Adimen artifizialak hainbat diziplinatan izan duen eragin handia kontuan hartuta, materialen fisikariak ikaskuntza automatikoko teknikak lantzen hasi dira euren eguneroko ikerketan. Gaur egun, ikaskuntza automatikoa erabiltzen ari da materialen propietateak iragartzeko soilik erregresio estatistiko-ereduetan oinarrituz, potentzial interatomiko zehatzak sortzeko, baita materialen ekuazio oinarrizkoenak ebazteko ere. Eskuizkribu honetan materialen zientzian ikaskuntza automatikoko ereduetan erabiltzen diren teknika nagusiak, aplikazio garrantzitsuenak eta etorkizuneko ikuspegiak aztertzen ditugu.

Gitza-Hitzak: Materialen zientzia. Neurona-sareak. Ikaskuntza sakona. Potentzial interatomikoak. Deskribatzaileak. Supereroankortasuna. Konputazio kuantikoa.

Teniendo en cuenta el gran impacto que ha tenido la inteligencia artificial en diversas disciplinas, los científicos y científicas de materiales han comenzado a incorporar técnicas de aprendizaje automático en su investigación diaria. Actualmente, el aprendizaje automático se utiliza para predecir las propiedades de los materiales basándose únicamente en modelos de regresión estadísticos, para crear potenciales interatómicos precisos y también para resolver las ecuaciones más básicas de los materiales. En este manuscrito analizamos las principales técnicas utilizadas en modelos de aprendizaje automático en ciencia de materiales, las aplicaciones más importantes y las perspectivas futuras.

Palabras Clave: Ciencia de materiales. Redes neuronales. Aprendizaje profundo. Potenciales interatómicos. Descriptores. Superconductividad. Computación cuántica.

Compte tenu du grand impact que l'intelligence artificielle a eu sur diverses disciplines, les physiciens des matériaux ont commencé à intégrer des techniques d'apprentissage automatique dans leurs recherches quotidiennes. L'apprentissage automatique est actuellement utilisé pour prédire les propriétés des matériaux en se basant uniquement sur des modèles de régression statistique, créer des potentiels interatomiques précis et également pour résoudre les équations les plus élémentaires des matériaux. Dans ce manuscrit, nous analysons les techniques utilisées dans les modèles d'apprentissage automatique en science des matériaux, les applications les plus importantes et les perspectives futures.

Mots-Clés : Science des matériaux. Réseaux de neurones. Apprentissage profond. Potentiels interatomiques. Descripteurs. Supraconductivité. Informatique quantique.

Materials Science Powered by Machine Learning

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Materials Science Powered by Machine Learning

1. Introduction

The advent of artificial intelligence in our society has been so fast in the last few years that it has permeated our everyday life without us being aware. Many of the world's citizens today have already used an automatic translator based on neural network technologies [Art18]. Or voice recognition software powered by machine learning [Den13]. Image recognition is applied by many of the most common applications to store photos, just to mention one of its more domestic and inoffensive applications. Artificial intelligence is thus expected to continue broadening its scope in the next few years and provide new functionalities to people in their everyday life, even if its development will pose profound societal and ethical questions that stakeholders need to address at the moment and decide the limits of these new technologies.

Artificial intelligence, or more precisely what it is understood as machine learning, has rapidly drawn the attention of the scientific community and it is more and more used in current research work. Materials science is not an exception and many groups around the world are incorporating these techniques into their research lines. Machine learning algorithms try to build computational models that can learn from a dataset to, afterwards, provide predictions that are too difficult or, better said, hidden for human capacities. More precisely, these algorithms try to reveal patterns in the training dataset to make predictions or decisions without having been programmed to perform such a particular task. Despite the application of these techniques is still in its early days, considering the outstanding capacities that machine learning methods have shown in other fields, nobody denies that it will be an outstanding tool for the advancement of materials science in the near future.

Despite many of the algorithms in which machine learning is based date back to the 80's [Hop82], it is in the last few years that applications of machine learning techniques have bloomed in materials science. There are several reasons for that. The most obvious is the rapid increase in the computational power worldwide that has happened in the last decades, which has enabled the application of deep learning techniques. Secondly, having in mind that successful machine learning techniques rely on broad, truthful, and unbiased data, the development of large curated databases in materials science has made it possible to turn datasets into materials discovery platforms [Him19]. Another less apparent but non-minor aspect of the advent of machine learning techniques in materials science is the culture of releasing computational codes as well as databases with open access, making them available free of charge to anybody. Thanks to this open software and data culture, which fortunately is expanding in the research community, new developments and applications are flourishing everywhere in the world, making these techniques more and more common.

