CURRENT TRENDS OF AI AND ML APPLICATIONS IN PHARMACY

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ABSTRACT : The integration of Artificial Intelligence (AI) and Machine Learning (ML) into pharmacy is revolutionizing the landscape of drug discovery, development, and clinical practice. This review highlights the current trends and advancements in AI/ML applications across various domains of pharmacy, including drug design, pharmacovigilance, personalized medicine, pharmaceutical manufacturing, and clinical decision support systems. With the aid of deep learning, natural language processing, and predictive analytics, AI and ML are enabling faster drug target identification, optimizing clinical trial designs, enhancing patient safety through adverse drug reaction detection, and supporting precision dosing. Moreover, the emergence of generative AI models and real-world data analysis is further pushing the boundaries of pharmaceutical innovation. Despite significant progress, challenges such as data privacy, algorithm interpretability, and regulatory compliance remain critical. This article provides an in-depth overview of the current state, ongoing research, and future directions of AI and ML in pharmacy, emphasizing their transformative potential and the need for interdisciplinary collaboration to ensure ethical and effective implementation.

Keywords :- Artificial Intelligence, Machine Learning, Pharmacy, Drug Discovery and Development, Pharmacovigilance, drug response, Clinical Trials, Clinical Decision Support, Pharmaceutical manufacturing, Deep Learning, Precision Medicine.

INTRODUCTION

Artificial Intelligence (AI) refers to the ability of computer systems or robotic devices to analyze information and produce outcomes in ways that mimic human thinking, including learning, decision-making, and problem-solving[1].

AI is a branch of computer science that initially focused on symbolic programming for addressing complex tasks. Over time, it has evolved into a powerful problem-solving discipline with wide-ranging applications across industries such as business, healthcare, and engineering[1]. Classification of AI:

1.Artificial narrow intelligence (ANI): This system is designed and trained to perform a narrow task, such as facial recognition, driving a car, playing chess, and traffic signaling. E.g.: Apple SIRI virtual personal assistance, tagging in social media.[2]

2.Artificial General Intelligence (AGI) or Strong AI: It is also called Human-Level AI. It can simplify human intellectual abilities.

Due to this, when it is exposed to an unfamiliar task, it can find the solution. AGI can perform all the things as humans.[2]

3.Artificial Super Intelligence (ASI): It is brainpower, which is more active than smart humans in drawing, mathematics, space, etc.; in every field from science to art. It ranges from the computer just little than the human to a trillion times smarter than humans.[2]

ML, a subset of AI, is utilizes a range of algorithmic techniques and statistical approaches to address problems without the need for explicit programming instructions. Many conventional machine learning models follow a single-layer design, which necessitates

extensive feature extraction and data preprocessing before the data can be effectively used by the

model. [3]

Types of Machine Learning:

1.Supervised learning: It involves training a model using labeled data—where both the input features and corresponding target values are known. The goal is to enable the algorithm to learn the mapping between inputs and outputs accurately. This approach is commonly used in developing predictive models, such as forecasting risks or improving the planning and execution of clinical trials.[4]

2.Unsupervised learning: It is utilized when the dataset contains only input variables, without any predefined output labels. One widely used technique in this category is clustering, which helps in uncovering hidden patterns or natural groupings within the data. These patterns can be valuable for making informed predictions about new cases, such as anticipating patient responses or understanding treatment behavior trends.[4]

3.Reinforcement learning: It differs from both supervised and unsupervised learning. In this approach, an agent learns to make decisions by interacting with an environment, receiving feedback in the form of rewards or penalties. Over time, the agent learns the optimal strategy to maximize cumulative rewards. This method is particularly useful in dynamic and complex scenarios where learning from direct experience is necessary.[4]

Historical Evolution in pharmacy :

Although ideas related to artificial intelligence (AI) emerged long before they were used in the pharmaceutical field, its impact on pharmacy began to grow significantly with advancements in computational technology. One of the earliest examples appeared in the 1960s with systems like Dendral, which used rule-based reasoning to help chemists infer possible molecular structures from mass-spectral data, establishing an early framework for computer-assisted drug design [5].

During the 1980s and 1990s, machine learning (ML) began establishing its place in pharmaceutical research as computational approaches matured. Researchers increasingly used statistical techniques—such as decision trees, support vector machines, and QSAR (quantitative structure–activity relationship) models—to forecast biological activities, drug–target interactions, and potential toxicities. These data-driven methods helped reduce dependence on traditional trial-and-error laboratory experiments [6].

