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# Machine Learning in Material Characterization

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## ABSTRACT

Machine learning has shown great potential applications in material science. It is widely used in material design, corrosion detection, material screening, new material discovery, and other fields of materials science. The majority of ML approaches in materials science is based on artificial neural networks (ANNs). The use of ML and related techniques for materials design, development, and characterization has matured to a main stream field. This paper focuses on the applications of machine learning strategies for material characterization.

***KEYWORDS:*** *machine learning, material characterization, artificial neural networks, artificial intelligence*

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## 1. INTRODUCTION

The rapid growth of material data from experiments, computations, and simulations is expanding beyond processable amounts. This massive amount of data may be due to the number of samples collected over time via experiments or simulations. It is not only an advantage to have a large data volume (a.k.a. big data) but it can also be a challenge to cope with tremendous amounts of data [1]. Machine learning methods have become inescapable in views this growing quantity of material data. In the era of big data, machine learning has become an integral part of our daily lives.

Due to the high cost of traditional trial-and-error methods in materials research, material scientists have relied on simulation and modeling methods to understand and predict materials properties. Traditionally, the field of materials science relies on experiments and simulation-based tools for material characterization. Simulations can be highly demanding in terms of time and resources. Recently, machine learning (ML) methods for property prediction and material design have attracted a lot of attention. ML algorithms have been successful in expediting, enhancing, and completing traditional modeling and simulation capabilities [2]. Materials engineers have leveraged machine learning tools to advance characterization methods in materials science and engineering.

## 2. OVERVIEW ON MACHINE LEARNING

Machine learning (ML) is an emerging branch of artificial intelligence that focuses on optimizing computer programs to improve algorithms through data and researching experience. It is the discipline that gives computers the ability to learn without being explicitly programmed. The term "machine learning" (ML) was initially coined in 1959 by Arthur Samuel, a computer scientist. Machine learning (or statistical learning) is part of artificial intelligence. It assists computers in estimating future events and modelling based on experiences gained from previous information. Machine learning (ML) focuses on how computers "learn" from data. It allows computers to learn from past examples and detect hard-to-discern patterns from large data sets. It describes a class of algorithms which learn model parameters from a set of training data with the purpose of accurately predicting outcomes for previously unseen data. ML

is a marriage between statistics and computer science [3, 4].

As shown in Figure 1, there are two types of learning: supervised learning and unsupervised learning [5]. Supervised learning focuses on classification and prediction. It involves building a statistical model for predicting or estimating an outcome based on one or more inputs. It is often used to estimate risk. Supervised ML is where algorithms are given training data. Learning from data is used when there is no theoretical or prior knowledge solution, but data is available to construct an empirical solution. In unsupervised learning, we are interested in finding naturally occurring patterns within the data. Unlike supervised learning, there is no predicted outcome. Unsupervised learning looks for internal structure in the data. Unsupervised learning algorithms are common in neural network models. A common application of such a process is to explore interrelationships between genetics, biochemistry, histology, and disease states. In addition to supervised and unsupervised learning methods, there are also growing method of semi-supervised learning.

Machine learning is a pure data operation. Its main objective is material prediction. Machine learning uses large amounts of data to continuously optimize models and to make reasonable predictions. The traditional machine learning methods (shallow learning) require features to be selected manually. They typically begin with raw data and end with a predictive model that can be used to make decisions. The process usually includes the following steps [6]:

1. *Data Gathering* to identify and collect input data.
2. *Data Cleansing* to standardize and clean the raw inputs.
3. *Feature processing* to transform the input data into formats that can be easily processed to identify the best predictor variables.
4. *Model Training* to train the model, using a wide range of potential algorithms.
5. *Model Validation* to test the model against historical data and assess its performance.
6. *Model Deployment* to load the model into an environment where it can make decisions.

The applications of machine learning are endless, including medicine, machine perception, computer vision, object recognition, natural language processing, cheminformatics, fraud detection, stock market analysis, games, robotics, health monitoring. Industrial leaders such Google, Amazon, and Microsoft are now offering numerous tools to enable beginners get started with building their own machine learning systems.

## 3. CHACTERIZATION OF MATERIALS

Characterization is a fundamental process in materials science. It refers to the general process by which a material's structure and properties are probed and measured [7]. Material characteristics such as strength, toughness, hardness, brittleness, or ductility are useful for categorizing a material. In materials science, researchers rely on experiments and simulation for material characterization.

Traditional material tests like tensile tests, compression tests, or creep tests are often time consuming and expensive to perform. Tensile properties indicate how the material will react to forces being applied in tension. Typical destructive tests are bend test, impact test, hardness test, tensile test, fatigue test, corrosion resistance test, or wear test.

In the past, characterization of the material, raw or processed, was done mainly by laboratory experiments, which can become costly. In recent times, computational models and high-fidelity simulations have made the process more efficient [8].

