A Review and Perspective on the Main Machine Learning Methods Applied to Physical Sciences

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Abstract: Several types of numerical simulations have been used over the years in the Physical Sciences, to advance the real-life problems understanding. Among the statistical tools used for this are, for example: Monte Carlo simulations, such mechanisms have been used in various areas, however, today another tool is used, Machine Learning, which is a branch of Artificial Intelligence (AI). This article reviews sets of work that encompass various areas of the Physical Sciences, to mention some such as particle physics, quantum mechanics, condensed matter, among many others that have used some Machine Learning mechanisms to solve part of the problems raised in their research. In turn, a Machine Learning methods classification was carried out and it was identified which are the most used in Physical Sciences, something that is currently done in very few studies, as it requires extensive review work. The analysis carried out also allowed us to glimpse which areas of the Physical Sciences use Machine Learning the most and identify in which types of journals it is published more on the subject. The results obtained, show that there is currently a good number of works that interrelate Machine Learning and the Physical Sciences, and that this interrelation is increasing.

Keywords: Machine Learning; Physical Sciences; review; interdiciplinary

1 Introduction

Machine Learning (ML) is a methodology aims to implement capable computational algorithms of emulating human intelligence by incorporating ideas of probability and statistics, control theory, information theory, neuroscience, among other. This has allowed successful applications in various fields, such as artificial vision, robotics, entertainment, biology, medicine, among others, so physical science could not be the exception. ML is basically integrated by 3 major learning paradigms [1]:

- ***Supervised learning:*** It creates a model that relates the output variables with those of the input. This function is used later to make predictions. This paradigm is generally used for regression and classification problems.
- ***Unsupervised learning:*** It has the objective of obtaining groups, such that in each of them there are homogeneous instances, while the groups are heterogeneous among themselves. In this learning there is no information from the past, it is the model itself in charge of making its own divisions. The tasks that cover this type of learning are grouping, dimensional reduction, association.
- ***Reinforcement learning:*** The algorithm learns, not with the previous information that has been provided, but with its interaction with the world that surrounds it, therefore, feedback is produced that modifies and refines its behavior.

Figure 1 shows the 3 paradigms of comprehend ML and some of the most common methods used in each category.

In addition to these three categories, in the present work the methods described below are also considered:

- **Ensemble methods:** These use the idea of combining several predictive models (supervised ML) to obtain higher quality predictions than each one of the models could provide individually. The most popular ensemble algorithms are Random Forest, XGBoost.
- **Neural Networks and Deep Learning:** Neural Networks are a subset of techniques that are inspired by the operation of connectionist systems, they are therefore within ML, the objective of Neural Networks is to capture non-linear patterns in data by adding layers of parameters to the model. Now the term Deep Learning comes from a Neural Network with many hidden layers and encapsulates a wide variety of architectures, for best performance Deep Learning techniques require a lot of data and a lot of calculations.

ML methods are designed to exploit large data sets in order to reduce complexity and find new functions in the data. Various Machine Learning algorithms have been used in the Physical Sciences, there are studies in the condensed matter physics area, such as Carrasquilla and Melko [2] that use a neural network with condensed matter model labels of low temperature and high temperature phase. The training set was given by an equilibrium configuration of the model obtained from Monte Carlo simulations.

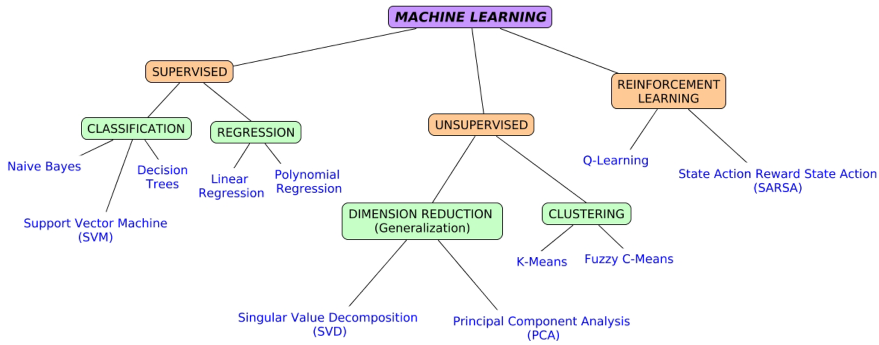

Figure 1
General ML scheme and some methods of each category

Another work used artificial neural networks to recognize different phases of matter and locate associated phase transitions, it is the work of Van Nieuwenburg, E. [3].

