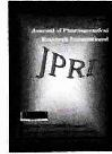


**Journal of Pharmaceutical  
Research International**



## Investigating the Impact of Machine Learning in Pharmaceutical Industry

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### Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

### Article Information

DOI: 10.9734/JPRI/2021/v33i46A32834

#### Editor(s):

(1) Dr. Jongwha Chang, University of Texas, College of Pharmacy, USA.

#### Reviewers:

(1) Boutheina Jilfi, University Manouba, Tunisia.

(2) K. Lenin, Prasad V. Potluri Siddhartha Institute of Technology, India.

(3) Vaibhav Godbole, University of Mumbai, India.

Complete Peer review History: <https://www.sdiarticle4.com/review-history/74285>

Received 01 August 2021

Accepted 07 October 2021

Published 11 October 2021

Review Article

### ABSTRACT

In the pharmaceutical and consumer health industries, artificial intelligence and machine learning played an important role. These technologies are critical for the identification of patients with improved intelligence applications, such as disease detection and diagnostics for clinical testing, for medicine production and predictive forecasts. In recent years, advances in numerous analysis tools and machine learning algorithms have led to novel applications for machine learning in several areas of pharmaceutical science. This paper examines the past, present, and future impacts of machine learning on several areas, including medicine design and discovery. Artificial neural networks are employed in pharmaceutical machine learning because they can reproduce nonlinear interactions typical in pharmaceutical research. AI and learning machines are examined in everyday pharmaceutical needs, industrial and regulatory insights.

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**Keywords:** Machine learning; consumer health; business change; cost-effective solutions.

## 1. INTRODUCTION

AI promises an ocean of untapped possibilities for business change in the pharmaceutical industry. Big Data, together with AI-driven analytics, has radically changed the innovative paradigm of the pharmaceutical sector [1].

Machine learning has the ability to promote innovation while at the same time enhancing productivity and achieving better results throughout the value chain (Nagy et al., 2019). The value proposition of pharmaceutical firms can be considerably improved by driving innovation and the development of new business models [2]. Drug managers are looking for ways to exploit artificial intelligence and machine learning in the health and biotechnology sectors [3]. Reports show that more and more companies are implementing existing applications leading to the digital future of technology in the industry. Top pharmaceutical enterprises cooperate and use AI technology in research, development and overall drug discovery with AI suppliers [4].

Reports show that nearly 62 percent of healthcare Organisation's plan to invest in AI in the near future, and 72 percent believe AI is essential to their future business practice [4]. Pharma News Intelligence examines existing AI applications, the best applications for AI and machine learning, and their future in order to get a better sense of AI's future in the field.

Every day, the amount of data generated, particularly pharmaceutical data, has increased dramatically. The term "big data" has gained increasing currency in a variety of research domains. Additionally, data-driven businesses are demonstrating how diverse industries can benefit from big data generation. Numerous definitions have been proposed for the term "big data." One of the most well-known definitions is "4 Vs." Douglas Laney offered the definition, which contains the "3 Vs" of volume, velocity, and variety [5]. IBM later expanded this definition to include the fourth "V." [6]. There is, however, no universally accepted and quantitative definition of "big data."

Due to the potential worth of data, it was dubbed the "new oil" [7]. Textbooks and publishing, social media, User Content, electronic health, genomics, and sensor networks all contribute to the richness and diversity of 'big data.' The

dramatic growth in data volume can be attributed to advancements in data storage and technical advancements [8]. Each year, almost 2.5 million new scientific papers are published [9]. Additionally, over 15,000 publications in the field of "pharmaceutical industry" were recorded in 2019. (PubMed).

Thus, in the pharmaceutical industry, "big data" can be viewed as both a challenge and an opportunity. Machine learning technologies, in which computers can 'learn' and perform tasks, have boosted the possibility for using big data in pharmaceutical industry. The scope of this review is unique for machine learning, as it is the most commonly employed AI technology in the pharmaceutical industry. Other branches of artificial intelligence, such as natural language processing (NLP), expert systems, and robotics, have grown in popularity in a variety of healthcare settings, including illness diagnoses, patient surveillance, and robotic surgery [10]. However, these technologies have not garnered the same level of interest in the pharmaceutical business as machine learning.

