it a suitable candidate to become the mainstream method in the future. Of course, there is a long path ahead to fully embrace these methods, as a complete simulation strategy is not easily available yet; further research on the coupling between molecular simulations and ML schemes is the primary way to achieve this.

6.2. Machine-learned potentials

In this new day and age, computer simulations are a standard technique to do research in CMP and its sub-fields. These simulations produce enormous quantities of data depending on the sub-field they are tasked in, for example, biophysics and applied soft matter have produced one of the largest databases—the Protein Data Bank [154]—that contain free theoretical and experimental molecular information as a by-product of research in specific topics. This explosion of immense data available to the public has attracted scientists to look into the ML methodologies that have been created for the sole purpose of dealing with the so-called *big data outbreak* [155] of recent years, and effectively uniting both fields to attempt to use such well-tested intelligent algorithms in the understanding and automation of computer-aided models.

One such task is that of constructing very complex *potential energy surfaces* (PESs) with the experimental and computational data available [12]. This has turned out to be a very successful application to materials science, physical chemistry and computational chemistry, as it allows scientists to obtain high-quality, high-precision representations of

atomistic interactions of all kinds of materials and compounds. In atomistic simulations and experiments, scientists are always very interested in obtaining a good representation of PESs because it guarantees the full recovery of the potential energy—and as a consequence, the full atomistic interactions—of a many-body system. The baseline technique that provides such information is the coupling of MD with the Density Functional Theory [156] which turns out to be a very computational demanding scheme, even for the simplest cases. This constituted the starting point in a long standing approach to use ML models that could compute such complicated functions effortlessly; the first attempt at this was done by Bank *et al* [157] where they proposed to fit FFNNs with information produced by some low-dimensional models of a CO molecule chemisorbed on a Ni(111) surface. They obtained very promising results, such as faster evaluation of the potential energy by means of the NN model compared to the original empirical model. The data sets used by Bank *et al* were composed with a range from two up to twelve features, or degrees of freedom, making it easy and simple to train the NN models.

But this is not always the case, in fact, one could argue that it is *never* the case, as systems like proteins consist of thousands of particles and electronic densities, hence a large number of degrees of freedom need to be computed simultaneously [158]. Another challenge for these type of ML potentials is that of the *descriptors* or *features* needed in order to be fed to an intelligent model. Data fed into ML models should account for all possible variations and transformations seen in real physical models to extend the generalization of the ML schemes and avoid bias in them.

It took more than ten years after the pioneering work of Bank *et al* for Behler and Parrinello [118] to undertake this challenge to a new level by proposing a similar methodology employing FFNNs, advocating now to a more generalized approach to computing the PES of an atomistic system by creating what they called *atomic-centered symmetric functions*. These functions had the role of atomic descriptors of all the possible physical interactions from the atoms or particles being simulated, with the special conditions that no matter what the orientation or position of each of the particles were, these functions could effectively be fed to a FFNN and be able to fit the data to produce the PES of the system. Another way to put it is that the trained NN encoded all possible information, such as electrostatic interactions, rotations, translation, and many other degrees of freedom, without the need to meticulously design this information by hand. This methodology introduced a paradigm shift because it was no longer a proof-of-concept that ML algorithms could be used in these research fields, and many other attempts have been carried out since then. Following the footsteps of Behler and Parrinello, Bartók *et al* [159] proposed a similar methodology, but with completely different ML schemes—in this case being Gaussian Processes [160] —which in turn needed new atomistic descriptors. We shall discuss atomistic descriptors in more detail in the next section.

The advantages of such techniques in all the sub-fields of CMP is manifold, the main one being that simulations are now faster, very precise and also completely reproducible;

by leveraging the retention of the learned features from the NN and employing *transfer learning* [161] the model does not need to be trained again to compute the same interactions it learned to compute. ML potentials have also been successfully applied to explaining very complex interactions, like the van der Waals interaction in water molecules and the reason this interaction results in such unique properties seen in water [162]. Another interesting application was the simulation of solid-liquid interfaces with MD [163], an application that was not thought of being computationally simple or even tractable. One of the remaining challenges in this area of research is a paradoxical one, being that these ML potentials require very large data sets that are computationally demanding in order to train the intelligent model, one possible approach to alleviate this issue is to build and maintain a decentralized data bank similar to the Protein Data Bank—which could be a cornerstone of modern computational materials science and chemistry—enabling anyone interested in this type of research to collect insights from the acquired data, without needing to run large-scale simulations or re-train complicated NN architectures to do so. This is a very interesting research field in the junction of many other specialized sub-fields which is also growing faster due to current computing processing power available, setting up the pathway for new and interesting intelligent materials modelling—which could surely become the future of materials science.

6.3. Atomistic Feature Engineering

So far, we have discussed the different ways in which scientists have been able to apply ML technology in different sub-fields of CMP, such as SM, but lattice systems seem to prevail, where most of the research done is reported with these systems—why is that?—.