A major acceleration in the use of machine learning came in the 2000s, driven by the growth of big data, advances in high-throughput screening, and enhanced computational power. These developments allowed ML techniques to be applied more extensively in predicting ADMET properties, guiding lead optimization, and performing virtual screening across large chemical libraries [7]. In the past decade (2010s–2020s), the adoption of deep learning (DL) and more sophisticated AI techniques has expanded significantly within pharmaceutical formulation and drug delivery. These approaches now support advanced predictive models for pharmacokinetics, formulation stability, and individualized dosing, enhancing precision in both development and patient care [8]. Recent literature from 2023 to 2025 emphasizes that AI applications in pharmacy now extend beyond drug discovery to include manufacturing processes, clinical trial planning, and supply-chain management. These studies also underline the growing significance of explainable AI and adherence to regulatory standards to promote safe, transparent, and ethically responsible use in pharmaceutical practice [9,10].

AI and ML, DL In Pharmacy

Artificial Intelligence (AI) is significantly transforming various sectors, and pharmacy is among the fields experiencing notable advancements. The adoption of AI technologies in pharmaceutical practice is reshaping how drugs are discovered, dispensed, and monitored—ultimately contributing to improved patient outcomes and increased operational efficiency. This overview explores the key innovations AI brings to pharmacy, with particular focus on its role in drug development, personalized treatment, and patient care. Through the use of sophisticated algorithms and machine learning models, AI empowers pharmacists to anticipate individual responses to medications, fine-tune dosage regimens, and enhance workflow efficiency. These developments not only accelerate the delivery and precision of pharmaceutical services but also help in lowering costs and raising the standard of healthcare overall.[11]

AI and ML are revolutionizing pharmacy by enabling predictive modeling for drug repurposing, optimizing clinical trial design, and monitoring real-time patient responses. Advanced algorithms can analyze genetic, biochemical, and clinical data to identify novel therapeutic targets, foresee adverse drug reactions, and personalize medication regimens. This accelerates drug development, reduces failure rates, and enhances patient safety, making pharmaceutical care more precise and efficient [12].

In the 2020 CASP14 competition, DeepMind's AlphaFold2 made a remarkable leap in predicting protein structures, significantly outperforming its closest rival. This breakthrough drew widespread media attention, often described using terms like Artificial Intelligence (AI), Machine Learning (ML), and Deep Learning (DL). AI broadly includes technologies such as computer vision and natural language processing (NLP), where systems interpret and respond to their environment to accomplish objectives. At its core, AI involves training systems using algorithms and data, allowing them to perform tasks and generate predictions or insights about future events.[13]

ML typically categorized based on learning types or by the nature of the algorithms. Deep Learning (DL), an advanced branch of ML, employs layered non-linear models that learn to identify relevant features from complex, high-dimensional data. The term "deep" reflects the number of layers in a neural network—more layers correspond to greater depth. Each layer processes input data into more abstract and higher-level representations. DL is often seen as an end-to-end learning method, meaning the model learns the entire task as a whole, rather than being divided into separate steps. Using input-output pairs during training, DL models optimize performance across the entire task, minimizing the error propagation issues seen in traditional ML approaches.[13]

Within ML, Deep Learning (DL) has emerged as a powerful subdomain that leverages artificial neural networks (ANNs)— structures inspired by the human brain—to detect intricate patterns and correlations in large-scale data. DL techniques have led to breakthroughs in areas such as image recognition, natural language understanding and speech recognition. Outlines the key distinctions among AI, ML, and DL, illustrating their specific roles and applications in revolutionizing drug discovery and delivery systems.[14]

Current Applications of AI and ML in pharmacy:

1.Drug Discovery and Development:
The process of developing new drugs includes several key steps: identifying drug targets, finding initial "hit" compounds, optimizing leads, and testing them in clinical trials for safety and effectiveness. Traditionally, this process relied on trial-and-error research methods, which are effective but often slow, expensive, and prone to failure [15].

Recently, artificial intelligence (AI), especially machine learning (ML), has started changing drug discovery. ML can handle and analyze large datasets from sources like genes, proteins, and chemical compounds. This improves target identification and speeds up early drug research [15].Fig. 1 shows AI in drug discovery.

One example is Atom wise, a biotech company that uses deep learning and convolutional neural networks (CNNs) to predict how small molecules interact with proteins. This approach has helped find potential treatments for diseases like Ebola and multiple sclerosis, reducing time and increasing success chances [15].

The chemical universe contains an enormous number of molecules (over 10^{60}), making it difficult to find viable drug candidates. AI-based methods have achieved up to 97% accuracy in predicting drug-target interactions and have helped discover new antibiotics from over 100 million chemical structures [16].

AI-based virtual screening uses ML to analyze large chemical libraries, predict biological activities, and prioritize compounds likely to succeed. This approach turns complex data into actionable insights, accelerating drug discovery [16].

Advanced technologies supporting drug discovery include:

• In silico ADMET platforms: These model drug absorption, distribution, metabolism, excretion, and toxicity. One method analyses   protein-compound interactions, while another uses ML with aggregated data. Both require careful data handling [17].
• Blockchain: Provides secure, transparent, and traceable data for clinical trials and supply chains. High costs and a shortage of trained professionals limit its adoption [17].
• 3D Printing: Advanced 3D printing techniques allow precise, on-demand production of pharmaceutical products [17].

