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Artificial intelligence and machine learning in pharmaceutical science

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Abstract

Artificial Intelligence (AI) and machine learning, in particular, have gained significant interest in many fields, including pharmaceutical sciences. The enormous growth of data from several sources, the recent advances in various analytical tools, and the continuous developments in machine learning algorithms have resulted in a rapid increase in new machine learning applications in different areas of pharmaceutical sciences. Large amounts of biological data stored in global databases are the building blocks for machine learning and deep learning methods. They make it easier to find patterns and models that can help find therapeutically active molecules with less time, work, and money. Machine learning and deep learning technology are vital in drug design and development. We have applied these algorithms to various drug discovery processes such as protein structure prediction, toxicity prediction, oral bioavailability prediction, de novo design of new chemical scaffolds, structure-based and ligand-based virtual screening, pharmacophore modelling, quantitative structure-activity relationship, drug repositioning, and clinical trial design. The integration of Artificial Intelligence (AI) and Machine Learning (ML) into pharmaceutical sciences has catalyzed transformative advancements across drug discovery, clinical development, manufacturing, and post-market surveillance.

Keywords: Artificial intelligence, machine learning, artificial neural network, deep learning, drug discovery, drug development and drug design

1. Introduction

With previously unheard-of efficiency and precision, the incorporation of Artificial Intelligence (AI) and Machine Learning (ML) into pharmaceutical sciences has transformed clinical trials, personalized medicine, and drug development. AI is now a fundamental component of contemporary pharmaceutical research thanks to developments in computing power, algorithmic complexity, and data accessibility during the last ten years. The scientific field of artificial intelligence, which focuses on intelligent machine learning, mostly includes sophisticated computer programs that mimic human cognitive processes. In general, this process includes gathering data, creating effective mechanisms for using the data, drawing precise or close-to-exact conclusions, and putting self-corrections and modifications into practice.

In general, machine learning is examined using artificial intelligence in a manner that mimics human cognitive activities, producing more precise assessments and insightful interpretations. Computational intelligence and a variety of statistical models are combined in AI technology. With its many useful uses, artificial intelligence (AI) technology has emerged as a crucial element in many technical and research domains.

2. Literature Review

- AI has revolutionized healthcare, including pharmacy, by improving data management, diagnostics, and treatment. Its applications in pharmacy include drug discovery, dosage design, and hospital pharmacy, enhancing efficiency and effectiveness.
- AI and neural networks are transforming drug development by predicting and optimizing medication compositions, reducing time and costs.

This approach enables personalized medicine by tailoring drug formulas to individual patient needs, improving treatment efficacy.

- AI in pharmaceutical formulation analyzes vast data to spot patterns, enabling discovery of novel targets and optimizing drug development. It predicts solubility, stability, and bioavailability, improving clinical trial success and patient outcomes.
- Artificial intelligence is transforming the pharmaceutical industry by automating and optimizing drug development, making it faster and more efficient. It predicts drug properties, toxicity, and bioactivity, improving precision and reducing costs in drug discovery and clinical trials.

3. Artificial Intelligence

Artificial Intelligence (AI) refers to the development of computational systems capable of performing tasks that normally require human intelligence, such as reasoning, learning, problem-solving, and decision-making. In pharmaceutical sciences, AI is applied in drug discovery, precision medicine, pharmacovigilance, clinical trials, and patient care optimization.

Three fundamental functionalities of artificial intelligence (about a computer or machine).

- Resolving problems,
- Reflecting on past experiences and adjusting and
- Dealing with novel situations and problems (generalization).

3.1 Classification of Artificial intelligence

Artificial intelligence can be categorised into two forms:-

- Based on their caliber
- Based on their presence

Based on the caliber, AI can be subdivided as follows:

- Weak AI, also known as Artificial Narrow Intelligence (ANI), is capable of carrying out a restricted program, such as traffic signals, chess practice, face recognition, and driving.
- **Strong AI or Artificial General Intelligence (AGI):** Human-level AI is the term for artificial intelligence that replicates human performance in every task. It could facilitate the completion of hitherto intractable mental tasks by humans.
- **Artificial Super Intelligence (ASI):** This extremely intelligent system outsmarts humans and demonstrates a significantly higher degree of complexity in domains like space exploration, painting, and mathematics.