It is mentioned by some authors [Hey09] that data-driven science brings a new, fourth, paradigm to the ultimate goal of materials science: the discovery of new materials. In the early times, material discovery was purely experimental based on trial and error. The development of the laws of thermodynamics brought a second paradigm, valid in the XVII, XVIII, XIX, and early XX centuries, in which model based theoretical science was implemented in the quest for new materials. The third paradigm arrived in the second half of the XX century with the development of practical implementations of quantum mechanics in material science based on density functional theory, which allowed the simulation of materials properties in the computer. The current paradigm based on machine learning tries to go beyond by predicting new materials seeking correlations on large datasets hidden to human intuition.

In the following we briefly overview the main concepts and methodologies used in machine learning algorithms for materials science, we review the main applications of these techniques in the field, and finally we discuss the prospects and future of these methods.

2. Basic concepts in machine learning methods for materials science

The applications of machine learning to materials science rely on what is called “big data” as well as on powerful machine learning algorithms, for instance, neural networks and deep learning.

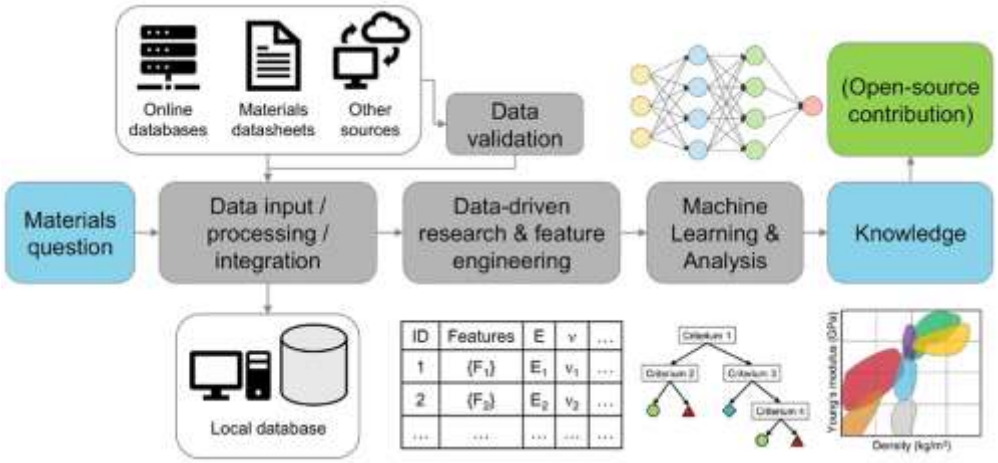
2.1 Big data

Data is crucial in materials science, where experimental observations and calculation results are continuously being collected or generated, stored, and analyzed. Materials data, if appropriately handled and exploited, are expected to be key in boosting materials development and discovery in coming years thanks to machine learning techniques. However, for this to happen, materials data must be made available and, ideally, open access to the community. Currently, efforts in this direction are being carried out worldwide and so-called *materials data infrastructures* are plentiful: the AFLOW consortium (http://aflowlib.org/) based at Duke University; the Computational Materials Repository (CMR, https://cmr.fysik.dtu.dk/), based at DTU; the Materials Project (https://materialsproject.org), based at LBNL; the NOMAD CoE project (https://www.nomad-coe.eu/), based at FHI/Max Planck Society. These are just a few of the many platforms developed in the last few years [Him19]. Besides collecting, storing and providing data, some of these data infrastructures also offer analytic tools for property prediction and materials discovery.

The rise of active materials data infrastructures, together with the growing rate of data collection and generation, has promoted the era of “big data” in materials science. The concept of big data primarily refers to the amount of data but, in a more general sense, it describes a data management strategy suitable for processing unstructured, time sensitive, or simply very large databases. Big data is usually characterized in terms of the so-called four Vs: volume, velocity (rate at which data is generated), variety (the heterogeneity of data type, format and meaning), and veracity (potential lack of data quality).