A review conducted in the area of particle physics by a research group [4] indicates that to date, the Large Hadron Collider (LHC) experiments have produced around 2,000 journal articles, providing a large library of examples for using ML with these kinds of complex data sets. In that work, for example, some highlights are discussed, including the role of ML in the discovery of the Higgs boson.

Challenges such as the 2014 Higgs Machine Learning Challenge and the Tracking Machine Learning challenge (TrackML) have even been carried out running on the Kaggle platform from March to June 2018 [5], which was a challenge for the ATLAS and CMS experiments, particularly for track reconstruction algorithms.

According to Zdeborová [6] every researcher in the Physical Sciences is clear that there are many numerical simulation types. Depending on the system and the interest question, knowledge and experience are required to find the correct numerical simulation and perform it carefully enough to be able to truly advance a given problem understanding. Under her consideration, the same goes for ML tool applications.

There are then various ML methods have been useful in the Physical Sciences, there are currently some review works such as Larkoski's [7] and Carleo [8] that show some ML methods applied to various areas, however, they do not perform a specific systematic review of a good number of methods used in various areas of the Physical Sciences. Therefore, the objective of this systematic review was to investigate the ML methods used in Physical Sciences, to detect the most used, in addition to identifying the Physical Sciences areas that the most take advantage of them, additionally to distinguish in what type of journals the most they are published.

The structure of this article continues with Section 2, where it explains the methodology used for the literature review. Section 3 shows the data analysis and research results. Finally, the last section addresses the conclusions and perspectives of the work.

2 Methods

2.1 Overview

For the representative review, the most relevant investigations were identified through a systematic search in various electronic resources, such as, ACM digital library, Annual Reviews, EBSCOHOST, IEEE Xplore digital library, Nature, ScienceDirect, Scopus, Wiley, Google Scholar, Web of Science and InSpire. These are 11 of the most used platforms for searching for information. The search ran through July 2021. The combined search terms included "Machine Learning", "Physical Sciences", "physics" and "review". The search was carried out with limited English language. Two of the reviewers performed the search independently, following the methodology of Snyder [9], titles, abstracts, as well as keywords were reviewed. The data collected from both searches was placed in a single directory.

In order to be included in this review, papers had to meet the following inclusion criteria: (1) be defined as research mentioning Machine Learning methods, (2) focus primarily on areas of Physical Sciences, (3) were included other previous review studies covering the intersection between ML and Physical Sciences, and (4) published in the period January 2005 and July 2021.

Referred scientific articles to any other area type not related to Physical Sciences, studies carried out entirely under a mathematical approach, as well as works that were complete books and those that were published in fields of knowledge other than physical and computational sciences they were excluded.

2.2 Data Extraction

The present article was carried out by two reviewers, the 11 electronic databases described above were used and 41 and 29 potentially relevant articles were found by each reviewer, giving a total of 70 articles in this phase. According to Snyder [9] the actual selection of the sample can be done in several ways, depending on the nature and scope of the specific review, in this case, the approach used was to perform the review in stages, firstly, the duplicate elements were deleted, leaving a total of 65 works, subsequently a preliminary analysis was carried out, based on the title, abstract and keywords, which reduced the number to 60, and finally the exclusion criteria were applied, to select the documents that could be eligible for this study, a total of 55 articles remained in this selection (see Figure 2). Once we had selected elements, we proceeded with the collection of the articles in full text for detailed analysis.

For each article included the following variables were identified: (1) Machine Learning methods mentioned in the work, (2) areas of physics addressed, (3) if the work is a review or not, (4) the journal where it was published.

The classification was carried out by two of the reviewers, and although in general there was a great agreement in the information collected, there were some studies where the vision of a third reviewer was necessary to clarify some discrepancies and reach a consensus.

The search and selection process for relevant works is summarized in Figure 2.

