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Original Article

The Role of Artificial Intelligence and Machine Learning in Revolutionizing Drug Discovery

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Abstract *- Today Artificial Intelligence (AI) is transforming the practice of drug discovery over a few years and has revolutionized the field. There are several artificial intelligence and machine learning techniques used in drug discovery. This paper describes the use of AI and ML in the development of drugs so that the results are more accurate and efficient. An organized evaluation of the review is carried out with the help of keyword searches in the available databases related to context, methods, and full text. The brief survey describes AI and ML in drug discovery making it cost effective both in time and money spent. The prevalent application of AI and ML methods indicates a blooming future for the drug industry. This will help researchers and the drug industry to utilize AI and ML in drug discovery growth.*

Keywords *- Artificial Intelligence, Drug Discovery, Explainable Artificial Intelligence, Generative Artificial Intelligence, Machine Learning.*

1. Introduction

The process of evolving new drugs is being completely transformed by incredible developments in artificial intelligence technology and processing capacity. In order to maintain their drug development programs, pharmaceutical companies can work with AI-powered discovery organizations. The medical care business recently has established artificial intelligence as a hot topic. The biopharmaceutical sectors are attempting to use AI to improve the drug discovery process, lower research and development costs, lower clinical trial failure rates, and ultimately produce better medications [1,2]. The way clinical evaluation and training are conducted is expected to change due to the growing use of Artificial Intelligence (AI). Incorporating medical professionals into the technology's development for the pharmaceutical and medical sectors will guarantee that the potential of AI has the potential to greatly enhance medical treatment [3]. Conventional AI technologies have been thoroughly explored in drug discovery, which includes supervised as well as unsupervised learning [4]. Even with huge investments and exciting discoveries, the process of creating a new drug is time-consuming and costly, and it is currently experiencing a silent crisis [5]. Numerous machine learning-based methods are employed for drug target prediction, including modelling the drug target's structure [6]. Artificial Intelligence (AI) has transformed the pharmaceutical industry in numerous ways. Among these are medication development and discovery, drug repurposing, increasing pharmaceutical productivity, clinical trials, etc., all of which lessen the strain on humans and enable quick target achievement [7,8]. AI and ML are making significant progress in drug discovery, but there is still a literature gap that should be addressed. Many AI models which are used for drug discovery are complicated and the reason behind their predictions is not clear. Enhanced research is required so as to develop AI models that can interpret the structure of drug molecules. To make accurate biological-related predictions so as to understand the disease processes, AI models should be developed to integrate this knowledge. Also, clinical research should be carried out to validate AI-based prediction in the real world. Currently, AI-based drug discovery is very powerful but with the drawback that it is inefficient to interpret biological content accurately and to validate real-world applications. To address these problems, it is needed to develop AI tools for finding medicines quicker.

2. Define the Research Question

Artificial intelligence is currently used to speed up improved medication research and development. The objective of this research is to identify and analyze the role of artificial intelligence and machine learning in the drug discovery process. The literature survey was carried out to

analyze and develop AI techniques for drug discovery and evaluation [9,10]. The research questions are formulated considering issues like advanced technology [11], machine learning [12], artificial intelligence [13] and emerging machine learning techniques.

RQ1: What are advanced technologies in drug discovery?
RQ2: How is machine learning used in drug discovery?
RQ3: How Artificial intelligence is used in drug discovery?
RQ4: What are emerging machine learning techniques?

Based on the research question, the approaches for artificial intelligence for drug discovery are presented, which are utilized to discuss systematic literature review. The framework, as shown in Figure 1, depicts three extends, which are advanced technologies in drug discovery, ML techniques in drug discovery, and AI techniques in drug discovery.

2.1. Advanced Technologies in Drug Discovery

The literature search findings related to RQ1 indicated that the pharmaceutical sectors are now using a variety of technologies and approaches to support drug research and manufacture.

Machine Learning techniques in drug discovery. It includes techniques like the chem-bioinformatic approach for drug discovery, blockchain technology in the pharmaceutical industry, and 3D printing in the pharmaceutical industry.