Within materials science, a pivotal step to benefit from the correlations contained in big data is to find the descriptors that determine a specific property or function of a material. For their use in machine learning strategies, such descriptors must be expressed in a machine-readable form. This involves what it is referred to as a “fingerprinting”, i.e. converting the raw data from the repositories to a machine-readable form. The fingerprints are basically strings of numbers, which, depending on the nature of the problem and the required degree of accuracy, are defined at different levels of so-called granularity. That is, if the problem does not require high accuracy the fingerprints may be given in terms of general properties of the materials (e.g. the band gap or the melting temperature), whereas for highly accurate predictions finer fingerprints containing atomic-level information are needed (e.g. atomic positions or electronic density) [Bat21]. Once the appropriate descriptors are identified and the conversion to a machine-readable form is completed, big data can be exploited for materials property prediction and screening, in particular employing machine learning tools as briefly sketched in Fig. 1.

Figure 1: Overall workflow of machine learning in materials science



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2.2 Main concepts in machine learning

Depending on the available data, machine learning can be divided into three main categories: supervised, unsupervised, and reinforcement learning. Supervised learning involves training a model with real input-output datasets to predict optimal outputs for new labelled inputs. Certainly, supervised learning is the most mature and powerful category, and it is widely used in materials science [But18]. For example, in the prediction of physical properties [War17, Isa17,Xie18,Sch19,Fab18,Gho19,Tod19] using as input the properties of a material or process (e.g. geometry, external conditions). As opposed to supervised learning, where labelled input data is used, in unsupervised learning only unlabelled input data is given to a model and the learning algorithm is focused on finding hidden patterns in the data. Unsupervised learning is often employed for preprocessing the input data [Zak18]. In reinforcement learning, a model is asked to find a set of optimal actions for a given goal in order to maximize a reward. In other words, it learns from interactions with the environment. Reinforcement learning is rapidly emerging in the field of materials science, and it can be very useful in tasks that demand machine creativity [Zhu18].

Furthermore, within the field of materials design and discovery, the machine learning strategy is commonly based on solving the so-called forward problem, which relies on screening a predefined list of materials candidates based on the properties predicted by machine learning. The list of materials properties that have been predicted using forward machine learning are truly immense as we will discuss below, and studied cases range from basic properties such as lattice thermal conductivity [Che19-1] to more exotic ones, e.g. superconductivity [Sta18]. Interestingly, in recent years the emphasis has shifted to strategies for solving the inverse problem, that is, directly generating material candidates starting from the target property or functionality [Tim18, Che19-2]. However, the materials space is huge and makes the inverse problems hard to converge. Moreover, one target property might correspond to multiple materials, which is referred to as "one-to-many" phenomena or "non-uniqueness". In order to tackle these problems, different strategies are being put forward [Bat21], and inverse design problems are expected to become ubiquitous in the near future.

Another crucial part of the machine learning process involves the choice of an appropriate algorithm to perform the analysis of the data. The spectrum of possible algorithms is enormous, ranging from linear

regression and nonlinear methods (kernel-based or Gaussian-process-based) to decision trees, support vector machines, and neural networks. Depending on the type of data and the question posed, various algorithms may be suitable for a given machine learning problem. Furthermore, it is often helpful to use an ensemble of different algorithms, or even of similar algorithms with different values for their internal parameters (known as 'bagging' or 'stacking'), allowing the creation of a more robust model.

In particular, neural networks (NN) are well established in materials science, where they have been successfully applied [Agr19, Li22], e.g. in the development of accurate interatomic potentials and in the mapping of complex materials behavior (flow stress, fatigue behavior, microstructure, etc.) to materials processing parameters (heat treatment, deformation, cold working, etc.). In the following, we briefly introduce the basics and the recent trends of NNs.

2.3 Neural networks and deep learning

Neural networks, also known as artificial neural networks, are inspired by the activity of the human brain and they mimic the way in which brain cells (neurons) signal to one another. A neural network consists of layers of nodes, containing an input layer, one or more hidden layers, and an output layer (see Fig. 2). Each node or artificial neuron is connected to another node by a direct link, which serves to propagate the data from one layer to the next. In fact, each individual node or neuron of a NN can be pictured as its own regression model, composed of input data, weights, a bias (or threshold), and an output (see Fig. 2). Once a set of inputs ($[x_1,...x_n]$) is established, weights ($[w_1,...w_n]$) are assigned to help determine the relevance of each variable. Then, all inputs are multiplied by their respective weights, summed, and shifted by the bias (b). Afterward, this summation (z) is passed through an activation function (σ), which defines the output of the node ($Y=\sigma(z)$). If that output exceeds the considered bias or threshold, the node is "fired" (or activated) and data is passed to the next layer in the network. Otherwise, no data is sent to the next layer of the NN. Within this approach, if the node is fired its output becomes the input of the next one. This process of passing data from one layer to the next defines this NN as a feed-forward network.