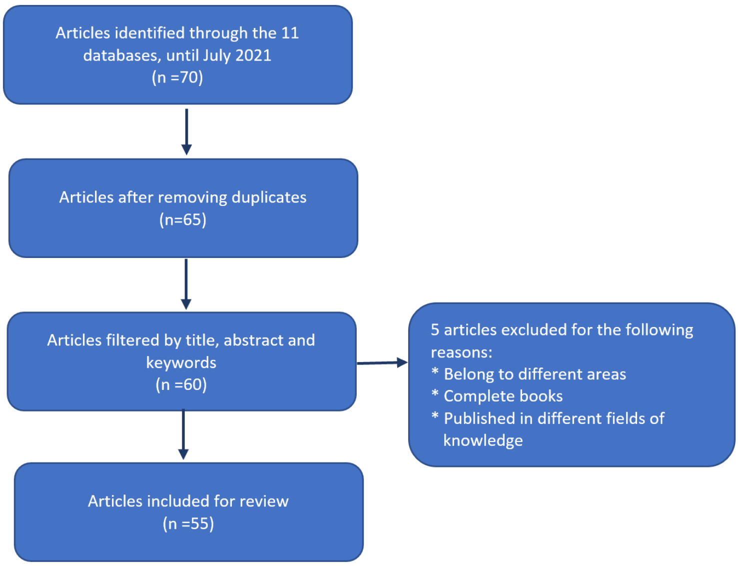

Figure 2

Search and selection strategy process flow chart

3 Results

3.1 Overview

Seventy records were identified through the electronic search carried out (see Figure 2). After removing duplicate items and applying the exclusion criteria, a total of fifty five articles were selected for further review. Once all the documents had been collected, it was necessary to identify the four variables described in the previous section for each work.

The following sections detail and explain the results obtained from the identification and classification of data according to the four variables, in particular Section 3.2 mentions the ML methods used or mentioned in each of the analyzed works, Section 3.3 mentions the areas of Physical Sciences that are covered in the articles, Section 3.4 describes the preceding review works and finally Section 3.5 illustrates in which type of journals they are most published, and a graph of the articles published as a function of time.

3.2 ML Methods

The articles analysis shows a great variety of ML methods, covering the 3 categories, both supervised, unsupervised and reinforcement learning, also including ensemble methods and deep learning. Table 1 shows each of the methods in detail, the total number of works where they were located and the main academic references where they are mentioned. It is important to note that in some studies more than one method is mentioned, even studies that included more than 10 methods were found, generally the review ones.

According to the results, it can be seen that the most used method is Neural Networks, which appears in 26 of the 55 references, which represents 47.27% of the total articles, in the second instance there are Convolutional Neural Networks that are mentioned in 21 articles, in third place we have both Vector Support Machines and Deep Neural Networks in 11 articles each, in fourth place are the Decision Trees that are mentioned in 10 articles and in fifth place are Generative Adversarial Networks mentioned in 8 works.

Among the less mentioned methods are Principal Component Analysis mentioned in 7 articles, followed by Random Forest mentioned in 6, and at the same level K-Nearest Neighbor and Recursive Neural Network with 5 mentions each, followed by three methods that have 4 mentions each, which are Gaussian Process Regression, K-Means, and Long Short-Term Memory.

Finally, it can be seen in Table 1 that there are several methods that are only named in one, two or three works, some of them are modifications or adaptations to the main methods such as Physics-Guided Recurrent Neural Networks that combines RNN and models based in Physics to take advantage of their complementary strengths and improve physical process modeling [10]. Others of them are a new proposal such as Lift & Learn [11] which is a physics-based method to learn low-dimensional models for large-scale dynamical systems.