Based on the presence, AI can be categorised as:-

- **Type 1 (Reactive machines):** Because they lack a memory system, reactive machines are made for specialized, limited-purpose applications and are unable to draw on prior experiences. IBM's chess program is an example of a reactive machine since it can recognize pieces on a chessboard and forecast outcomes based on the state of the game.
- **Type 2 (Limited Memory System):** A limited memory system can solve new issues by drawing on prior knowledge. This system in autonomous cars can make choices based on previously captured observations that direct later actions, although these records are not kept on file forever.

Type 3, The "Theory of Mind" serves as its basis. This implies that people's intentions, thoughts, and desires influence their choices, something AI systems are currently unable to do.

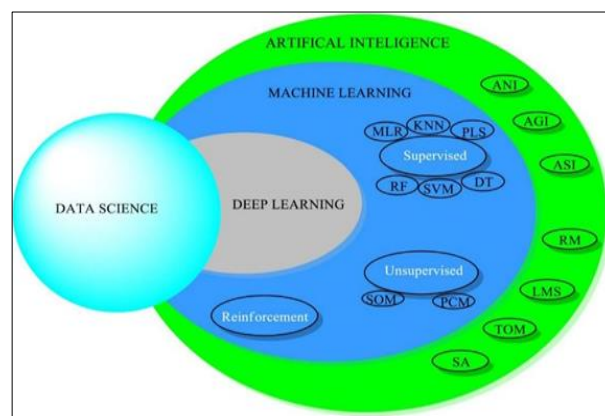


Fig 1: Machine learning and deep learning are subsets of artificial intelligence linked with data science.

3.2 Significance of AI in Pharmaceutical Sciences

AI is transforming the pharmaceutical industry by enhancing drug development, patient care, and healthcare efficiency across multiple areas:

- **Drug Discovery and Development:** Accelerates identification of potential drug candidates by analyzing large datasets and predicting drug efficacy.
 - **Drug Interaction Analysis:** Improves accuracy in predicting potential drug interactions.
 - **Personalized Medicine:** Enables customized treatments based on genetic, lifestyle, and environmental factors.
 - **Drug Safety Monitoring:** Enhances pharmacovigilance through better post-market safety surveillance
- Overview of Artificial Intelligence

Artificial Intelligence (AI), often linked with robotics and automation, refers to the ability of machines to exhibit human-like intelligence such as learning, reasoning, problem-solving, perception, and language understanding. While robotics involves building machines for repetitive or physical tasks, AI focuses on enabling these machines or computer systems to perform intellectual and cognitive functions autonomously. Currently, most AI systems are Weak or Narrow AI, designed for specific tasks like voice recognition, facial detection, internet search, or autonomous driving. The ultimate goal is Strong or General AI, capable of performing any cognitive task that humans can, potentially even surpassing human intelligence.

3.3 Basic Concepts and Scope of Artificial Intelligence

Artificial Intelligence (AI), first introduced at the 1956 Dartmouth Conference, was defined as the ability of machines to think and act intelligently. Over time, AI has evolved from perceptual machines to advanced models like Support Vector Machines (SVMs), Random Forests (RF), and Artificial Neural Networks (ANNs). Machine Learning (ML) and Deep Learning (DL) are major branches of AI DL being an advanced form of ML. With modern hardware advancements, AI is now widely applied across fields such as healthcare, pharmaceuticals, robotics, and data analysis, making it a rapidly growing and impactful technology.