The activation function defined above is a critical component of a NN. If the function σ is taken to be linear, the neuron performs linear regression or classification. Because of its limited power, using linear activation functions it is not possible to create complex mappings between inputs and outputs of the network. Therefore, typically σ is chosen to be a nonlinear function, which enforces a nonlinear regression and allows to solve classification problems that are not linearly separable. Commonly employed nonlinear activation functions include sigmoid, hyperbolic tangent (tanh), and rectified linear unit (ReLU) [Cho22]. The choice of an activation function is very relevant, as it can significantly affect the efficiency of the training as well as the final accuracy.

Figure 2

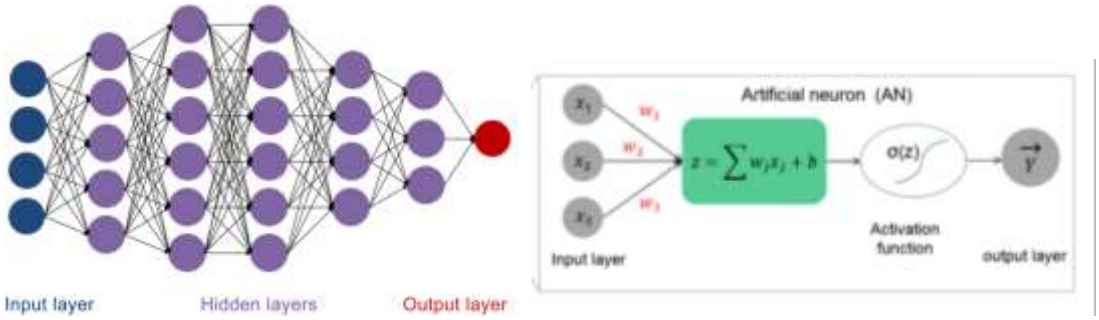

Figure 2: (Left) Illustration of a general neural network with multiple hidden layers, adapted from [Agr19]. (Right) Schematic representation of a single node's functioning within a NN, adapted from [Li22].

Another key component of the learning process is the loss function (also known as an objective function or empirical risk), which is used to evaluate the accuracy of the NN. The loss function is calculated by comparing the output of the neural network and the known target value data, and depending on the problem different loss functions can be used, e.g. mean squared error (MSE), negative log likelihood (NLL), or binary cross entropy (BCE). The ultimate goal is to minimize the loss function until the desired accuracy, which is typically done by iteratively adjusting the weights via gradient descent algorithms such as stochastic gradient descent (SGD), Adam, Adagrad, etc. [Cho22]. Remarkably, many modern NN frameworks make use of so-called back-propagation (or backward propagation of errors) to obtain the partial derivatives of the loss function with respect to the weights through recursive application of the chain rule, iterating back from the last layer. The high efficiency of the back-propagation method makes it possible to employ gradient methods for training multilayer NNs.

Multilayer NNs are characterized by the depth of layers, that is, the number of hidden layers it incorporates. A neural network that consists of many layers, typically 5-100 including the input and output layers, is considered a deep learning (DL) algorithm. Deep learning is one of the best-performing machine learning techniques, as its wide success in computer vision and speech recognition has demonstrated [Lec15]. Remarkably, in recent years DL has also emerged as a game-changing method in the field of materials science [Li22]. The potential of deep learning can be mainly attributed to its ability to generate representations that capture the most relevant aspects of the data, while disregarding the nonessential details. Besides, DL is highly flexible, with a large spectrum of available model architectures, each of them suited for a particular type of input-data. However, the high representation power of DL requires a large training dataset to fit the models and achieve accurate results. In this sense, efforts are being made to benefit from the inherent structure in materials sciences to reduce the amount of data needed in DL algorithms in this field [Bat19].

A critical issue regarding deep learning is that this method is not readily interpretable, i.e. it is challenging to achieve a detailed explanation on how the model arrives at its predictions. Usually, DL generates black-box models that one would ideally wish to open and understand. Moreover, interpretability is also relevant for debugging machine learning models and for taking informed steps towards their improvement. Enhancing interpretability is indeed an essential ingredient for the broad deployment of DL in all fields, including materials science. Within this scenario, several methods to interpret DL methods have been proposed recently [Zil18,Bac15,Kum17,Mon18].

Regardless of the above-mentioned issues, DL is clearly outperforming other machine learning techniques in various scientific areas, and it is rapidly becoming an essential tool in materials science. An evident proof of this is the recent successful application of DL to solve a wide variety of problems in materials science,[Gha15,Mor16,Sch17-1,Rya18,Xie18,Zil18] as well as the development of custom neural network architectures in this field [Xie18,Sch18,Gho19].