Sometimes, statistical machine learning tools are trained on the available experimental results, and then used in place of the real experiments. The application of ML approaches is considered helpful for an easier generation of material property information. ML methods are trained on experimental datasets to accelerate the characterization of materials. The majority of early ML applications to materials science employed simple-to-use algorithms, like linear kernel models and decision trees. To solve material problems using ML requires datasets to help detect target features.

The guiding ideology of materials science can be summarized in four paradigms. The first paradigm is the empirical trial and error method. The second paradigm is physical and chemical laws. The third paradigm is computer simulation, and the fourth paradigm is big data-driven science. The fourth paradigm can perfectly unify the other three paradigms in the aspects of theory, experiment, and computer simulation [9]. Figure 2 shows an application of machine learning in materials science [10].

Materials scientists have demonstrated success in utilizing ML-based methods in two major categories: (1) to accelerate the prediction of material properties for specific

applications and (2) to accelerate the on-demand design and the optimization of material composition. The superior effectiveness of ML techniques is demonstrated, compared to traditional simulation or experimental approaches [11]. Machine learning has been applied in studying the properties of inorganic materials. For metallic biomaterials, an attractive application of ML in recent years is in medical implant. It is expected that machine learning is applied in bio-related material science [12].

## 4. BENEFITS

Machine learning (ML) is widely used in several aspects of material science such as new material discovery, detection of material properties, material prediction, material design, inverse design, corrosion detection, material screening, and data preprocessing (data collecting and data cleaning) [13]. ML can be used to predict proper new compounds. A major advantage of applying ML approaches is that it is not necessary to postulate a mathematical model at first. Machine learning allows one to replace the traditional tests with simple and fast tests. ML techniques have been utilized to predict material fatigue life for steel. They have become efficient tools for analyzing materials in the new field of material discovery. They can be applied in material discovery including data preprocessing, feature engineering, and machine learning algorithms. They have also been employed along with physics-based simulations to combine information from different sources. Experiment- and simulation-based data mining in combination with ML tools provide great opportunities to enable identification of fundamental interrelations within materials for characterization. The development of deep learning has made new progress in the application of materials science. Deep learning has high potential in the inverse design of materials. It is needless to say that we are only scratching the surface of what is possible with machine learning.

## 5. CHALLENGES

There have been many challenges in implementing ML techniques in materials science. At present, the ML approach is confronted with many challenges: the messy datasets must be preprocessed; the accuracy of the model is limited by its algorithms; the high-intensity computation places pressure on computing resources; etc. Complex ML algorithms are often treated as black boxes and lack novel understanding and knowledge arising from their use. There is often the problem of small data in material characterization, because the experimental or simulative generation of data is complex and expensive. For some applications, there is a lack of benchmarking datasets and standards.

## 6. CONCLUSION

The commonly used traditional trial-and-error approaches rely on personal experience and do not apply for new materials due to their long development cycles, low efficiency, and high costs. Recently, using machine learning to explore new materials is becoming popular. Various machine learning methods have successfully been

used for the prediction of materials properties. More information on materials characterization using machine learning can be found in the books in [14] and the following related journals:

- Materials Characterization
- International Journal on Materials Structure and Behavior.
- Machine Learning: Science and Technology

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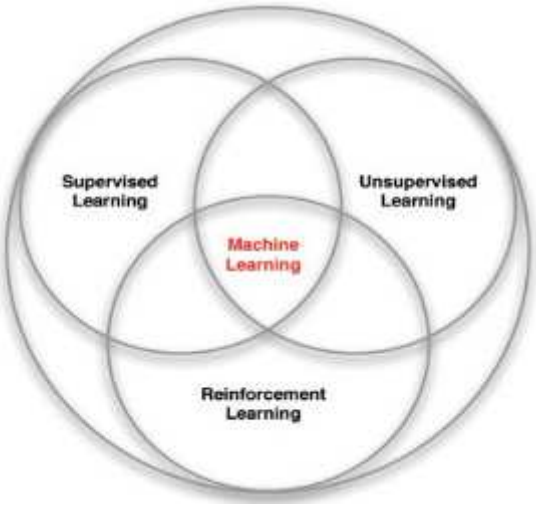


**Figure 1 Branches of machine learning [5].**

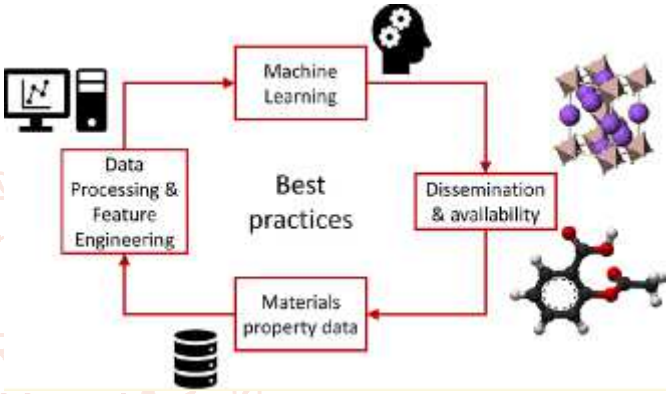


**Figure 2 Machine learning in materials science [10].**