3.4 Neural Networks

Recent advancements in computer science and mathematics have led to the development of three potential solutions:

- The goal of fuzzy logic is to mimic how the human brain makes judgments and generates answers when presented with ambiguous or insufficient information.
- Neural Networks: These models mimic how the human brain works by utilizing evolutionary tactics and genetic algorithms that support biological systems' self-organization and adaptability.

3.4.1 Features of Neural Network

They are capable of handling an array of tasks through their versatile applications:-

- **Associating:** Neural networks may link unknown patterns to the most similar versions they have learned through training on a variety of patterns, and they can switch to those versions as necessary.
- **Classification:** Neural networks are used to sort patterns or data into predetermined categories.
- **Clustering:** They categorize the data by identifying a distinguishing feature without having any prior knowledge of the data.
- **Prophecy:** Using the input given, they obtain the expected result.

3.5 Artificial Neural Networks (ANN)

Artificial Neural Networks (ANNs) form a core part of machine learning (ML) and deep learning (DL). They are inspired by the structure and functioning of the human brain, consisting of interconnected units called neurons or perceptrons arranged in layers. Each neuron processes input data and passes the output to the next layer, enabling the system to learn patterns and make predictions. The Multilayer Perceptron (MLP) is a common ANN architecture, where input variables (X_1 , X_2 , and X_3) are processed through hidden layers to generate an output (Y). ANNs are widely used for pattern recognition, prediction, and data classification across scientific and industrial applications.

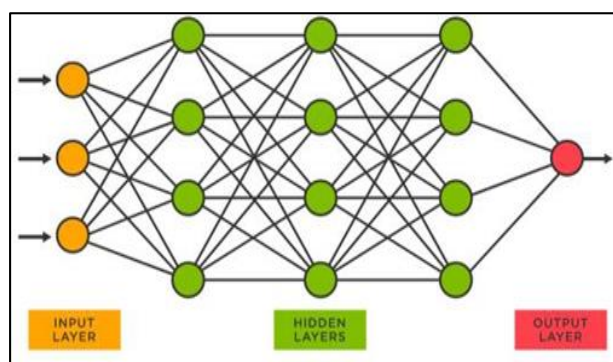


Fig 2: Schematic diagram of artificial neural network

3.6 Artificial Intelligence in Drug Discovery

Artificial Intelligence (AI) significantly accelerates drug design and development by analyzing data from genomics, proteomics, and metabolomics to identify potential drug targets like proteins or enzymes. It enables virtual screening of vast chemical databases and uses structure-activity relationship (SAR) analysis to predict how structural changes affect biological activity, optimizing drug potency and safety.

AI also predicts toxicity early, eliminating unsafe compounds, and improves clinical trial efficiency by selecting suitable patients using biomarkers and demographic data.

The AI-driven drug discovery process involves:

- Defining the problem and preparing data.
- Selecting the model: SVM, Random Forests (RF), or Neural Networks for discriminative tasks; DBM, DBN, GAN, VAE, or AAE for generative tasks.
- Training and evaluating models to minimize errors.
- Continuous optimization of data and model design for improved prediction ACCURACY.

3.7 Artificial Intelligence in Drug Development:

AI replaces the traditional trial-and-error approach in drug formulation by applying computational tools such as QSPR (Quantitative Structure-Property Relationship) to address challenges like solubility, porosity, and stability. Decision-support systems use rule-based algorithms to select optimal excipients and formulations, adjusting processes through feedback loops. Artificial Neural Networks (ANNs) streamline formulation development by correlating formulation parameters with desired outcomes through back propagation learning.

Expert systems assist in decision-making for formulation design, while computational methods like CFD (Computational Fluid Dynamics), DEM (Discrete Element Modeling), and FEM (Finite Element Method) help analyze powder flow, tablet compression, and disintegration behavior. Integrating these mathematical models with AI greatly enhances the speed, precision, and efficiency of pharmaceutical product development.