Table 1
Various ML methods found in analyzed works

Acronym	Meaning	Totals	Main Academic References
BDT	Boosted decision trees	3	[8] [12] [13]
BM	Boltzmann machine	2	[6] [8]
CNN	Convolutional neural network	21	[2] [4] [5] [6] [7] [8] [10] [14] [15] [16] [17] [18] [19] [20] [21] [22] [23] [24] [25] [26] [27]
DBN	Deep belief network	1	[23]
DCN	Deep convolutional network	2	[8] [15]
DF	Decision forests	1	[6]
DNN	Deep neural network	11	[5] [7] [8] [12] [13] [19] [20] [23] [24] [28] [29]
DQL	Deep Q-learning	2	[16] [23]
DQN	Deep Q-networks	1	[23]
DRN	Deep residual network	1	[23]
DT	Decision trees	10	[16] [19] [20] [26] [30] [31] [32] [33] [34] [35]
EML	Ensemble Machine Learning	2	[32] [36]
GAN	Generative adversarial networks	8	[7] [8] [12] [15] [20] [23] [26] [29]
GBDT	Gradient-boosted decision trees	2	[35] [37]
GBRT	Gradient boosting regression trees	2	[8] [19]
GDL	Geometric deep learning	1	[5]
GPR	Gaussian process regression	4	[8] [25] [26] [38]
GRNN	Generalized regression neural network	1	[39]
GRU	Gated recurrent unit	1	[40]
K-means	K-means/medians	4	[16] [31] [41] [42]
KNN	K-nearest neighbour	5	[19] [20] [31] [33] [34]
LiR	Linear regression	1	[43]
LL	Lift & learn	1	[11]
LoR	Logistic regression	1	[19]

LSTM	Long short-term memory	4	[5] [10] [23] [40]
MCTS	Monte carlo tree search	1	[5]
MEM	Matrix element method	1	[12]
MLP	Multi-layered perceptron	1	[44]
MPR	Multivariate polynomial regression	2	[33] [45]
NB	Naive Bayes	2	[19] [20]
NN	Neural network	26	[3] [4] [6] [7] [8] [13] [14] [16] [20] [22] [26] [31] [32] [33] [34] [42] [43] [44] [46] [47] [48] [49] [50] [51] [52] [53]
PCA	Principal component analysis	7	[3] [8] [29] [34] [42] [47] [54]
PDML	Physics-driven Machine Learning	1	[55]
PGRNN	Physics-guided recurrent neural networks	1	[10]
PNN	Parsimonious neural networks	1	[56]
RBFN	Radial basis function network	1	[28]
ReF	Regression forests	1	[57]
RF	Random forest	6	[19] [26] [40] [41] [43] [53]
RM	Regression models	1	[16]
RNN	Recursive neural network	5	[7] [10] [15] [23] [40]
SVM	Support vector machine	11	[6] [8] [16] [18] [19] [23] [31] [32] [34] [37] [43]
SVR	Support vector regression	2	[40] [54]
VAE	Variational autoencoder	2	[7] [29]
XGB	XGBoost	1	[28]

3.3 Areas of Physics Addressed

In order to group the articles, the following classification was proposed, consisting of 2 categories that cover several areas of Physics. The first was Basic Physics and the second was Applied Physics. Figure 3 shows the classification made in this study and the percentage of works found by areas of Physics. It is important to note that all publications make use of ML as an extremely powerful tool to reach a conclusion or result in one or more areas of the Physical Scienes.

In Figure 3 it can be seen that the areas of knowledge concentrated in the publications are in first place Particle Physics (16%), followed by Materials Science (15%), in third place Quantum Mechanics (12%), later Condensed Matter (9%), Physical-Chemistry (6%), Atmospheric Physics (6%), Astrophysics (4%), later, Mathematical Physics, Mechanics, Fluids, Statistical Physics, new Physics, Geophysics, Energy Systems with 3%, and finally with 1% each of the remaining areas.