3. Applications in materials science

The ultimate goal of machine learning applications in materials science is the discovery of new materials with physical properties that outperform current ones. New advanced functional materials will be crucial to tackle the huge challenges the world is facing in this century, mostly related to the climate crisis, increasing energy demand, and exhaustion of natural resources. Considering that the estimated number of possible materials is as large as a googol (10^{100}) [Wal15], it seems inconceivable that there are no synthesizable materials out there with, for example, a larger thermoelectric efficiency than current best thermoelectric materials or a higher critical superconducting temperature. The capacity of unveiling hidden correlations to human capacity makes machine learning a formidable tool in this daunting task. Although the applications of these techniques are still somewhat primordial and a larger impact is expected in the coming years, there are already promising results that have led to the discovery and experimental realization of new interesting materials [Teh18]. It is clear that this data driven new approach towards materials discovery is a promising alternative to the traditional way based exclusively on experimentation, theory, and/or computation.

The success of machine learning techniques will depend on their capacity of predicting physical and chemical properties of unknown materials based on datasets, as well as in the possibility of incorporating artificial intelligence techniques into the calculation of properties that at the moment are too complex or expensive for first-principles methods. Current efforts in the application of artificial intelligence to material science are thus focused on estimating materials properties based on existing datasets, on the development of empirical potentials to describe the interactions between atoms in a material, and the ultimate solution of the Schrödinger equation in systems with few electrons. In the following we will briefly overview some of the main results obtained thus far in each of these areas.

3.1 Prediction of materials properties based on datasets

There are about a few millions of materials cataloged and hundreds of millions of properties calculated for them already [Cur12]. This does not mean, however, that all properties of all known materials are classified: there may be known materials that have unknown properties, which may be remarkable. The use of artificial intelligence can help to calculate the properties of materials that have not been studied thus far, in order to unveil if an already known material existing in the databases has an interesting unknown property. Also, based on analogies to the compounds in the databases, the existence of new materials can be predicted.

Unless the problem is well framed with suitable descriptors, machine learning algorithms will not succeed in this task. The standard descriptors used currently in the machine learning prediction of materials properties are related to the elemental properties and the chemical environment. The elemental descriptors can be the period and group in the periodic table of the element, the ionization potential, the covalent radius, the electronegativity, and so on. It is noteworthy to state that elemental descriptors should be uncorrelated. Thus, it is not surprising that sometimes better results are obtained by simply

considering the group and period of the element instead of a large set of elemental descriptors [Sch17-2]. The descriptors of the chemical environment are more difficult to determine, since they do not depend exclusively on one particular atom, but on the other atoms in the vicinity. Different descriptors have been developed in the last years that face this difficulty. However, it is not given that a descriptor is better than another one: the suitability of them may be problem dependent. Some of the most common descriptors for the chemical environment are those based on the Coulomb repulsion between atoms [Rup12], the radial and angular functions introduced by Behler and Parrinello that determine the atomic neighbors of a given compound [Beh07], or the smooth overlap of atomic positions (SOAP) that is constructed by centering Gaussian functions at each atomic sites [Raf12].

Figure 3: (a) Predicted superconducting critical temperature by machine learning versus the measured critical temperature. (b)-(e) Predicted critical temperature versus the experimental critical temperature when the machine learning training is performed exclusively in one superconducting family