4. Machine Learning

Machine Learning (ML) is a subset of AI that uses algorithms and statistical models to identify patterns in data and make predictions or decisions without being explicitly programmed. In pharmaceutical sciences, ML is widely used in drug-target interaction prediction, biomarker discovery, molecular property prediction, adverse drug reaction detection, and personalized therapy.

4.1 Types of machine learning in pharmaceutical science

1. Supervised Learning, 2. Unsupervised Learning, 3. Reinforcement Learning

- **Supervised Learning:** Algorithms learn from labeled datasets to predict outcomes. Examples include random forests for toxicity prediction and support vector machines (SVMs) for classifying active/inactive compounds
- **Unsupervised Learning:** Algorithms identify hidden patterns in unlabeled data. Clustering methods like k-means are used to group compounds with similar properties, while dimensionality reduction techniques (e.g., t-SNE) visualize high-throughput screening data
- **Reinforcement Learning (RL):** Agents learn optimal actions through trial-and-error interactions with environments. RL has been applied to de novo molecular design, where models generate novel compounds by maximizing reward functions tied to drug-likeness.

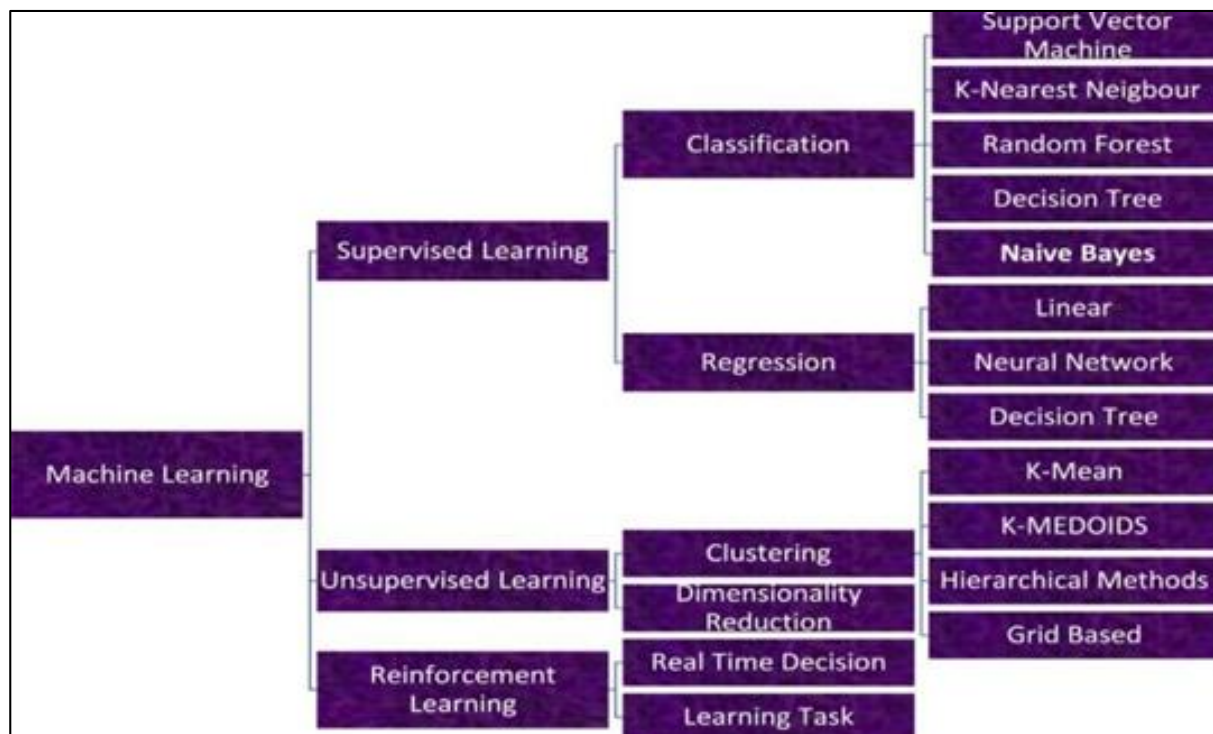


Fig 3: Brief overview of supervised and unsupervised and reinforcement learning

4.2 Principle of artificial intelligence and machine learning

The goal of machine learning (ML), a subfield of artificial intelligence (AI), is to develop models and algorithms that can handle massive volumes of data. Machine learning (ML) is the specialized process of creating software that can learn from data and make predictions or judgments, even if not all AI techniques are ML^[49, 50]. Scientists can forecast significant physical, biological, and chemical characteristics of novel compounds by utilizing various machine learning methods. Supervised learning and unsupervised learning are the two primary categories of machine learning.

4.3 Evolution of Artificial Intelligence and machine learning in life sciences