This article discusses numerous machine learning techniques that are frequently employed in various domains within the pharmaceutical industry.

## 2. MACHINE LEARNING AND PHARMACEUTICAL INDUSTRY

However, the mainstream AI definition is still unavailable. But AI's fundamental goal is to computerise human intelligence. A computer model of artificial neurons was created by Warren McCulloch and Walter Pitts in 1943. Artificial neurons, like human neurons, turn on or off when stimulated [11]. A.I. was first used by John McCarthy in 1956 at the Dartmouth Conference [12]. Since then, AI has had its ups and downs [13]. Health care [14], engineering [15], and transportation [16] have recently used AI [16]. Big data in healthcare and the rapid development of analytical tools spurred this increased focus on AI applications [10].

Supervised and unsupervised machine learning algorithms approach uses generalisations in supervised learning. An input-output dataset. Targets are known-good output data (or correct). Finally, the machine learning model predicts a win [17].

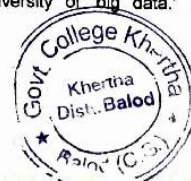


Table 1. Parametric model vs non-parametric model

Parametric Model	Non-parametric Model
<p><b>Definition</b> A learning model summarizing data with a set of fixed size parameters is called a parametric model (depending on the number of training examples). No matter how often data we throw on a parametric model, how many variables it needs does not change its mind [22].</p> <p><b>Popular Algorithms</b></p> <ul style="list-style-type: none"> <li>• <b>Logistic Regression-</b> It is possible to predict a data value using logistic regression, which is a statistical analytic approach based on previous observations of a data collection. To predict a dependent data variable, a logistic regression model examines the relationship between one or more already-existing independent variables [23].</li> <li>• <b>Linear Discriminant Analysis-</b> Dimensionality reduction is frequently used for supervised classification problems, and it is also known as linear discriminant analysis (LDA), normal discriminant analysis (NDA), or discriminant function analysis (DFA). In this context, it refers to differences between groups, such as those that exist between two or more classes. It's a technique for bringing features from a higher-dimensional realm down to a more mundane (geeksforgEEKS.org).</li> <li>• <b>Naive Bayes-</b> The Naive Bayes method, unlike the others on this list, is based on the Bayes theorem, which takes a probabilistic approach. The algorithm does not go immediately into the data since prior probabilities have been specified for each of your target's classes. The programme creates the posterior probability by updating these prior probabilities depending on the new information we have provided (edureka.co ,2021).</li> </ul> <p><b>Benefits</b> Simpler: it is easier to understand and interpret these methods. Speed: Data can be used to learn parametric models reasonably quickly. Less data: We don't require as much learning and we can work well even if we don't fit the data precisely.</p> <p><b>Limitations</b> Constrained: these procedures are extremely limited to the stated form when selecting a functional form. Complexity limited: Methods are better adapted for simpler issues. Low fit: the approaches will probably not match the fundamental transformation matrix in practice.</p>	<p><b>Definition</b> Nonparametric techniques are suitable if we have a large amount of data and no prior information, and we do not want to be concerned with finding the exact right functionality [22].</p> <p><b>Popular Algorithms</b></p> <ul style="list-style-type: none"> <li>• <b>k-Nearest Neighbors- KNN</b> is a non-parametric learning algorithm since it makes no assumptions about the underlying data distribution. The "training" phase of lazy learning is brief. Its purpose is to use a large number of data points classified into several groups to predict the categorization of a new sample point.</li> <li>• <b>Decision Trees-</b> On the Decision Tree, each node represents an attribute test, and each branch reflects the outcome of that test. This is how the Decision Tree can be summarised. The leaf nodes include the predicted labels. The comparison of attribute values continues until we reach a leaf node, at which point we return to the tree's root (edureka.co ,2021).</li> <li>• <b>Support Vector Machines-</b> An SVM is the only one of its kind since it seeks to sort the data with the widest possible margins between two groups. Max margin separation is what it's called. A final thing to bear in mind is that SVMs only employ the support vectors to plot the hyper plane, as opposed to linear regression, which makes use of the entire dataset (edureka.co ,2021).</li> </ul> <p><b>Benefits</b> Flexibility: fit many useful forms. Power: no following function assumptions (or weak assumptions). Performance: Can lead to higher performance prediction models.</p> <p><b>Limitations</b> More data: Requires a lot more training data to estimate the mapping function. Slower: Far slower to train, because they often have far more parameters for the train. Overfitting: It is tough to describe more risks of overfitting the training data and why certain predictions are made.</p>