2.1.1. Chem-bioinformatic Approach for Drug Discovery

The silicon ADMET is the chem-bioinformatic approach. ADMET encompasses adsorption, distribution, metabolism, elimination, and toxicity.

ADMET thus assesses a drug's efficacy, safety, absorption, excretion, and metabolic behaviour [14]. In order to manufacture novel medicinal compounds, this method simulates pharmacokinetic and physicochemical outcomes. ADMET uses two methods. The first approach analyses the result in the context of interactions between target chemicals and proteins. However, it needs individual proteins to have effects that are unmistakably the ADMET outcome, such as cost-effectiveness and safety [15]. In the second method, secondary data is collected and collated based on the known parameters for diverse compounds used to manufacture proteins. Using the data, complex and hybrid deep learning models can be developed using artificial intelligence and machine learning. The drawback with this method is that it requires huge manual maintenance and keen attention to tackle. Even a very small mistake can cause wrong results and conclusions, which is time-consuming and costly.

2.1.2. Blockchain Technology in the Pharmaceutical Industry

A sophisticated database system called blockchain technology makes it possible for information to be shared transparently inside a company network. The term "blockchain" comes from the fact that blockchain is a type of data structure that is created by gathering and organizing records into blocks that are then joined to one another in a chronological manner to form a chain [16]. Blockchain has several features that make it possible for the pharmaceutical business to adopt it. Permanence, decentralization, clarity, and recognizability are these elements. The term "permanence" describes the constant and irreversible characteristics of the blockchain's data. The term "decentralization" refers to the possibility of several entities handling data within a system.