AI in life sciences began in the 1980s with early expert systems like MYCIN, which used rule-based algorithms for medical decision-making. Progress was limited until the 2000s, when the genomics revolution and high-throughput technologies produced vast biological datasets.

In the 2010s, Deep Learning (DL), powered by Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs), revolutionized image analysis, natural language processing (NLP), and predictive modeling. Achievements like Alpha Fold's protein structure prediction showcased AI's capability to solve complex biological problems.

4.4 Role of machine learning in drug discovery

Machine Learning (ML) is a vital tool in modern drug discovery, capable of analyzing complex biological data to

predict and optimize drug candidates. Supervised learning methods like Support Vector Machines (SVMs) and Random Forests predict drug-target interactions, toxicity, and ADMET properties, enabling virtual screening of large compound libraries.

Unsupervised learning helps cluster compounds with similar features and discover new chemical scaffolds, while reinforcement learning aids in optimizing synthesis pathways. Integrating ML with high-throughput screening and OMICS data accelerates target identification and candidate prioritization, reducing cost and development time.

4.5 Machine learning in drug development

Drug development is traditionally a costly, time-consuming, and high-risk process, often taking more than a decade and billions of dollars for a single drug to reach the market. Machine learning (ML), a branch of artificial intelligence (AI), offers powerful tools to accelerate pharmaceutical research by analyzing large-scale biological, chemical, and clinical data to improve decision-making at all stages of drug discovery and development.

Drug development is a complex, multi-phase process encompassing target discovery, preclinical testing, and clinical trials. Traditionally, this pipeline requires 10-15 years and costs over USD 2 billion to bring a single new chemical entity (NCE) to market, with a high failure rate due to poor efficacy or toxicity. Despite challenges such as data quality, bias, and over fitting, ML significantly improves the efficiency, precision, and success rate of drug discovery.

