

## Chapter 2

# Deep Learning and Machine Learning and Their Application on Computational Chemistry

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### **ABSTRACT**

*Machine learning (ML), coined by Arthur Samuel in 1959, is now a versatile tool in various fields like data mining, computer vision, and medical diagnosis. It builds models from training data for predictions without explicit programming. Deep learning (DL), a subset of machine learning, utilizes neural networks like DNN, CNN, and RNN. In health and safety research, ML applications started in the mid-1990s, focusing on toxicity. Challenges in chemical health and safety research, such as primitive algorithms and skill requirements, limited its early use. Recent advancements in AI and computer science have highlighted the significance of ML and DL. Improved data, computing power, and algorithms have led to autonomous data analyses, transforming solutions in structural engineering (MPSE). In integrated computational materials engineering (ICME), ML and AI are assimilated into efforts like the materials genome initiative (MGI), accelerating autonomous experiments and improving data analytics.*

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## 1. INTRODUCTION

Artificial intelligence (AI) has started with Bayes' statistics and Laplace's least squares, and Markov chain derivatives. Machine learning (ML) was initiated by Arthur Samuel in 1959 (Samuel, 1959). It has since improved the existing data mining strategies, computer science, natural language processing and developed the means of biometric recognition, medical diagnosis, credit-card fraud detection, stock market analysis, speech and handwriting recognition, strategy games, and robotics (Pierson and Gashler, 2017; Jiao et al., 2020a).

Machine learning works on mathematical models, as it uses many mathematical tools, including probability theory, statistics, approximation theory, convex analysis, algorithm complexity theory, and many others (Jiao et al., 2020a).

Deep learning (DL) is a multi-layer algorithm that exploits data using artificial neural networks and creates an abstract feature. It is a newer area of ML and is structured by several frameworks: deep neural network (DNN), convolutional neural network (CNN), and recurrent neural network (RNN) (Jiao et al., 2020a; LeCun et al., 2015).

Practical ML applications have started quite recently, in 1990s, and in health and safety (Lee et al., 1995). Related research aimed at classifying toxic materials and future predictions. Swift developments in artificial intelligence and computer science allowed the use of ML and DL algorithms in cumbersome statistical calculations. By the turn of the century, these algorithms have been used in automated/autonomous data analysis (Pan et al., 2008; Pan et al., 2009).

Today, machine learning is deeply involved in the process and structural engineering (MPSE) application fields, in making machine-based autonomous decisions. This involves simultaneous and sequential operation steps: (i) perception of a knowledge space (ii) anticipation of perceived space, and (iii) unsupervised action of a robotic system (Dimiduk et al., 2018).

In existing MPSE operations, "Big Data" often refers to the data itself and the data sources. Data collection, and the accuracy of the collected data constitute very important issues. The "semi-structured" MPSE data is then used by industrial developers and designers. Here, ML/AI tools can again lead to transformations in the improvement of this data structure problem, as the application of these tools to the collected data, in turn, help their evolution and improve the performance of the users (Dimiduk et al., 2018).

The scale of depth depends on the number of independent observations on the states of a system. Independent observations essentially involve the creation of experimental data. This step is rather costly and all of created data must be utilised. Thus, developing ML/AI technologies could also be used in data mining in the near future. Such developments are needed in the creation of models in order to reduce the experimental workload and its cost. Here two types of data are created, by measurements and by synthesis. MPSE users might thus need to develop data production methods to fulfil the needs ML/AI data structuring efforts (Dimiduk et al., 2018).

Although ML/AI is promptly integrated into ICME, integrated computational materials engineering, and in the MGI, Materials Genome Initiative, efforts, the application of ML/AI in ICME and MGI still seems to be in progress. While material data has been a focus of interest in MPSE for some time, ML/AI has not been stated in available ICME reports (National Science and Technology Council Committee on Technology Subcommittee on the Materials Genome Initiative, 2011; National Science and Technology Council Committee on Technology Subcommittee on the Materials Genome Initiative, 2014).

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