ML is increasingly used across drug development to streamline high-throughput screening, reduce costs, and possibly reduce the need for animal testing. Effective ML models require large chemical and biological datasets, including toxicity, efficacy, pharmacokinetics, and enzyme activity data [17].

AI also plays a key role in protein analysis. Predicting 3D protein structures is complex and expensive. Deep learning helps improve predictions of protein structures and protein-protein interactions, which are essential for designing effective drugs [18]. Challenges in drug discovery include:

• Drug–Target Interactions: Understanding how drugs bind to proteins.
• Drug–Drug Similarity: Comparing structures and functions of compounds.
• Side Effects: Predicting adverse effects from drug combinations.
• Drug Sensitivity and Response: Predicting how patients or cell lines respond [19].

Digital Twins (DTs) are virtual models that mirror real-world systems. In pharmaceuticals, DTs combined with AI and IoT can improve efficiency, innovation, and decision-making [19].

AI in healthcare and pharmaceuticals supports human work rather than replacing professionals. It assists with administration, diagnostics, imaging, robotic surgeries, and drug development. In pharmaceuticals, AI helps with drug dosage accuracy, rational drug design, personalized medicine, and clinical data management [20]. This study aims to review scientific literature on how AI algorithms are applied in drug discovery and clinical trials [20].
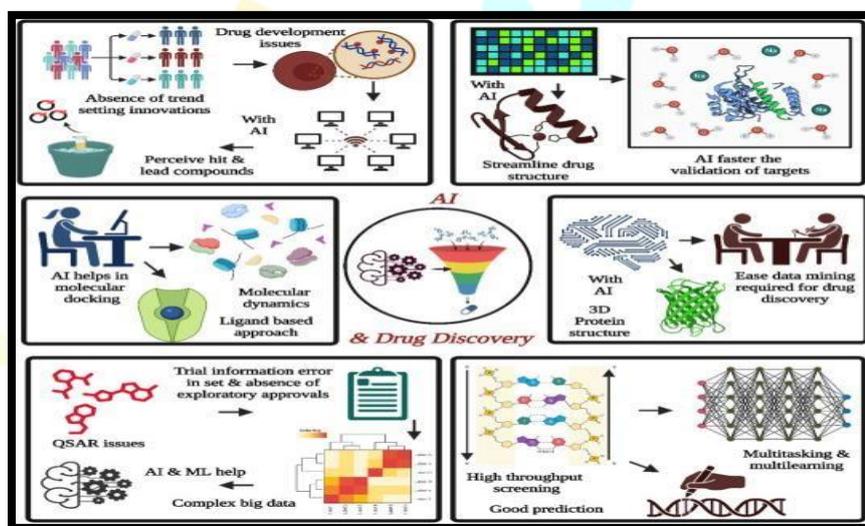

Fig No.1: AI in Drug discovery

2. AI Technologies in Pharmacovigilance Systems

Pharmacovigilance (PV) involves the scientific and practical activities aimed at detecting, assessing, understanding, and preventing adverse effects or other problems related to pharmaceutical products. The main goal of PV is to protect patients from harm caused by side effects, whether drugs are used as approved or off-label, throughout the product's life cycle [21].

PV helps ensure medicines are used safely and effectively by continuously providing updated information about drugs, healthcare providers, and patients. This contributes to better public health outcomes [21].

Monitoring drug safety is crucial to identify and manage risks associated with medications. A proactive approach improves patient protection, helps detect potential safety issues early, and maintains public trust in the healthcare system [21].

Drug safety surveillance also ensures compliance with regulatory standards, supports post-marketing evaluation, aids evidencebased decision-making, and reinforces public confidence in healthcare products and services (see Fig. 2) [21].

AI technologies provide major advantages in handling repetitive and routine PV tasks. They can assist in data entry, detecting adverse events (AEs), identifying drug–drug interactions, and recognizing subtle trends in data. AI can also convert unstructured safety information, such as free-text reports and handwritten documents, into standardized, machine-readable formats [22]. AI can streamline tasks like Medical Dictionary for Regulatory Activities (MedDRA) coding, finding duplicate case reports, classifying submissions as physician- or consumer-reported, and Distinguishing serious from nonserious cases. Advanced AI systems can analyze unstructured documents, extract important information, and generate automated clinical narratives. This reduces the need for manual review and lowers the workload for signal detection and validation [22].

AI tools can retrieve and interpret individual case safety report (ICSR) data from multiple sources, including medical literature, published case reports, online medication reviews, social media, electronic health records (EHRs), and hospital discharge summaries. Studies show AI accelerates data processing, performs previously impractical tasks, and saves both time and resources [22].