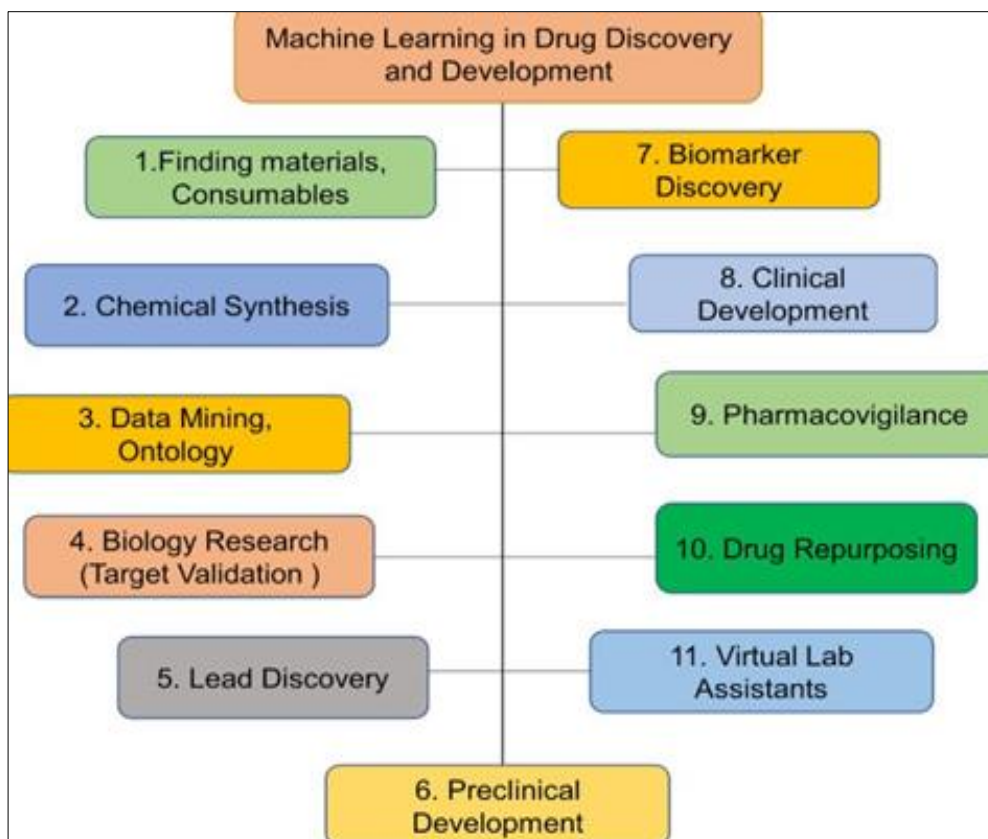


Fig 4: Machine learning in drug discovery and drug development

5. Advantages and disadvantages of artificial intelligence and machine learning

Advantages

- It perform unstoppable job throughout life span.
- It do not require any type of break and do not ask for holiday.
- Only one time investment and maintenance at certain interval require.
- No dependency on others.
- It provide more accuracy and precision in any task. Maximum output can be achieved. Speed of work
- Cross contamination can be avoided, in particular, sterile area or parentral products manufacturing, as AI stay all the time in premises.

Disadvantages

- Encouraging human laziness Job displacement.
- It is too much costly. Maintenance cost is too high or replacement of any spare part become costlier affairs.
- It replace human job placements.
- It does not generate any new idea and work as per programmed.
- Malfunctioning spoil the work, procedure and system too. To take instance, mixing of wrong raw materials in manufacturing department lead batch failure.

6. Applications

The most important aspect of production facilities is cleanliness. The machine is capable of carrying out this task continuously, repeatedly, and frequently.

AI can be used in a variety of manufacturing processes, such as balancing the weight of active ingredients and excipients, moving ingredients from one location to another, mixing ingredients, and moving materials from a container to a

machine and back again after the task is finished. For example, materials may be moved to a mass mixer to mix different ingredients, and vice versa. It could run simple machines and serve as a machine operator's assistance.

Additionally, the packaging section uses an intelligent machine to insert packed strips into a secondary pack, and AI then transports the prepared dosage forms to the finished goods storage room.

The department of pharmaceutical chemistry is where drug compounds are synthesized. Synthesis steps involve weighing of chemicals and reagents, mixing, heating for longer period of time (sometimes overnight stay), cooling and many more. If AI is properly programmed, it can accomplish the aforementioned goal. It lessens the workload for scientists, who must spend the night watching substances boil. Additionally, machines aid with the cleaning of glassware, chemical handling, and the synthesis of reagents that are hazardous to humans, such as bromine gas in CCL₄.

7. Conclusion

Artificial Intelligence (AI) has become a transformative force in pharmaceutical sciences, revolutionizing how drugs are discovered, developed, and delivered. By analyzing vast experimental data, AI accelerates drug research and formulation, reducing both time and cost. AI models help predict absorption, distribution, metabolism, and excretion (ADME) properties, improving drug efficacy and safety. It also enables drug repurposing by identifying new therapeutic uses for existing medicines, saving significant resources.

Overall, AI enhances efficiency, precision, and innovation across the pharmaceutical pipeline. As AI technologies continue to advance, the future of pharmaceutical sciences promises faster, smarter, and more personalized healthcare solutions.

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