Unsupervised machine learning includes regression, SVMs (Support Vector Machines), random forests, and ANNs (Artificial neural network). Unattended learning extracts functions



without examples using MCA (Multiple correspondence analysis) [17]. (PCA). SVMs and ANNs can support supervised models (Lo et al., 2018). PCA (Principal component analysis) is an unattended dimensional reduction method used to find a smaller-dimensional collection of axes in unlabeled data [12].

Pharmaceutical scientists employ fluffy logical algorithms to study machine learning. Fuzzy set membership is represented using logical expressions [12]. This method reduces the requirement for system expertise, data noise consideration, and predictability [18]. Gene expression prediction models using fuzzy logic [18]. GA is a population-based optimization technology. GA is often used in pharma research to pick QSAR (Quantitative structure-activity traits) [19,20]. Non-conventional pharmaceutical machine learning approaches like machine light gradient boosting (lightGBM). This machine learning algorithm offers many advantages over others. Transfer learning is a modern AI method. It retrains an existing model to achieve a new goal [21]. For good transfer learning, a big original model dataset is important. Machine learning models are classified as parametric or non-parametric.

Table 1 shows Parametric model vs non-parametric model.

### 3. ANN AND DEEP LEARNING

ANNs are biologically inspired computer models that learn from experience. Our brains contain thousands of neurons, or processing units. Synapses connect these neurons, allowing them to communicate fully [24]. Axons are lengthy threads that carry info from one cell to the next. A neuron is a biological cell that [24].

Coefficients (weights) link artificial neuron to human neuron in an ANN (artificial nervous system) [24]. Three structural components define an ANN on average. Hidden and visible input layers Artificial neurons have dendrites that match those of organic neurons. Between the input and output layers is a concealed layer. The hidden layer links the two layers (weights). Thousands of neurons cover every layer (also called nodes). The number of neurons in the supervised layer of ANNs is generally determined by test-and-ander [25]. Too few or too many neurons in the hidden layer might cause over-storage or over-composition of the training data, reducing ANN generalisation.

DL (Deep Learning) is a representation learning machine [26]. DL uses modern neural network technology. With DL, there are more hidden layers (typically 3+) and nodes per layer. So DL uses several representation layers to learn complex functions. Large training sets are required for DL, which limits its application. Many neural network topologies have been examined extensively elsewhere, including CNNs, RNNs, and fully connected feed forward networks (FCFF) [27]. To produce medication formulations [28], drug discovery [29], DL was famous and interested in several pharmaceutical research areas [29]. They outperform other master learning approaches like SVMs and RF (Radio Frequency), in terms of prediction and overall performance [28].

### 3.1 Applications of AI and ML in Pharmaceutical Industry

AI may be used in practically every element of pharmaceutical production, from medication discovery to marketing. Incorporating AI technology into fundamental workflows can help pharma organisations run more efficiently, cost-effectively, and smoothly. The best part is that AI systems are meant to improve outcomes as they learn from fresh data and experience, making them a formidable tool in pharmaceutical research and development.

Here are a few notable AI uses in the pharmaceutical industry:

- **R & D**

Pharma businesses deploy powerful ML and AI algorithms to streamline drug discovery procedures. These intelligence technologies are meant to find complex patterns in huge data sets to tackle biological network problems.