As the amount of electronically stored drug-safety data grows, integrating AI into pharmacovigilance workflows can reduce effort, speed up processing, cut costs, and improve the quality of safety data, making AI a transformative tool for future PV activities [22]. AI and machine learning (ML) help overcome traditional PV challenges by providing faster and more accurate ways to analyze data, detect safety signals, predict risks, and develop new tools for improved drug safety monitoring.
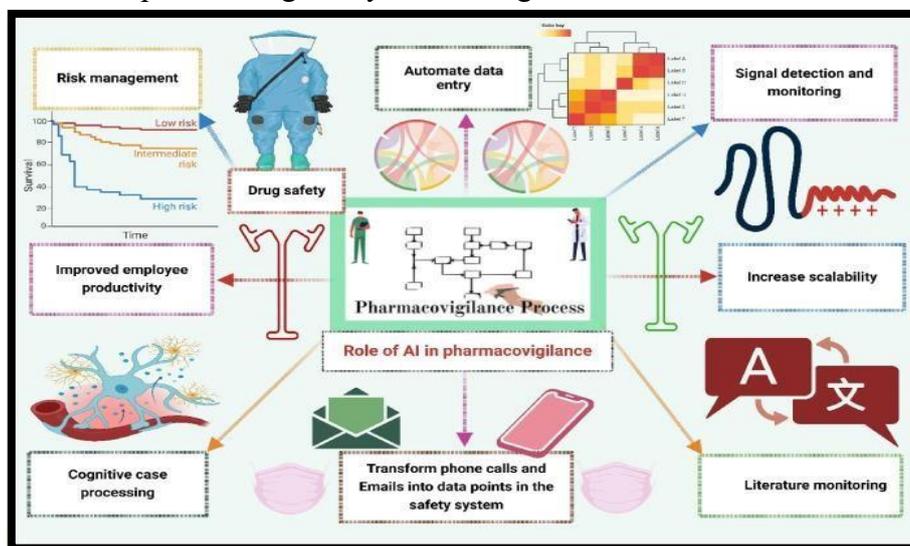

Fig No.2: AI in Pharmacovigilance
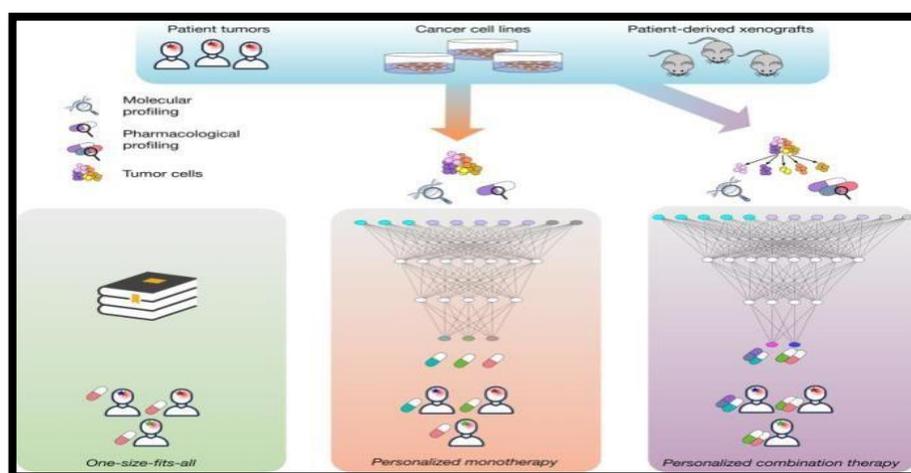
3. AI in Drug Response :

Predicting how cancer patients will respond to specific drugs is crucial for selecting the best therapy. However, conducting largescale clinical trials across all cancer types is difficult due to cost and logistics. To address this, cancer cell lines are widely used as experimental models, which has led to the creation of major pharmacogenomics databases. Resources like the Cancer Cell Line Encyclopedia (CCLE) and the Genomics of Drug Sensitivity in Cancer (GDSC) allow researchers to train artificial intelligence (AI) models to predict drug responses [23].

Many studies use these databases to build models that estimate drug efficacy, often using measures like the half-maximal inhibitory concentration (IC50) for individual drugs. Genomic information from cancer cell lines—such as mutations and gene expression— is commonly used as model input. While traditional machine learning (ML) methods are widely applied, it remains unclear whether ML or deep learning (DL) provides better accuracy for single-drug response predictions [23].

A key challenge is identifying which genomic features most influence model predictions. Explainable AI (XAI) methods are increasingly used to interpret model outputs by highlighting important biological features driving drug sensitivity predictions. However, few studies have applied XAI in the context of patient-derived genomic data. Developing interpretable, drug-specific prediction models is therefore a pressing need [23].

