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SCOPE OF MACHINE LEARNING IN SOLID STATE MATERIAL: A COMPREHENSIVE REVIEW

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Abstract

The machine learning is one of the most exciting instrument that have joined the material science toolbox in recent years. This set of statistical methods has already proven to be able to accelerate both fundamental as well as applied research considerably. We are currently experiencing an explosion of work that generates and applies machine learning to solid-state systems. In this arena, we are providing a detailed overview as well as the review of the most recent study. We are incorporating machine learning principles, algorithms, descriptors, and databases in materials science as a starting point. We continue with the overview of various approaches to machine learning to discover stable materials and to predict their crystal structure. In various quantitative structure-property relationships and different techniques, study is then addressed to replace first-principle methods with machine learning. We review how it is possible to apply active learning and surrogate-based optimization to enhance the rational design process and related application examples. The interpretability of and the physical understanding obtained from machine learning models are still two big questions. The numerous aspects of interpretability and their meaning in the science of materials are therefore considered. Finally, in computational materials science, we suggest ideas and possible study directions for different problems.

Keywords: *Algorithms, Machine Learning, Types of Learning, Supervised Learning, Unsupervised Learning.*

I. INTRODUCTION

Machine learning is used to teach computers how to more effectively manage data. Often, we do not interpret the pattern or extract information from the data after viewing the data. We apply machine learning in that situation [1]. With the abundance of available datasets, the

market for machine learning is growing. Machine learning is used by many industries, from medical to military, to extract relevant knowledge [2].

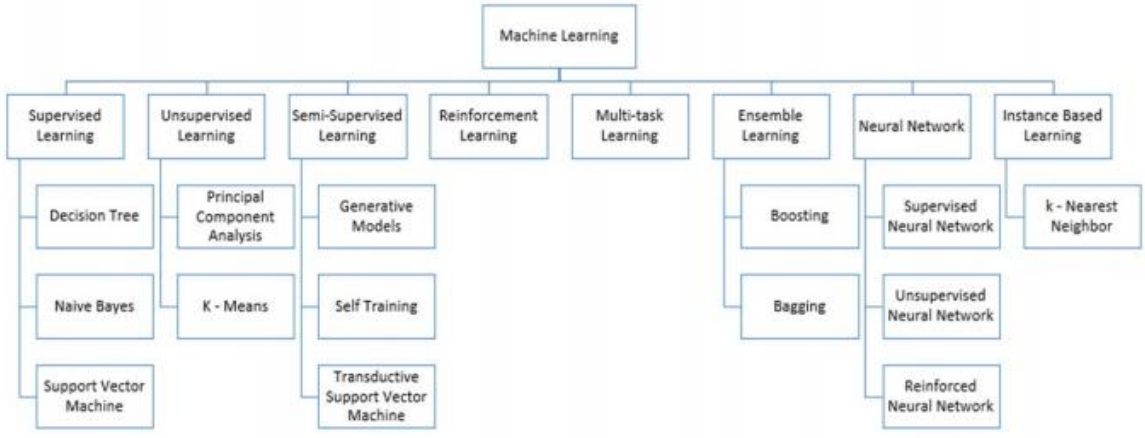

Fig.1 Illustrates the types of learning [3].

A. Supervised Learning:

The machine learning algorithms that are supervised are those algorithms that need outside assistance. The input dataset is split into a dataset of trains and tests. There is an output variable for the train dataset that needs to be predicted or graded [4]. For prediction or classification, all algorithms learn some kind of patterns from the training dataset and apply them to the test dataset [5].

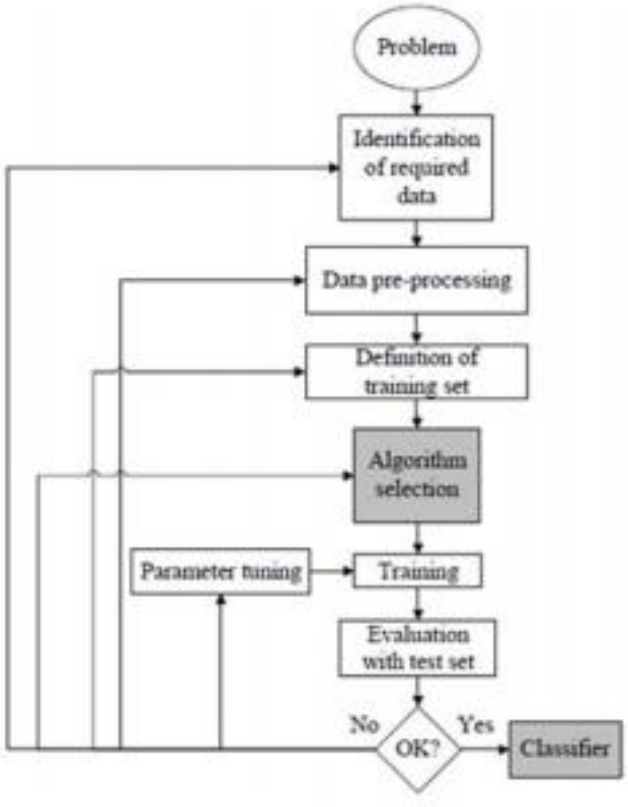

Fig.2 Illustrates the workflow of the supervised machine leaning algorithm [3].