This is a great approach to look at disease patterns and see which treatments work best for which ailments. Thus, pharmaceutical companies can focus on developing medicines that are most likely to treat a disease or medical condition.

- **Drug development**

AI has the potential to improve R&D. AI can accomplish everything from discover novel compounds to validate and identify targeted treatments.

The MIT study found that only 13.8% of medicines pass clinical testing. A pharmaceutical



company must also approve a medicine after completing a clinical trial that costs between \$161 million and \$2 billion. Pharmaceutical companies increasingly use AI to increase new drug success rates, create more cheap ad treatments, and most importantly, lower operating expenses.

- **Diagnosis**

They can collect, process, and analyse massive amounts of patient data. Worldwide healthcare providers use ML technology to safeguard cloud patient data or a central storage system. These are medical computerised records (EMRs).

These records can help doctors understand the health effects of a genetic trait or a drug. ML systems can use EMR data to predict real-time diagnosis and treatment. The potential of ML to quickly collect and analyse enormous amounts of data can help save millions of lives.

- **Disease prevention**

Pharmaceutical businesses can use AI to heal common and rare diseases like Alzheimer's and Parkinson's. The ROIs for rare disease treatments are poor compared to the time and money necessary to develop medicines for uncommon diseases.

Nearly 95% of uncommon diseases have no FDA-approved therapies. But AI and ML's inventive skills are fast changing the situation.

- **Epidemic forecasting**

Many healthcare providers and companies utilise AI and ML to track worldwide outbreaks. These technologies use data from the web to investigate the links between geological, environmental, and biological elements, and public health in diverse geographical areas. Less developed countries lack healthcare infrastructure and financial foundation for epidemic management. An example of this AI application is the ML-based outbreak prediction model, which helps healthcare providers detect and respond to impending malaria epidemics.

- **Remote Monitoring**

A stride ahead in the pharmaceutical and healthcare industries. Companies have created AI devices to remotely monitor patients with life-threatening disorders. Tencent Holdings, for

example, has created an AI solution with Medopad to remotely monitor Parkinson's patients and minimise engine function evaluation time from 30 to three minutes. Using AI technologies and smartphone apps, patients' hands can be opened and closed remotely.

A smartphone camera detects hand motions and records the intensity of symptoms (Parkinson's). Patients' severity is determined by movement frequency and amplitude, allowing doctors to remotely alter medications. An alarm will be sent to the doctor if the condition worsens. These remote technologies can reduce travel and patient waiting time to the doctor's office.

- **Manufacturing**

Pharmaceutical businesses can employ AI to increase drug production productivity, efficiency, and speed. AI can be used to control and improve any component of the industrial process.

- ❖ Quality control
- ❖ Predictive upkeep
- ❖ Waste reduction
- ❖ Design optimization
- ❖ Process automation

AI can help pharmaceutical companies promote their goods faster and cheaper than traditional approaches. AI also reduces human error by restricting human participation in the production process, while enhancing their ROI.

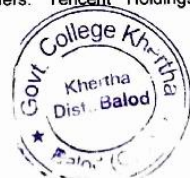
- **Marketing**

AI can be a useful tool in pharmaceutical sales and marketing. Pharmaceutical firms can design AI-based marketing tactics that increase revenue and brand awareness.

Marketing technology (leading transformation) drives visits to sites and converts them into buyers. AI can help you plan your client journey. This allows pharma businesses to focus on marketing techniques that increase conversions and profits.

To determine which marketing strategies are the most cost efficient, AI can analyse historical outcomes. This saves time and money by designing current marketing campaigns. As well as predicting marketing campaign success or failure.

While AI quickly transforms the pharmaceutical sector, it is not without obstacles. Most pharma companies' present IT infrastructure is built on



legacy technologies that are not AI-ready. Also, integrating and adopting AI requires industry competence, which is still lacking. This step can help the pharmaceutical industry use AI: Partnering with AI R&D Academic Bodies to assist AI Pharmaceutical Companies Profit from AI-powered discovery firms' expert advice, powerful tools, and industry experience. Educate R&D and production teams on AI tools and technology

#### 4. THE CURRENT IMPACT OF PHARMACEUTICAL INDUSTRY

The wide range of applications mentioned in this analysis will considerably assist the pharmaceutical sector. AI can be used in practically every phase of medication development, from concept to marketing.