In this study, two integrated datasets were created by combining CCLE drug response profiles with gene expression and mutation data from CCLE and GDSC. These datasets were used to build drug-specific response prediction models for 24 drugs. ML and DL methods were compared for predictive performance, and XAI techniques were applied to the best models to identify the genomic features most associated with drug sensitivity [23].

AI-Driven Prediction of Drug Response in Cancer Therapy: (fig.3)

Fig No.3: AI drive prediction of drug response in cancer therapy

Limited patient data makes predicting individual drug responses challenging. To overcome this, researchers often use model systems such as immortalized cancer cell lines and patient-derived xenografts (PDXs) as surrogates for real tumors

Most cancer treatments currently follow standardized approaches based on cancer type or subtype. While effective, this approach does not consider molecular and genetic differences between patients. Personalized monotherapies, which target tumor-specific mutations, have shown promise but are suitable for fewer than 20% of patients [24].

Computational models can integrate data from model systems and available patient datasets to predict the most effective drugs for a broader patient population. These models aim to expand the benefits of personalized medicine beyond the small subset eligible for monotherapy [24].

However, monotherapies may be limited by tumor heterogeneity and acquired drug resistance, reducing long-term effectiveness. This has increased interest in predicting synergistic drug combinations. Early models used bulk gene expression data, but recent single-cell technologies provide more detailed insights into intra-tumor variability and potential treatment responses [24].

4. AI-Driven Automation in Pharmaceutical Manufacturing

Artificial intelligence is revolutionizing pharmaceutical manufacturing by enabling intelligent automation, particularly in areas such as equipment maintenance, process optimization, and supply chain management.[25]
a.Smart Sensors and Predictive Maintenance
The integration of Internet of Things (IoT) sensors into manufacturing equipment allows for the continuous collection of operational data in real time. These sensors—monitoring factors like motion, vibration, and temperature—supply information to machine learning algorithms that can detect early indicators of equipment degradation.[25]

For example, Novartis utilizes IoT-enabled machinery alongside AI models to anticipate mechanical failures before they happen. This predictive approach has significantly decreased unexpected equipment downtime and enhanced the overall efficiency of production systems.[25]

Typically, such predictive maintenance systems employ supervised learning methods, such as random forests or neural networks, trained on labeled historical sensor data to distinguish between normal operation and conditions that precede failure. However, the effectiveness of these systems heavily relies on the accuracy and reliability of the input data. Poorly calibrated or noisy sensor inputs can result in false positives or missed detections, highlighting the importance of rigorous data preprocessing and quality assurance processes.[25]
b. AI in Batch Process Control and PAT Systems
Process Analytical Technology (PAT) is central to ensuring quality in pharmaceutical batch manufacturing by enabling real-time monitoring and control. The integration of artificial intelligence, particularly machine learning, into PAT systems enhances their ability to interpret complex and non-linear interactions between process variables and product outcomes.[25]

Artificial neural networks (ANNs) are frequently applied in this context. As reviewed by Nagy et al. (2022), ANNs have been successfully used in PAT for tasks such as predicting tablet hardness and optimizing crystallization processes. These models often rely on real-time sensor data—such as pH, viscosity, or spectroscopic readings—to anticipate critical product attributes and dynamically adjust operational parameters.[25]

For instance, an ANN could process Raman spectroscopy data to estimate the uniformity of a powder blend and trigger automated changes in mixing settings when deviations are detected. This form of intelligent control aligns with the Quality by Design (QbD) framework, as machine learning enables adaptive learning and consistent product quality despite variability in raw materials.[25] While many academic studies highlight promising proof-of-concept applications, scaling these systems for full regulatory compliance remains a challenge. Rigorous validation procedures are required to meet industry standards. Emerging research areas, including transfer learning (to generalize models across different production batches) and hybrid control strategies that blend traditional PID controllers with machine learning, aim to improve the adaptability and robustness of batch process control systems.[25]

c. AI-Driven Supply Chain Optimization

Artificial intelligence is also transforming pharmaceutical supply chain management, particularly in the areas of demand forecasting and inventory optimization. Machine learning models—such as long short-term memory (LSTM) neural networks and gradient boosting algorithms—are increasingly used to analyze sales trends, epidemiological data, and external signals to anticipate product demand more accurately than conventional forecasting techniques .[25]

During high-demand scenarios, such as the COVID-19 vaccine rollout, adaptive AI models were used to integrate case count data and distribution metrics to forecast regional surges in demand. This allowed for more efficient allocation of resources, minimizing both shortages and overstock situations. Companies like McKesson have leveraged predictive analytics to detect potential drug shortages early, enabling timely procurement decisions .[25]

More advanced strategies, including reinforcement learning for multi-echelon inventory management, are being explored to optimize the entire supply chain network. These systems continuously learn from real-time logistics and demand data, aiming to minimize delays and reduce waste across multiple levels of the supply chain.[25]