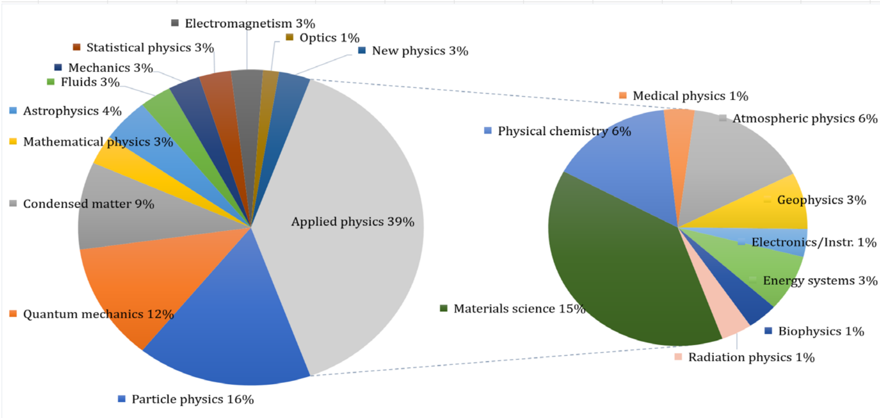

Figure 3
Areas of Physics that use Machine Learning

It is convenient to mention that it was possible to establish a methodology to identify the intersections of the Physical Sciences with Machine Learning, through which the publications in this regard were identified and based on this it becomes clear that Machine Learning is becoming an important tool in the Physical Sciences. This crossing is very novel, it can be explained by the ML strengthening and the use of GPUs. On the other one hand, due to the need for new tools to solve highly complex problems in the Physical Sciences, which alone cannot it is possible to solve them with traditional tools.

Something very interesting for the Physical Sciences is that, by qualitatively analyzing the works [30] [50] [51], a new strategy is observed to identify new Physics methods (such as new experiments in Quantum Mechanics or Physics beyond the model standard) using Artificial Intelligence. This is something completely new, Physics has never been built by AI. We can suggest the term AI Physics.

3.4 Review Articles

Most of the analyzed works are original articles, in which the result of an investigation is reflected with clarity and objectivity. On the other hand, 8 review works were located, some of them do not explicitly say “review”, however, they encompass a large number of works and show an overview of various aspects of ML methods applied in some fields of the Physical Sciences. These broadly contextualize the issue. Around 14.54% (n = 8) of the analyzed papers are review articles, the methods mentioned in such papers are summarized in Table 2. As can be seen in the study by Carleo et. al [8], includes more than 10 methods, among them the most used as NN, GAN, CNN and SVM. It can also be seen that neural networks is the method most mentioned in the review papers.

Table 2
Review works and ML methods included in each of them

Study	ML methods mentioned
Larkoski et. al. [7]	NN, CNN, RNN,DNN,GAN, VAE
Carleo et. al. [8]	PCA, BM, GAN, NN, DNN, DCN, BDT, CNN, GPR, SVM, GBRT
Guest et. al. [15]	DCN, CNN, RNN, GAN
Radovic et. al. [4]	NN, CNN
Dunjko and Briegel [16]	NN, SVM, RM, K-means, DT, CNN, DQL
Zhang et. al. [32]	NN, SVM, DT, EML
Ng et. al. [43]	LiR, RF, SVM, NN
Cheng and Yu [23]	DNN, RNN, SVM, CNN, DQL, DQN, GAN, DRN, DBN, LSTM

3.5 Journals Where the Investigations were Published

The vast majority of the analyzed articles were published in Physical Science journals (see Figure 4), with 69% of the total, including: Physics Reports, Reviews of Modern Physics, Annual Review of Nuclear and Particle Science, Journal of Physics: Conference Series, Contemporary Physics, among many others. On the other hand, it can be observed in Figure 4 that only 20% of the investigations are in journals in the field of Computer Science, among them are: Applications of Artificial Intelligence, Procedia Computer Science, Computers & Fluids and some in as IEEE 14th International Conference on e-Science. However, 11% of the papers were published in journals considered interdisciplinary, such as: Nature communications, Scientific Reports, Nature.

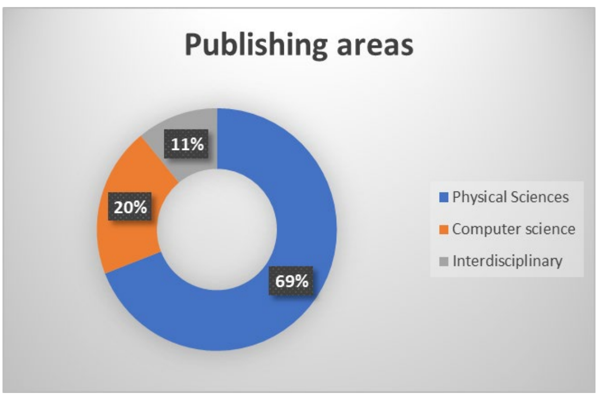

Figure 4
Journal types where it is mostly published

The publications are well referenced in databases that record articles of high academic quality; It is worth noting that several of the articles belong to the journals with the greatest impact in the Physical Sciences such as "Nature" [2-4] [6] [13] [20] [30] [35] [51]). Approximately 96% of these publications are cited in the "Journal Citation Reports 2020" [58].