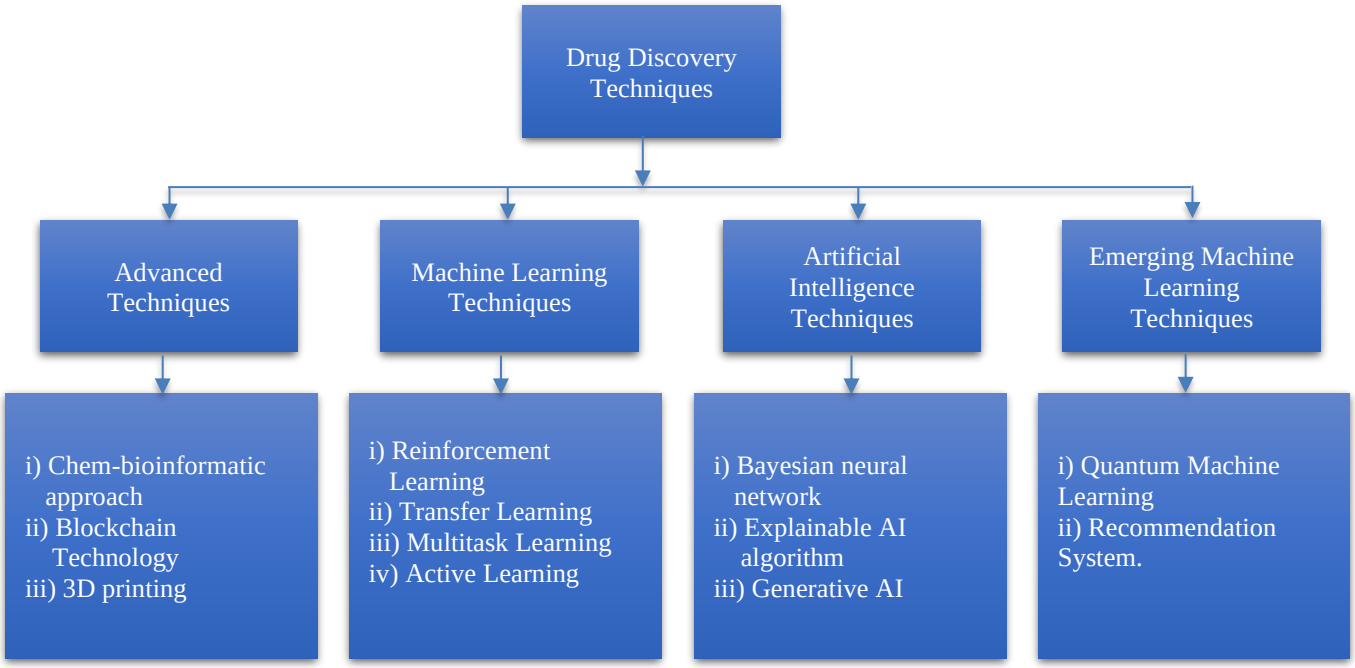

Fig. 1 Drug discovery framework using artificial intelligence techniques

The term "clarity" describes how transparent data is kept in a blockchain and how a user can access all of the data maintained throughout the blockchain. The capacity of a blockchain user to track data recorded in the blockchain with unquestionable timestamps is known as " recognizability ".

The drug manufacturer can view and track the data whenever they want using these factors. Being a recent technology, blockchain has vast installation and preservation costs, which are high-priced for small businesses [17].

2.1.3. 3D Printing in the Pharmaceutical Industry

3D printing is an innovative method that uses blue light instead of white light and thus expands accurateness owing to its lingering volume to the transmission of impedance. Because modern 3D printing is widely available and practical, it also makes it possible for a wide range of people and companies to produce goods on-site and as needed [18].

3. Machine Learning in Drug Discovery

Machine learning has techniques according to RQ2 like reinforcement learning, transfer learning, multitask learning, and active learning.

3.1. Reinforcement Learning

Designing and creating molecules that are both safe and effective is essential for the medical chemistry industry. It is a challenging task that involves many properties with orthogonal trends. Reinforcement learning is based on the actor-critic model, used to create unique compounds with the best attributes [19], as shown in Figure 2. Reinforcement learning is concerned with how the agent takes action in an environment to maximize the rewards [20]. Temporal difference [TD] learning is utilized in actor-critic models, where an agent's behavior is accessed by a critic model, which provides feedback on the agent's performance. Figure 2 shows the actor-critic model for designing and creating molecules.