Nonetheless, implementing AI in pharmaceutical logistics comes with challenges. Irregular demand patterns, regulatory stockpiling mandates, and limited transparency from suppliers can reduce model accuracy. Despite these hurdles, industry consensus suggests that AI-powered forecasting and supply chain visibility will be essential for competitive operations by 2025—especially if models are continuously retrained with updated data .(sees in fig.4.)[25]
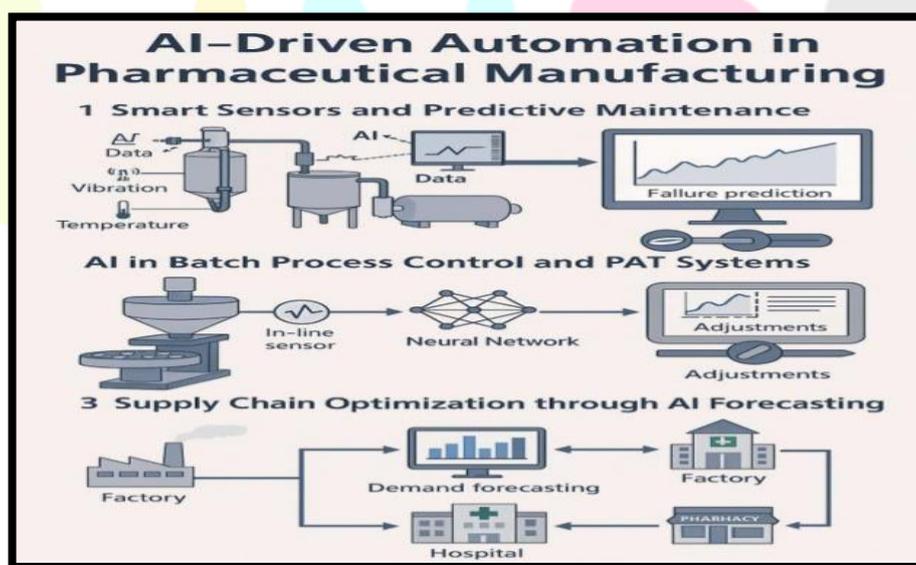
Fig No.4 : AI drive automation in pharmaceutical manufacturing

AI-driven automation is transforming pharmaceutical production by merging machine-learning systems, robotics, and advanced process-control technologies to simplify operations and reduce the likelihood of

human error. These tools provide real-time oversight of key quality parameters, enable predictive equipment maintenance, and improve consistency from one batch to the next. As a result, companies can boost productivity and reliability while adhering to strict regulatory requirements for product safety and quality.[26] In addition, AI-enabled analytics platforms enhance continuous manufacturing by examining large volumes of data generated from sensors, manufacturing equipment, and laboratory systems to identify irregularities before they become critical issues. Automation also speeds up formulation development, lowers operational expenses, and strengthens traceability throughout the supply chain. As adoption grows, AI is increasingly becoming a core catalyst for innovation and long-term competitive strength across the pharmaceutical sector.[27]

Advantages :

1.Reduces Cost

Automation lowers long-term manufacturing costs by replacing large workforces with fewer supervisors and machines. After the initial investment, expenses mainly involve maintenance and energy. AI and data analytics also help cut costs by guiding better production decisions.[28]

2. Increases Productivity

Automated lines divide tasks across multiple stations, allowing robots to perform repetitive and complex actions quickly. This speeds up processes such as material handling, equipment operation, and product assembly, leading to faster overall production.[28]

3. Enhances Quality

Automated systems deliver consistent and precise output with extremely low error rates. Continuous monitoring and adaptive controls help maintain accuracy throughout every stage of production.[28]

4 Improves Industrial Safety

Robots handle heavy, dangerous, or high-risk tasks, reducing workplace accidents. Sensors track conditions like temperature and send alerts when abnormalities occur, helping protect workers.[28]

5.Ensures Accurate Results

Automation depends on reliable data. AI and machine learning analyze this information to support precise decision-making and create self-learning systems that consistently produce accurate results.[28]

6. Better Working Conditions and Value Addition

Automation maintains steady production and quality. Flexible systems can be quickly reprogrammed for new designs, reducing downtime and eliminating long retraining periods for workers.[28]

7. Industrial Communication

Industrial communication is essential for automation. It helps control machines, manage power, and monitor production lines.