One of the fundamental parts of using a ML method is that of *data input* with specific features; for instance, images are described by *pixels* in a two-dimensional grid where the pixels are the features that numerically represent the image, these pixels are then fed to a ML model, e.g. a classifier; another clear example are numerical inputs that can be readily used in regression tasks, and then used as a prediction model. We wish to obtain a similar representation for physical systems, so as to ease the use of ML models in condensed matter systems. Recall that the intrinsic features of lattice systems are spins (σ_i), these spins do not change location they actually stay put and only change their spin value taken from a finite, discrete set of values. We can easily see a link between images and pixels, and a lattice system and its spins; both can be described by a set of discrete features that do not change their values as the system is evolving and changing. But we cannot say the same about atomistic and off-lattice systems, thus we cannot use the same representation as lattice systems because atomistic systems are described primarily by the constant movement of their atoms and particles, and their many degrees of freedom—for instance, for a three-dimensional system, one has $3N$ translational degrees of freedom with N being the total number of particles—. By using the raw positional coordinates, velocities or accelerations we might not be able to convey the true features that the system possesses; if even possible, they could be

conveyed in a *biased* way, e.g., by defining an arbitrary coordinate system or by not being invariant to translation and rotations. In order to overcome this limitation, a special mechanism needs to be developed to feed this data to the ML algorithms. It is this *encoding* of raw atomistic data into a set of special features that has seen a strong surge in recent years when dealing with soft matter and materials.

Atomistic descriptors have been studied heavily throughout the years [164, 165, 166, 167, 168, 169, 170] because they are the gateway to applying ML methodologies in atomistic systems. The reader is referred to these reviews [12, 171] for more information on the topic. Descriptors are a systematic way of encoding physical information in a set of *feature vectors* that can then be fed to a ML algorithm. These encodings need to have the following properties: a) the descriptors must be invariant to any type of point symmetry, for example translations, rotations and permutations; b) the computation of the descriptor must be *fast* as it needs to be evaluated for every possible structure in the system; and c) the descriptors have to be differentiable with respect to the atomic positions to enable the computation of analytical gradients for the forces. Computing these descriptors is essentially called *feature selection* in the ML literature, and most of the time these procedures are carried out in an automated way in a normal ML workflow. Once a particular descriptor has been used, all the methodology from ML that we have seen applied to lattice systems can now be employed on atomistic and off-lattice systems.

6.4. Phase transitions

Phase transitions are the cornerstone of ML applications to lattice systems, but with the use of atomistic descriptors these can easily be extended to off-lattice systems. Jadrich, Lindquist and Truskett [172, 173] developed the idea of using the set of distances between particles as a descriptor for the system, and used unsupervised learning—in particular, Principal Component Analysis—on these descriptors. They wanted to test whether a ML model was able to detect a phase transition in hard-disk and hard-sphere systems. When the unsupervised method was applied, the output from the model was later found to be the positional bond order parameter for the system [174, 175], which effectively determines whether the system has been subject to a phase transition. In other words, the ML model was able to automatically compute the order parameter without having been told to do so. A similar approach but to colloidal systems was done by Boattini and coworkers [176]. Instead of using inter-particle distances, they computed the orientational bond order parameters [177, 178], then they used a DL unsupervised method —a FFNN based autoencoder—to obtain a latent representation of the computed order parameters. With all these preprocessing steps, they fed the encoded data to a clustering algorithm and obtained detailed descriptions of all the phases of matter in the current system. This methodology is systematic and leads itself nicely to an automated form of phase classification in colloidal systems.

6.5. Outlooks

As we have discussed so far, the fundamental step to applying ML to soft matter and off-lattice systems is to define and use a set of meaningful descriptors, but the choices for descriptors are large as well as system-dependent. In order to fully embrace ML in soft matter and colloidal systems a more automated approach will need to be developed, posing it as new and fascinating research area. Recently, DeFever *et al* [179] developed a generalized approach that does not use hand-made descriptors; instead, a complete DL workflow is used with raw coordinates from simulations and it is able to obtain very promising results about the phase transitions, both in and out of thermodynamic equilibrium, in soft matter systems. This scheme is a great step forward towards a fully automated strategy for off-lattice systems, as it reduces the amount of bias a scientist might introduce while using certain descriptors for given systems. Similarly, Terao [180] used CNNs to analyze complex structures in soft matter, like liquid crystals, as well as different types of solid-like structures, by computing special descriptors for the system. The only downside to employing these types of DL methodologies is the large amount of data needed, so maybe in future research can we see approaches where we can use a small amount of data to obtain similar results.

7. Perspectives

ML and CMP have created a very enriching and prosperous joint research area. Modern ML techniques have been applied to CMP with outstanding results, and Physics has given fruitful insights into the theoretical background of ML. But in order to embrace and fully adopt ML tools into standard physics workflows, some challenges need to be achieved.

Currently, there is no standard way to couple both ML and Physics simulation software suites; the main approach is to use available software and hand-craft code that can use the strengths of both parts. Physicists have seen the great advantage that is the use of standard simulation software suites like LAMMPS [181] or ESPResSO [182], but these are not meant to be used with ML workflows. A universal, coupling scheme might be able to simplify research in this exciting scientific area.

Quantum systems have also seen a great deal of advances with ML applications [10], thus it might be interesting to see if the same schemes can be modified and applied to larger-scale systems, such as soft materials, as we have seen it was possible in the topic of phase transitions.

New interesting theoretical insights have also been proposed to explain ML by applying not only CMP, but other Physics frameworks, like the AdS/CFT correspondence [183]. Physics is full of these rich and rigorous frameworks and new research into the area might be able to give a full and thorough explanation of the theory of Deep Learning and its learning mechanisms.

All in all, ML and CMP are just starting to convey ideas to each other, creating a

fertile research area where the work done is towards an automated, faster and simplified workflow that will enable condensed matter physicists to unravel the deep and intricate features of many-body systems.

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