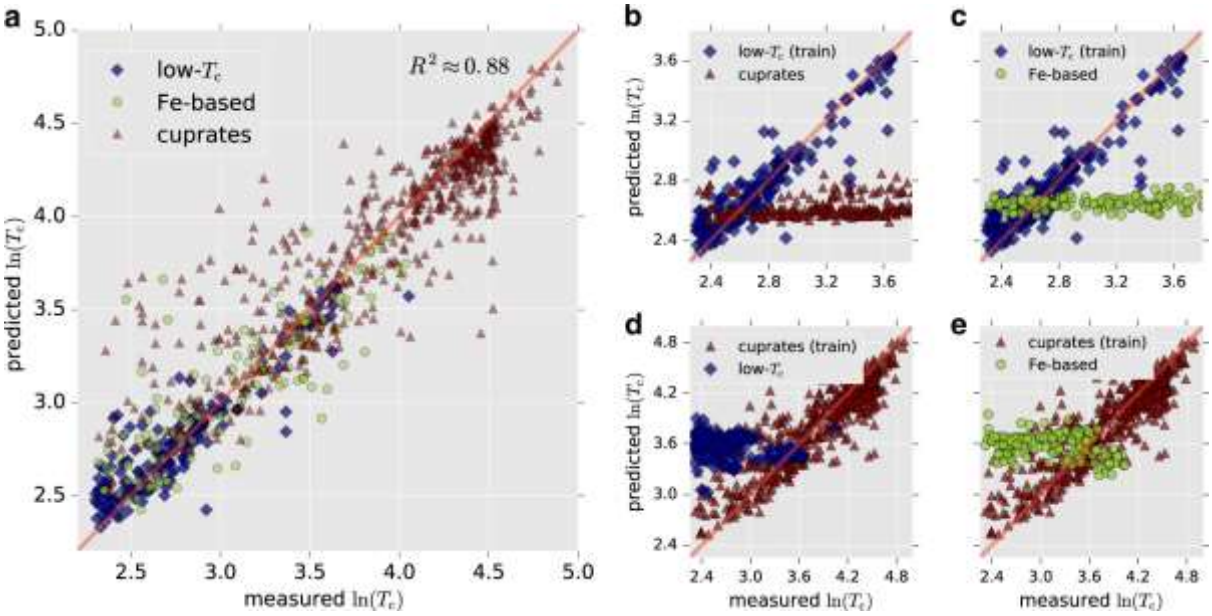

Figure taken from Ref. [Sta18].

Making use of these descriptors and large databases, machine learning techniques have been applied to the prediction of many physical properties of materials already. The list is large and growing [Sch19], and includes predictions of electronic, mechanical, magnetic, and vibrational properties such as the Curie temperature [Bal18], vibrational free energy and entropy [Leg17], electronic band gap [Xie18], lattice parameter [Pil18], heat capacity [Isa17], thermal expansion coefficient [Isa17], thermal conductivity [Car14-1], local magnetic moments [Pha17], melting temperature [Sek14], magnetocaloric effect [Zha18], grain boundaries [Kik18], Seebeck coefficient [Gau16], thermoelectric figure of merit [Car-2], bulk and shear moduli [Xie18, Teh18], electrical resistivity [Gau16], density of states [Sch14], metal-insulator classification [Shi16], topological invariants [Zha17], and superconducting critical temperature [Sta18].

Some of these first applications of machine learning techniques to the prediction of materials properties based on databases are quite remarkable already. The performance of the models in predicting experimental electronic band gaps lies between standard approaches for dealing with electronic correlation and more advanced methods [Xie18]. By screening more than 100,000 systems for superhard materials, a recent work was able to predict new superhard compounds, two of which were actually

synthesized a posteriori [Teh18]. Another remarkable application sketched in Fig. 3 was the creation of a regression model for the critical temperature (T_c) of superconductors, including low-Tc as well as high-Tc cuprates and pnictides [Sta18]. A very interesting result is that a model trained in one type of compound is unable to predict the T_c of other types of superconductors. This points to the fact that the superconducting mechanism is different for low-T_c superconductors, pnictides, and cuprates.

3.2 Development of empirical potentials based on machine learning

Based on databases and elemental and chemical environment descriptors, the prediction of crystal structures simply from the chemical composition has also been attempted by machine learning techniques [Fab16, Kim18]. This is one of the ultimate goals of materials discovery, as the crystal structure is the starting point for any other characterization of a material. However, the approaches so far purely based on databases focus on specific types of compounds, like Heusler compounds [Kim18] or perovskites [Sch17-2]. Considering that the databases used are formed by already known materials, these approaches are not expected to be able to predict fully novel crystal structures with unexpected properties. More traditional crystal structure prediction techniques based on the density-functional theory (DFT) calculation of formation enthalpies [Pic06, Goe04, Gla06, Wan10], which are not biased by the recurrence of particular types of compounds in databases, are more prone to new unexpected discoveries. The problem of the latter approach is that it requires a huge computational effort, already very intensive for ternary compounds and probably unfeasible for quaternaries.