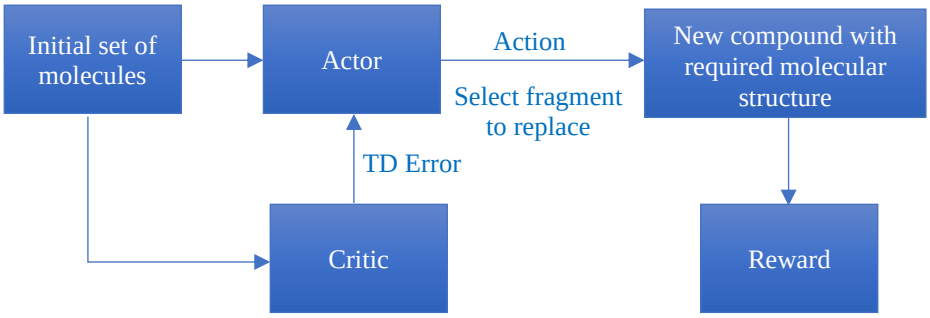

Fig. 2 Actor-critic model for designing and creating molecules

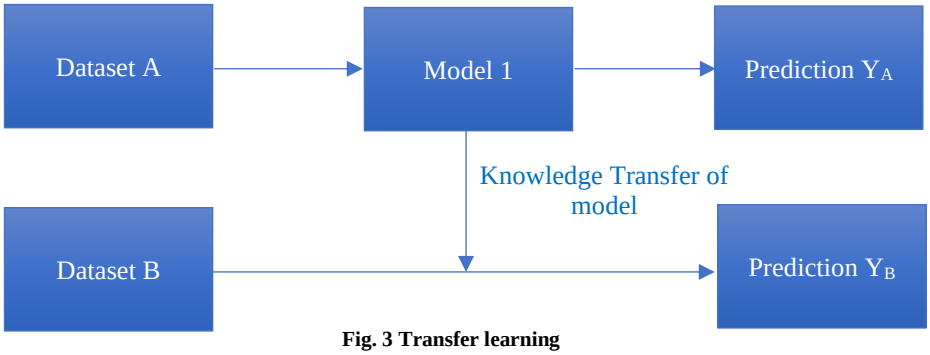

Fig. 3 Transfer learning

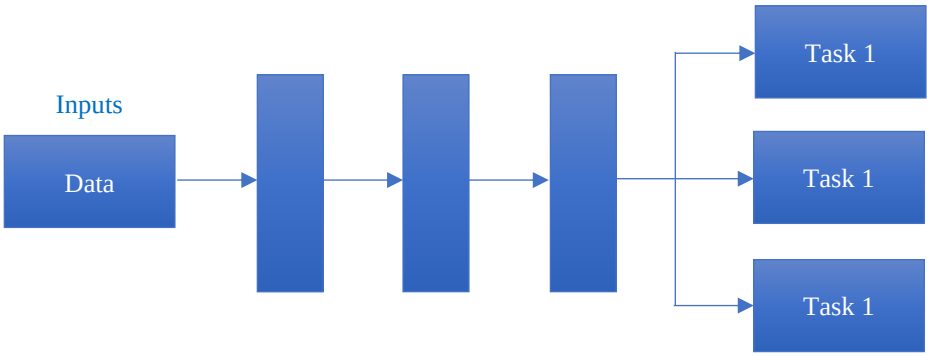

Fig. 4 Multitask learning

3.2. Transfer Learning

In silico drug discovery investigations frequently have a low data volume. Consequently, a significant barrier to the usage of artificial intelligence in drug development is the availability of labelled data. Creating algorithms capable of handling comparatively diverse and sparse data is one way to address the issue. Machine learning techniques such as transfer learning allow for the application of prior information from connected tasks to a particular activity that lacks sufficient data. In the arena of drug discovery, deep transfer learning is the most widely utilized method and has made significant advancements. The purpose of this viewpoint is to give a general understanding of transfer learning and its claims in drug development [21]. The use of transfer learning is a common technique in drug discovery. Three primary phases of drug discovery involve the application of transfer learning: forecast of molecular assets and happenings, molecule production, and structure-based simulated run. Most apps make use of feature-based and fine-tuning techniques. A Recurrent Neural Network (RNN) variant known as the Long Short-Term Memory (LSTM) model consists of various memory blocks, or cells, that together can hold considerably longer sequential data than an RNN can since information passed through cells can remain unmodified [22]. The procedure of refining the learning of a new task by using knowledge from a formerly learned related activity is known as transfer learning. The method controls the features produced from a large data set, A, that is used to predict its target variable, YA. It serially transfers the information to predict a dissimilar target, YB, from a data set, B, which has inadequate data. Figure 3 describes the transfer learning.

3.3. Multitask Learning

Multitask learning considers numerous similar biological targets collected and makes joint information transfer crosswise from one task to another, thus refining learning as well as prediction efficiency [23]. Multitask learning is useful when the volume of the dataset is low and has significant noise [24]. When there is little information required for each work, the multitask learning method has been introduced to help with knowledge exchange among activities. In multitask learning, the output is several unseen layers conforming to the number of tasks forecasted. The linked tasks may be uncorrelated at the output layer but are correlated at the interior level. There is an inductive transfer of information among tasks, thus optimizing multiple damage functions that enable models to improve and generalize crosswise numerous tasks [25,26]. Figure 4 illustrates multitask learning. Multiple tasks can learn from each other and filter appropriate and inappropriate features, mainly wherever very few data are present or insignificant noise is present, as shown in the figure. Moreover, because the various tasks are learned collaboratively, bias and overfitting are reduced [27]. When there is overfitting, multitasking learning enables the many tasks to support one another in establishing a more seamless reliance on shared characteristics. It is possible to apply multitask learning for both supervised and unsupervised learning [28]. It can be realized with Bayesian multiple linear regression [29], Support vector machine [30], K-nearest neighbor, deep learning, and neural networks.

3.4. Active Learning

Today, active learning is widely used in drug discovery. Besides experimental design, it also helps to remove redundant information [31, 32]. It addresses low-labelled datasets using user feedback. It is perfect where there is plenty of unsupervised training data, which necessitates expensive and resource-exhaustive experimentations to label. Active learning has the potential to consider fewer labelled data and hence speed up the drug discovery process and minimize the cost [33,34]. Active learning models can be constructed as predictable models like support vector machines deep learning.