B. Unsupervised Learning:

The algorithms of unsupervised learning learn few features from the data. It uses the previously learned features to identify the class of the data when new data is added. It is used primarily to cluster and minimise functionality. In Figure 3, an example of the workflow of unsupervised learning is given [6]. Figure 1 shows the types of learning. Figure 2 shows the workflow of the supervised machine leaning algorithm. Figure 2 shows the workflow of the supervised machine leaning algorithm. Figure 4 shows the examples of unsupervised learning.

II. LITERATURE REVIEW

Lee et al. conducted a survey on Machine Learning applications of artificial intelligence: analysis and prospect. One of the most exciting new Artificial Intelligence technology is machine learning. Learning algorithms that we use every day in many applications. One of the reasons why it works so well is that a learning algorithm, one introduced by Google or Microsoft, has learned how to rank web pages every time a web search engine such as Google or Bing is used to search the internet. That's also machine learning every time Facebook is used and it recognises the pictures of friends. Email spam filters prevent the user from having to wade through loads of spam emails, which is a learning algorithm as well. A brief analysis and

potential outlook of the vast applications of machine learning has been provided in this paper [7].

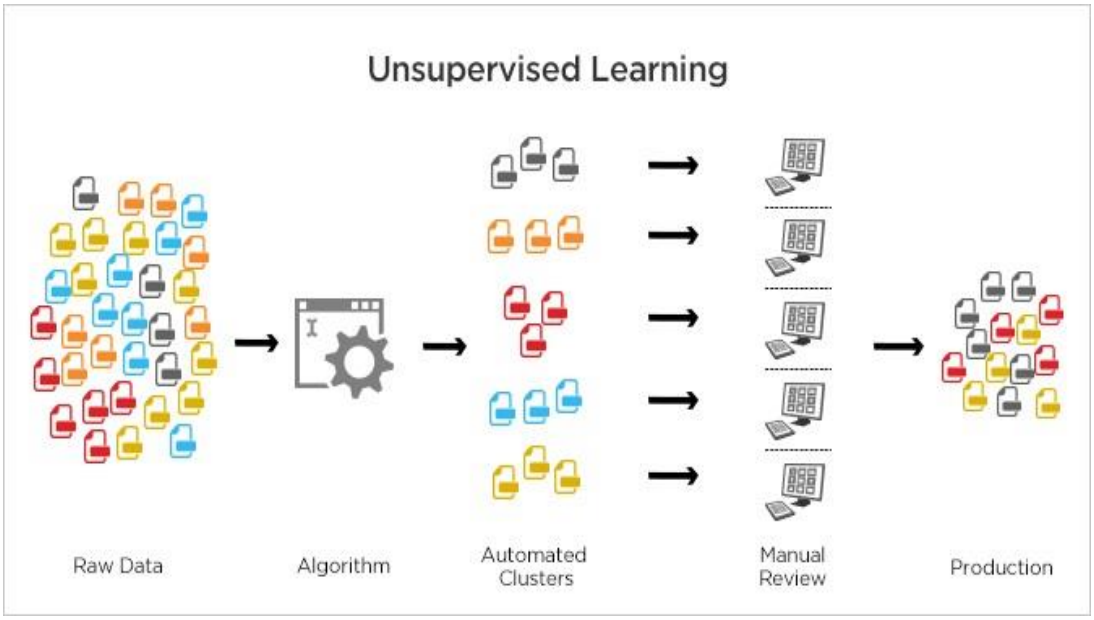

Fig.3 Illustrates the examples of unsupervised learning.

III. DISCUSSION AND CONCLUSION

This paper surveys different algorithms for machine learning. Today, each and every individual consciously or unknowingly uses machine learning. From having a suggested product to updating images on social networking sites while shopping online. This paper provides an introduction to most of the common algorithms for machine learning. To conclude, we analysed the new machine learning applications in the field of materials science. In the past few years, these implementations have been mushrooming, fuelled by the unprecedented success that machine learning algorithms have found in many different science and technology fields. It is our firm belief that this set of powerful statistical instruments is also capable of significantly accelerating both fundamental and applied science. As such, they are undoubtedly more than a fleeting fashion and will probably influence the science of materials for years to come.

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