Machine learning techniques can however help in this task, but in a different way: with the development of empirical machine learning potentials which can calculate the energies, atomic forces, and lattice stresses in a fraction of time compared to DFT. Machine learning potentials use structural descriptors to fit a force field on a training set built with forces usually calculated with DFT on different atomic configurations, which are in most cases generated by *ab initio* molecular dynamics. There have been several different machine learning potentials developed in the literature since Sumper *et al.* used for the first time neural networks to create an empirical potential [Sum92]. One of the most successful machine learning potentials are those developed by Behler and Parrinello [Beh07], in which the total energy of the system is represented as the sum of individual atomic contributions. This has become standard in other more modern machine learning potentials because it allows a very fast calculation of the forces and, thus, it makes possible the application of these potentials to very large systems. Other types of highly used machine learning potentials are the so-called Gaussian approximation potentials (GAP) [Bar10], which make use of Gaussian regression by exploiting the fact that the forces on the training set are usually distributed according to a Gaussian. GAP potentials have been used in many systems, such as boron [Der18], iron [Dra18], graphene [Row18], and so on.

All these machine learning potentials have DFT accuracy, obviously at the DFT level used to train them. Having fast but accurate potentials can give the option to study the thermodynamic properties of large systems, with thousands or even millions of atoms, as well as their dynamics, by running molecular dynamics simulations for times unaffordable to DFT. Machine learning potentials can also be useful for crystal structure prediction according to recent works [Pic22]. Whether machine learning potentials based crystal structure prediction becomes standard will depend on the capacity of these potentials to describe different crystal structures even if the chemical environment is different. This is one of the biggest challenges in the field, which is of utmost importance for the sake of materials discovery.

3.3 Solving the electronic Schrödinger equation with deep neural networks

The advantage but also the problem of current machine learning potentials is that indeed they have DFT accuracy. However, due to the approximations assumed by DFT for the electronic exchange and correlation part of the electron-electron interaction, the DFT calculations used to build the potential may not yield good atomic forces, hindering their accuracy and predictability. This is a difficult problem to overcome because calculating accurately the electronic wave functions requires very complex and expensive calculations with quantum Monte Carlo, coupled clusters, or full configuration interaction (FCI) methods. It is hard to believe that machine learning can help to solve the electronic problem itself, but recent deep neural network applications have shown that the Schrödinger equation of spin Hamiltonians as well as simple fermionic problems can be solved making use of neural networks [Car17, Pfa20]. Applications have been limited to very simple systems like molecules, but have reached accuracies comparable to FCI with a reduced computational cost. These results are promising and show that neural networks can be applied to the core problem as well, by helping to solve the most basic equations that govern matter.

The scalability of these methods to larger systems will determine the future of these techniques. If researchers manage to make these techniques efficient also for systems with a large number of electrons, one can think of training machine learning potentials on these calculations. This can yield an unprecedented accuracy for materials simulations and a bright future for materials science.

4. Prospects and future

The capacity of machine learning techniques to unveil hidden correlations in datasets and to perform predictions based on them, examples of which have been discussed above, challenges one of the most basic pillars of science. Scientific progress up to now has been based mostly on the idea that understanding the reasons behind a given physical phenomenon opens the possibility of making new predictions and discoveries. In other words, the comprehension of physical laws precedes the prediction of physical properties. With machine learning methods, however, this is no longer true, as predictions can be made without having an understanding. And these predictions may be perfectly right. Causality, which is at the core of scientific construction, is therefore questioned by machine learning approaches.

Such a radical statement, however, is not totally exact because, as it has been described above, defining accurate descriptors is necessary for machine learning methods to work. And in order to define accurate descriptors a physical understanding of the problem at hand is necessary, which helps determine the right variables at play. Therefore, no machine learning method will be successful without a clear prior understanding of the physical problem. Moreover, despite the obscurity of machine learning predictions, the deep causal understanding of the problems will always be essential and, thus, the quest for the deepest causal reasons in materials science will not disappear from the research community.

A clarifying example of the need for fundamental laws and understanding is provided by the machine learning predictions on superconductivity. Despite machine learning regression models are capable of reproducing experimentally observed critical temperatures in high-temperature superconducting cuprates [Sta18], no new superconducting material with a higher critical temperature has been predicted and later synthesized thanks to machine learning predictions. The main reason is probably that the physical mechanism behind superconductivity in these compounds remains a mystery. On the contrary, record superconducting critical temperatures above 250 K have been measured in high-pressure hydrides [Dro19], following earlier theoretical predictions performed without any help of machine learning

techniques [Pen17]. The latter calculations are possible only because in these compounds the coupling is the well-known electron-phonon interaction, which is fundamentally quite well understood, and the physical understanding of the problem is sufficient to guide the quest for higher T_c materials.