4. How Artificial Intelligence is Used in Drug Discovery

The RQ 3 expresses an enormous amount of data generated by public health organizations, pathology records, molecular screening profiles, etc. This produced data could benefit from artificial intelligence techniques to speed up and prevent failures in the drug discovery pipeline. It includes methods like the Bayesian Neural Network, Explainable Artificial Intelligence algorithms, and Generative Artificial Intelligence.

4.1. Bayesian Neural Network

Bayesian neural network is used to build a robust model by approximating the data vagueness. The model accomplishes improved predictions of interactions amongst molecules and proteins [35]. BNN models [36] are also used to recognize the genes that are accompanied by drug understanding for 24 anticancer drugs. At the earliest possible stage of drug development, pharmaceutical companies want to avoid erosion due to drug effects. BNN is used to guess noxiousness from assay data and physiochemical properties of compounds [37]. BNN handles small data sets because of their capability to evade overfitting through former probability distribution to figure the average across plentiful models throughout training, which results in a regularization outcome to the system [38]. Even though BNN reports some of the inadequacies of neural networks, they need huge efforts to design the neural net.

4.2. Explainable Artificial Intelligence Algorithm

An alternative story for the machine language used in the molecular sciences is needed, and this has created a need for "explainable" artificial intelligence techniques [39]. Together, medicinal chemists, chemo informaticians, and data scientists will be able to find and develop new drugs more effectively thanks to XAI. Should XAI prove effective, it might offer crucial assistance in evaluating and interpreting progressively intricate chemical information, along with developing novel

pharmaceutical theories, all while circumventing human prejudices [40,41]. A simple, fast, reliable method was proposed by [42] termed Multi-Descriptor Across for emerging together precise and understandable models that were abstractly associated with the KNN method but usages dissimilar kinds of chemical descriptors instantaneously for resemblance valuation. When quality structure-activity relationship modelling was used as an example of explainable machine learning, semi-supervised regression trees originated to perform better than supervised regression trees [43].

4.3. Generative Artificial Intelligence

Generative models are proficient in producing new samples. They can also be cast off as separate techniques [44]. Generative models are accomplished by creating new samples for distribution. This is in contrast to discriminant models, which indicate the likelihood of the categorized data being present in the data example irrespective of whether the data example is effective or not [45]. Topical research has demonstrated the potential of deep-learning models to not only generate new computational units but also to augment data once working with minor data sets and to decrease dimensionality [46,47].

5. Emerging Machine Learning Techniques for Drug Discovery

With its remarkable outcomes, Machine Learning (ML) and Artificial Intelligence (AI) are becoming more and more popular in the drug development field. The emerging drug discovery techniques rendering to RQ 4 use machine learning, including quantum machine learning and recommendation systems.

5.1. Quantum Machine Learning

The primary benefit of quantum computing lies in its ability to handle intricate problems with efficiency that traditional computers would find unaffordable [48]. In traditional models, processing units calculate bits, which are in the form of 0 and 1, while in quantum computing, the qubits are in overlaid state together in 0 and 1 [49].

Logic gates are used to process qubits, resulting in the prevention of loss of information [50]. Quantum reinforcement learning can effectively explain value-based decision-making [51]. Using a quantum accelerator, a routine that runs on a quantum computer, enables the encoding of a probability distribution. A reinforcement learning setup is then used to encrypt the distributions that drive achievement selections [52].

Advances in quantum machine learning algorithms present intriguing substitutes for traditional machine learning methods, potentially benefiting the biochemical investigations associated with initial drug discovery stages [53,54].

To help researchers employ hybrid quantum ML, Google LLC provided an open-access quantum machine learning framework for Python. Hybrid-quantum machine learning's promise in the pharmaceutical sciences will, therefore, probably soon be achieved [55,56].