With a 10-year average of \$2.6 billion [30], AI may make significant investments to speed up and optimise this process. The number of pharmaceutical businesses and start-ups adopting AI has increased dramatically during the last decade. Companies like Novartis and Pfizer partnered or purchased IBM Watson AI technologies [31]. Mak & Pichika [32] provided a comprehensive overview of AI and pharmaceutical firms, including medication discovery and reuse. Pharmaceutical businesses are currently researching automation, robotics, and AI marketing [31]. Advanced algorithms and high, complicated data availability help sustain industrial efficiency and fast data digitization. So AI can help us make better decisions and ultimately generate better treatments. A shortage of expertise, changing to alternative science methodologies, and lack of investments were cited as reasons/challenges by Henstock [31]. To overcome these issues, the author proposes internal data management and AI expertise [31].

Mary and her colleagues performed a survey in 2019 to better understand the impact and deployment of AI in pharma and biotech firms. The usage of AI for patient selection and recruiting, as well as medication data gathering, have been identified in 217 organisations. Main reasons for non-use include lack of skilled employees; safety; regulation; and budget constraints [4].

#### 5. CHALLENGES

Machine learning in the pharmaceutical business faces various challenges. Here are a few examples:

- A transparent method is required in order to assemble onerous limits on medication improvement. Causal reasoning is essential for use behind machine deduction.
- The pharmaceutical sector relies heavily on people with data science skills. It's vital to build a solid talent pipeline.
- An important topic right now is data governance. In any case, medical records are private, and this is hardly a legal means of gaining access to them. According to this, the privacy data is taken for granted.
- Even while there is direct financial benefit from adjusting or supporting research, the pharmaceutical business has historically been reluctant to do so [33].

#### 6. CONCLUSION AND FUTURE ASPECTS

In various pharmaceutical applications, the expanding interest in artificial neural networks (ANNs) showed substantial potentials. In medicine and gene delivery this is already happening. Medicines are often delivered to cells via peptides (CPPs). ANNs were recently used to research and analyse the efficacy of CPP. This model also provided 13 critical predictions and evaluations [34]. These technologies can also help reuse medicines [35].

The first AI drug is not yet available, but the COVID-19 epidemic is still present. Anti-COVID-19 drug discovery requires IA. Benevolent AI [36] discovered COVID-19 medications in clinical trials using engine learning.

According to latest surveys, most global healthcare organisations will use AI by 2025. Investment in chronic diseases and oncology will increase. The chronic afflictions of America kill most A.I. is used more and more to improve treatment of chronic diseases while decreasing costs. Future chronic diseases, including kidney, diabetes, cancer and IPF, will be treated. As a result, AI will influence the progress of medicine. AI guarantees top candidates that patients can be promptly screened and the best prospects for the test are found [37-40].

A large test group is not essential by minimising components that may impair clinical investigations. AI also helps with patient diagnosis and screening. AI can extract mammograms and MRI pictures from data. AI and machine learning will continue to support the



development of medicines. The pharmaceutical and production systems are also entered by Artificial Intelligence (AI).

In short, the application of AI and machine learning may be maximised in digitising pharmaceutical research. In pharmaceutical firms, machine learning is rapidly used, exhibiting its adaptability. In practice, the type of data and the quantity of a dataset might influence the method of learning. Therefore it is task-specific. High-value AI applications can become routine with enough data. Cost-effective solutions will thrive in future digital pharmaceutical research [41-44].

#### CONSENT

It is not applicable.

#### ETHICAL APPROVAL

It is not applicable.

#### COMPETING INTERESTS

Authors have declared that no competing interests exist.

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Peer-review history:  
The peer review history for this paper can be accessed here:  
<https://www.sdiarticle4.com/review-history/74285>



  
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