3.5.1 Scientific Publications of ML and Physics as a Function of Time

Figure 5 shows the research articles analyzed in this work, as a function of time, covering the period January-2005 and July-2021. It highlights the significant and accelerated increase of publications in the last 5 years, which corresponds to 85% of the publications.

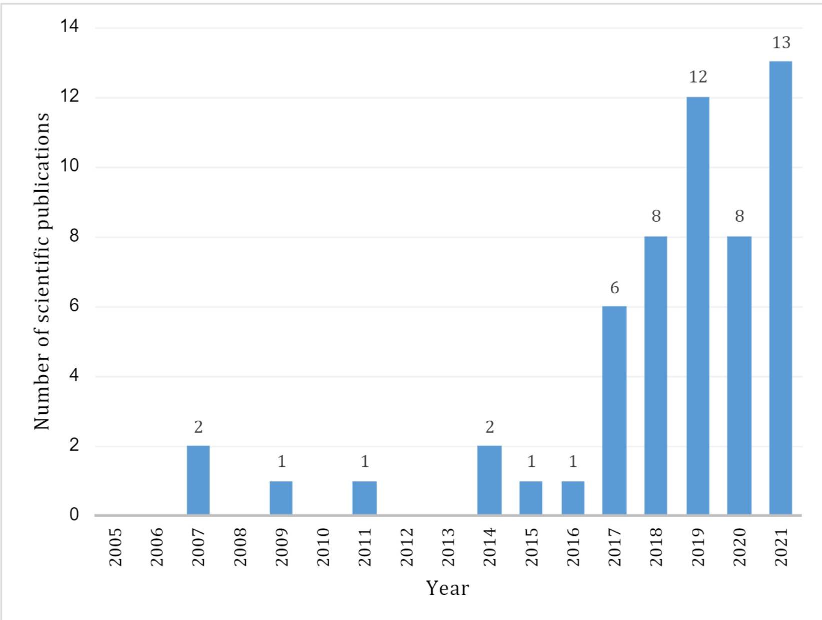

Figure 5
Number of publications in Physics using ML

Conclusions

In general, the results show that there is a good amount of work that connects Machine Learning and the Physical Sciences. It can be seen that there is a wide variety of ML methods that are used both for supervised and unsupervised learning, as well as for reinforcement. Those mentioned to a greater extent are Neural Networks, Convolutional Neural Networks, Vector Support Machines, Deep Neural Networks, Decision Trees and Generative Adversarial Networks. Some works that carry out new proposals were also found, such as Physics-Guided Recurrent Neural Networks that combines RNN and Physics-based models and another such as Lift & Learn, which is a Physics-based method to learn low-dimensional models for large-scale dynamic systems.

On the other hand, according to the results, it can also be seen that there is an area of great variety of the Physical Sciences that use ML methods, among the most Particle Physics, Quantum Mechanics, Condensed Matter, which are considered within basic Physics. However, jobs were found within applied Physics, particularly in the areas of Materials Physics, Physico-Chemistry, among others.

Part of the research was to find other articles that were for review, few were found, in fact, just a total 8, which denotes that there is little research that considers the various areas of the Physical Sciences, most of the works are original articles, that are results of particular investigations.

Another contribution of this work was to differentiate the types of journals where the investigations were published, which helped us realize that most of them are from Physical Sciences and not, as could be expected, in the Computational area.

The work carried out shows that the interaction between Machine Learning and the Physical Sciences has shown growth in recent years, and this growth can be expected to continue in the coming years, especially in the areas of the Physical Sciences, where it has not yet been greatly applied, in order for interesting results to be generated.

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