Table 1. Overview of drug discovery techniques

Sr.no.	Technique	Methods	Application
1	Advanced Technique in Drug Discovery	i. Chem-bioinformatic approach [14]	Assess drug efficacy, safety, absorption, excretion, and metabolic behaviors.
		ii. Blockchain [16]	Transparency in sharing information outside the company.
		iii. 3D printing [18]	Improves accuracy due to lingering capacity.
2	Machine Learning in Drug Discovery	i. Reinforcement Learning [19]	Design and create safe and effective molecules essential for the medical chemistry industry.
		ii. Transfer Learning [21]	Creating algorithms capable of handling diverse and sparse data.
		iii. Multitask Learning [23]	Transferred shared information from one task to another, thus improving prediction efficacy.
		iv. Active Learning [31,32]	Remove redundant data
3	Artificial Intelligence in Drug Discovery	i. Bayesian neural network [35]	Build a robust model by estimating data uncertainty.
		ii. Explainable artificial intelligence [40,41]	Evaluate and interpret intricate chemical information.
		iii. Generative artificial intelligence [45]	Capable of creating new samples for distribution.
4	Emerging Machine Learning Techniques in Drug Discovery	i. quantum machine learning [49]	Capable of handling intricate problems.
		ii. Recommendation system [58,59]	Used in e-business. Capacity to manage sparsity in data and forecast the event in which historical data is unavailable.

5.2. Recommendation System

A recommendation system is a machine learning framework that connects between the customers and the products [57]. The recommendation system is profoundly used in e-businesses such as Amazon and YouTube to initiate their sales [58]. The benefits of these methods include their capacity to manage sparsity in data, forecast in the event that historical data is unavailable, and offer transparency by elucidating the recommendation system's decision-making process. Medical recommender systems, which suggest the best sequence of acts built on a patient's medical antiquity, have been studied [59]. On the other hand, there are currently no documented uses in medication research and discovery. In order to forecast compound-target interactions for the purpose of medication research and discovery. In order to forecast compound-target interactions for the purpose of finding antiviral drugs, Sosnina et al. created a recommender system [60]. A content-based cleaning recommender system, which works well with scarce data and interpretability, was employed by the authors. Table 1 Gives a brief overview of the drug discovery techniques.

6. Aspects of Healthcare, Including Drug Discovery, Reshaped by Artificial Intelligence and Machine Learning

6.1. Data Analysis

There is an enormous amount of data, such as patient histories, clinical experimental results, and genetic data, that can be analysed using Artificial intelligence and Machine learning methods [61]. This analysis enables the researchers to better understand the diagnosis of diseases so that possible treatments can be suggested to find patterns, relationships, and intuitions which cannot be visualized using conventional methods [62].

6.2. Predictive Analysis

Using patient history data, AI techniques can help to predict a situation and how the patient reacts to treatment and side effects. This enables the predictive analysis to direct efforts in the direction of drug discovery [63,64].

6.3. Precision Diagnostics

The ability of the AI systems to accurately diagnose helps in the early detection and exact diagnosis of diseases based on patient's genetic characteristics and medical history [65].

6.4. Drug Discovery

To find new drugs, an enormous amount of data is analysed in order to forecast the efficiency and safety of new enhanced drug designs. Artificial intelligence and Machine learning help in speeding the process of drug discovery. By using these technologies, it becomes easier for scientists to discover chemical materials and biological methods so as to come out with exact and potential treatments [66].

6.5. Treatment Optimisation

With the help of AI-driven decision support systems, doctors adapt treatment plans for patients based on their medical history and symptoms. This minimizes the negative side effects and improves the treatment results [67,68].