Anyway, machine learning techniques are a fantastic tool for the advancement of science, also materials science, and will become more and more common in the field. The development of empirical potentials based on machine learning techniques, for instance, offers an unprecedented technique in materials science. As calculating forces and energies with these potentials is orders of magnitude faster than with DFT, but keeping DFT accuracy at the same time, systems with a very large number of atoms can be simulated, or very long molecular dynamics simulations prohibitively expensive for DFT can be ran. Therefore machine learning potentials can open the way for the study of, for instance, biological systems with DFT accuracy, considering that the length and time scales of biological processes are too large for DFT calculations. Also, machine learning potentials can be highly efficient for pure crystal structure predictions in materials with a complex chemical formula, for instance, ternary compounds. The chemical space is too large for DFT standard crystal structure prediction methods [Zha17-2, Oga19]. Despite it may be obscure why machine learning potentials give its values, their use, after benchmarking them rigorously, can allow us to perform calculations that were not feasible before, opening new avenues in research. In that sense, machine learning potentials are not that different from the current use a large part of the research community gives to DFT calculations: without clearly understanding why it is giving these results it is perfectly valid in research studies.

An emerging subfield of machine learning that is expected to have a strong impact on a broad range of scientific areas is quantum machine learning (QML), which lies at the intersection between quantum computing and machine learning [Bia17]. Quantum computing is envisioned to solve intricate problems that classical computing cannot; this is what is known as “quantum advantage” or “quantum speed-up”. Undoubtedly, the enormous speed-up in computational efficiency provided by quantum computers and quantum algorithms holds a great potential to boost the performance of machine learning systems.[Hua22] As such, QML might enable improving and often expediting classical machine learning techniques, which is referred to as achieving quantum advantage in QML. This has motivated the development of a host of quantum machine-learning algorithms like quantum supervised and unsupervised learning [LLo13], or quantum reinforcement learning [Dun16]. Similarly, research has been carried out for neural networks aimed at discovering unforeseen quantum advantages [Wie15, Ami18, All20]. In particular, following Feynman’s idea [Fey82], quantum computation is expected to play a key role in the simulation of quantum systems with many degrees of freedom. Such is the case of materials science, where QML algorithms are expected to be a promising alternative to their classical counterparts. For instance, shallow neural networks using quantum algorithms have already been applied to obtain accurate molecular potential energy surfaces [Xia18], or to simulate excited states of monolayer transition metal dichalcogenides both on classical and quantum computers [Saj21]. With the rapid development of new quantum algorithms and larger-scale quantum computers, QML techniques are expected to become powerful tools to perform electronic structure calculations or to design new materials. As such, QML is expected to be a game-changer in the future of materials science.

As it was mentioned above, the prospects of machine learning techniques are intrinsically linked to the quality of the datasets used in the models. In fact, these methods usually require large data sets for the learning to be effective. This is normally not a problem in fields such as image recognition, where millions of input datasets are available. However, in materials science the amount of high-quality data points is normally limited to hundreds or thousands, which may not be enough in some cases. Besides, current data infrastructures contain mostly computational and hardly no experimental data. Hence, the scientific community, including researchers, journals and funding agencies, need to make a serious effort in building relevant data repositories to fully exploit the potential of not only machine learning, but of data-

driven materials science in general. In this vein, the open science movement – which aims to make research more accessible and usable by everyone – has been and will certainly be crucial in enabling the advancement of this field [Him19]. Remarkably, with the aim of providing aid in data management, the FAIR Data Principles were established: findability, accessibility, interoperability, and reusability [Wil16, Dra18]. Despite all these initiatives, materials data infrastructures face various challenges today –relevance, completeness, standardization, acceptance, and longevity– that still need to be addressed [Him19].

An alternative solution to the problem of limited datasets relies on meta-learning, a subfield of machine learning also known as "learning to learn". In other words, meta-learning learns from experience of solving different problems and makes inferences about transformations useful in different contexts [Jan11]. Based on this approach, developments have been made that allow to achieve high-level performance on learning problems with limited data [Gra14, Dua17, Lak15]. This can have important consequences on materials science, where data are scant and normally slow and expensive to achieve. Indeed, meta-learning is a growing approach that has provided interesting applications in materials science in recent years, ranging from the fingerprint of nanoporous materials for hydrogen storage [Sun21], the iterative of peptides for bio-materials [Rai21], and the guided synthesis of flash graphene [Bec22], just to name a few.

In conclusion, provided that international efforts to gather large and open access databases continue in the coming years, materials science will be powered more and more by machine learning methods. Even if the causal understanding of physical phenomena will continue to be crucial for the development of the field, the incorporation of machine learning techniques into materials science will boost the discovery of new advanced materials.

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