Common protocols include Fieldbus, Profibus, EtherCAT, and Ethernet/IP, enabling fast data analysis and real-time decisions.[28] 8. Monitoring and Predictive Maintenance

Sensors constantly track temperature, pressure, sound, and other factors on the production floor. When changes occur, alerts are sent so technicians can fix issues early. This prevents major breakdowns and reduces downtime.[28] 9. Equipment Monitoring

Automated systems use sensors and cameras to monitor equipment from a distance. They detect faults early, improve safety, reduce the need for many operators, and extend machine life in industries with large, complex machines.[28]

5.Clinical Trials

Artificial Intelligence (AI) uses techniques like Machine Learning (ML), Deep Learning (DL), Natural Language Processing (NLP), and Optical Character Recognition (OCR) to enable intelligent systems. AI is increasingly transforming clinical trials by improving patient selection, predicting trial outcomes, and reducing costs and timelines [29].Fig.5 shows AI and ML in clinical trials. Traditional clinical trials are slow, costly, and have low success rates. AI can analyze real-world data to classify patients better, optimize study design, and improve recruitment by matching patient characteristics to eligibility criteria. It also helps identify drug candidates more likely to succeed and links diverse datasets such as electronic medical records (EMRs), publications, and trial databases [29].

AI also enhances patient monitoring during trials. Wearable devices and EMR data can be analyzed in real time to track health and detect adverse events. Additionally, AI can generate real-world evidence (RWE) by

mining EMRs, automating medical imaging interpretation, and assessing long-term drug safety and effectiveness [30].

Digital twins—virtual patient models—are another AI application, allowing simulation of treatment responses for personalized therapy [30]

Key AI Applications in Clinical Trials:

Patient Enrollment: AI uses predictive analytics to estimate recruitment rates by analyzing factors like disease prevalence, trial complexity, and adverse events [31].

Risk-Based Monitoring: AI predicts site performance based on historical and real-time data, helping optimize trial outcomes by managing underperforming or high-performing sites [31].

Chatbots: AI-driven chatbots assist patients, site staff, and researchers by providing instant responses and reducing workload [31]. Data Management: AI automates data checks by identifying inconsistencies or anomalies in trial databases and learning from past corrections to improve accuracy [31].

Overall, AI and ML streamline clinical trials, making them faster, safer, more cost-effective, and more accurate in decision-making.
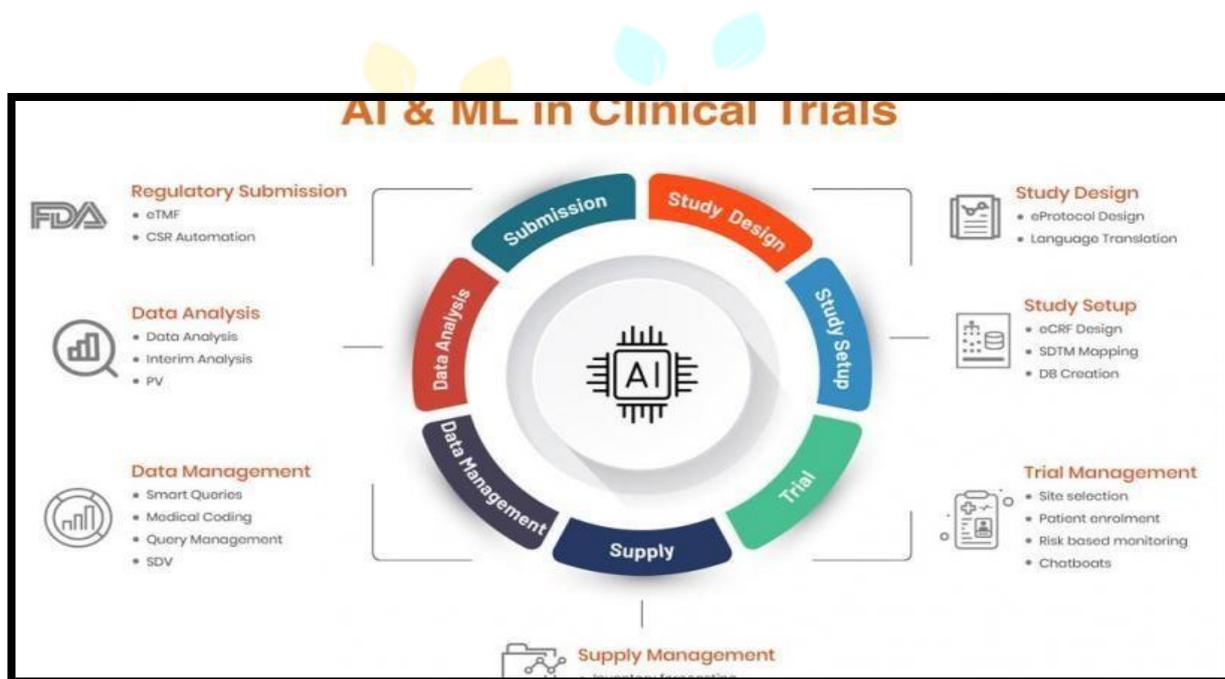
Fig No.5 : AI and ML in clinical trials