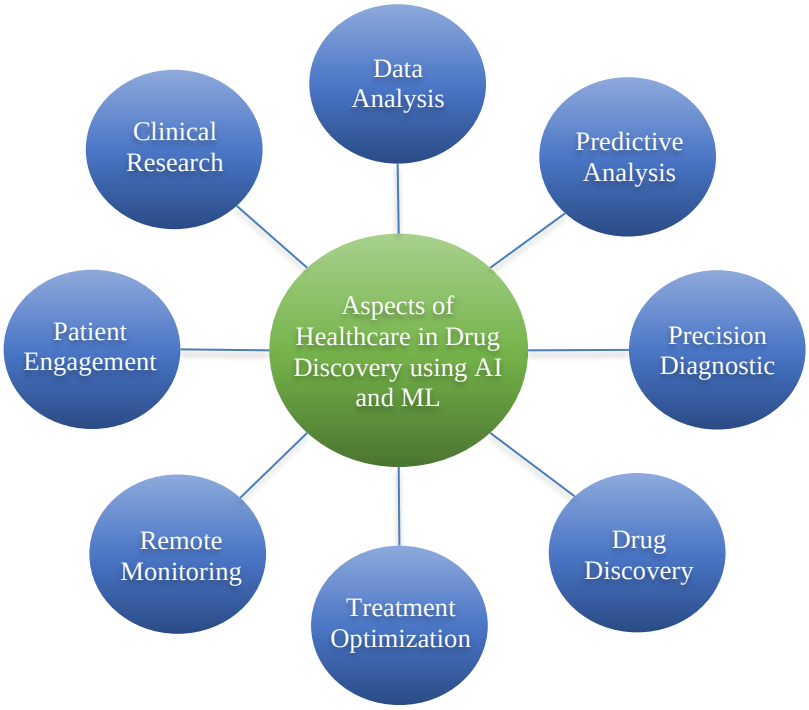

Fig. 5 Aspects in Healthcare, including drug discovery by AI and ML

6.6. Remote Monitoring

AI-powered remote monitoring equipment, such as wearable sensors, can continuously trace the patient's data outside of outdated clinical settings. This collection of data in real-time disease management, early diagnosis, and well-planned treatment of the patient [69].

6.7. Clinical Research

Artificial intelligence and Machine Learning are enabling clinical research by analysing huge and complex datasets. This helps to accelerate the research at a lower cost and improves the medicines which are based on evidence [70]. Figure 5 describes the aspects of healthcare, including drug discovery by AI and ML.

7. Construct Validity

In the context of drug discovery techniques, RQ1: What are the advanced technologies in drug discovery? The authors [14,16,19] have validated by chem-bioinformatic approach, blockchain, and 3D printing methods. Many authors have worked with machine learning in drug discovery, which answers the research question RQ2: How is machine learning used in drug discovery? Reinforcement learning [19], transfer learning [21], multitask learning [23] Active learning [31] constructs its validity. The RQ3: How artificial intelligence is used in drug discovery is validated through the methods of Bayesian neural network, explainable AI, and generative learning [53,40,45]. The validity constructs for RQ4: What are emerging techniques in drug discovery is satisfied by quantum machine learning and recommendation systems [49,58]. ScienceDirect, IEEE, Research Gate, scientific reports, springer, National Library of Medicine, and MIT press papers and articles are included which show good quality.

8. Conclusion and Future Scope

In summary, many important factors have an effect on AI and ML in drug discovery. They help the development of the drug industry so that time and money consumed on research and expansion can be reduced to increase efficiency.

An organized literature analysis has been carried out to recover the production and accurateness of drug discovery. Techniques such as advanced technologies, machine learning, artificial intelligence and emerging machine learning supplement the efficiency of the process. Molecular structure study also helps researchers in the advancement of drug discovery. Complex data can be utilised to develop hybrid deep learning models using AI and ML. Blockchain 3D printing also works as a recent technology. Reinforcement learning, transfer learning, multitask learning, and active learning play a vital role in the progression of drug discovery.

Bayesian neural networks, explainable AI, and Generative AI techniques are used to prevent failures in drug discovery. Quantum ML, and recommendation systems are the emerging techniques that will help the drug industry to come up with affordable methods.

Today AI and ML are helping drug discovery to revolutionise the development. Still, there are hurdles like complex unstructured datasets, which slow down drug discovery development. Once the hurdles are detached, AI and ML can be very widely and rigorously utilised in the new era of the pharmaceutical industry.

With the rapid developments in natural language processing, reinforcement learning, deep learning and generative AI, the AI and ML techniques are developing at a faster rate. These advanced technologies have the capacity to deal with complex problems in drug development, such as mixing the multi-omics data, diagnostic of infrequent diseases and suggesting drugs.

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Author Contributions

VDJ: Conceptualization, Methodology, Writing-Original draft preparation, DRD: Field study, Reviewing, Visualization, AB: Conceived, Investigation, Validation SND: Writing-Reviewing and Editing. All authors read and approved the manuscript.

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