## 5.Data Integration Challenges for Machine Learning in Precision Medicine

Precision Medicine aims to personalize diagnostics and treatments by integrating vast amounts of data about the molecular and environmental causes of diseases. Artificial intelligence (AI) and machine learning (ML) play key roles in analyzing this complex, heterogeneous data to predict individual health outcomes. However, efficiently managing and integrating large, diverse datasets— ranging from genetic information to clinical records—remains a major challenge.[32]

Biomedical research has increasingly become data-intensive, relying on large projects like The Cancer Genome Atlas and the UK Biobank that produce massive datasets combining genetic, clinical, and environmental data. Alongside genomics, clinical data— especially electronic health records (EHRs)—are crucial but complicated, as EHRs were originally designed for hospital administration rather than research, resulting in heterogeneous, unstructured data.[32]

Successful AI/ML applications in Precision Medicine must handle this data diversity and scale while addressing practical constraints like computational resources, confidentiality, and ethical considerations. A major obstacle is integrating varied data types and formats into unified models that can be used in research and clinical practice.[32]

Metadata—data describing the characteristics and context of other data—is increasingly important for understanding and managing these datasets. Proper data integration requires standardized protocols and collaborative infrastructures to support scalable analysis.[32]

Finally, addressing these challenges will enable AI/ML to transform healthcare by providing personalized, evidence-based medical insights that improve patient outcomes and public health policies.(Sees in fig.6).[32]
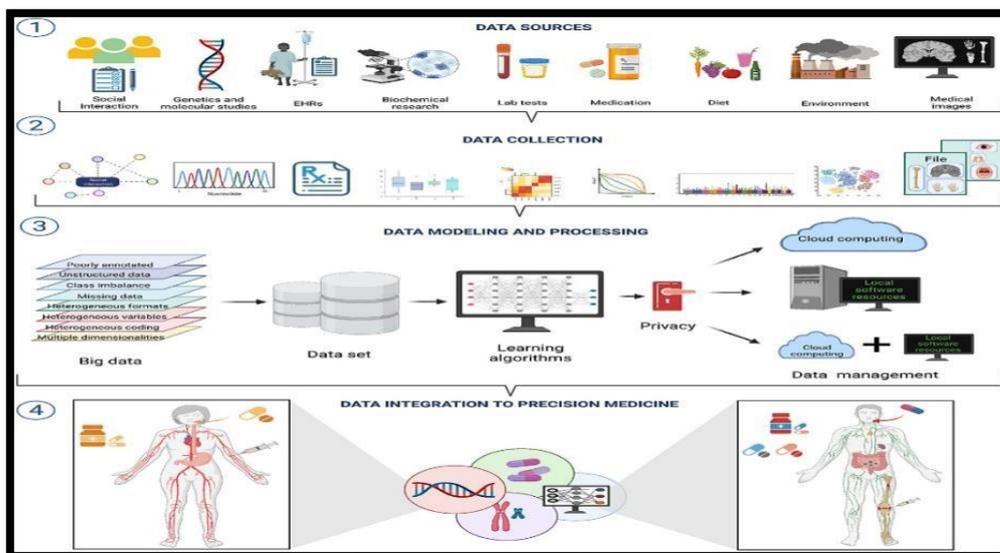
Fig No.6: Data integration to precision medicine

AI and ML support personalized disease prevention and treatment strategies. These technologies are transforming many aspects of precision medicine, including medical imaging, risk assessment, phenotype prediction, and gene expression analysis.[33]

Precision medicine focuses on identifying distinct subgroups within larger populations, characterized by differences in disease risk, progression, detection, and treatment response due to variations in environment, physiology, and other factors. The goal of personalized medicine is to tailor prevention, diagnosis, and therapy based on an individual's genetics, phenotype, epigenetics, and lifestyle. Achieving this requires detailed characterization—or deep phenotyping—of each patient prior to intervention.[33] Access to multimodal datasets enhances the ability to uncover disease-related phenotypic and genotypic traits that inform predictions of dose-response, risk, prognosis, and treatment outcomes. Recently, AI/ML methods have shown encouraging results in predicting disease risk, phenotypes, and treatment responses in areas such as neurology, oncology, and cardiology, with notable precision and reliability.[33]

Moreover, AI-driven decision-making integrates three critical elements of big data: multimodal data analysis, scientific knowledge, and decision support systems. AI and ML approaches in precision medicine also facilitate identification of single-cell characteristics, including genomic and epigenomic profiles, proteomic signatures, immune markers, and morphological features, which aid in selecting targeted therapies.[33]

Nonetheless, one major limitation of computational precision medicine is the need for advanced computing infrastructure to process complex multimodal data. The core challenges of big data in biomedical and health informatics are often summarized by the "V's": volume, velocity, variety, veracity, variability, and value. Together, AI, ML, precision medicine, and big data are advancing healthcare by delivering highly accurate and precise interventions.[33]
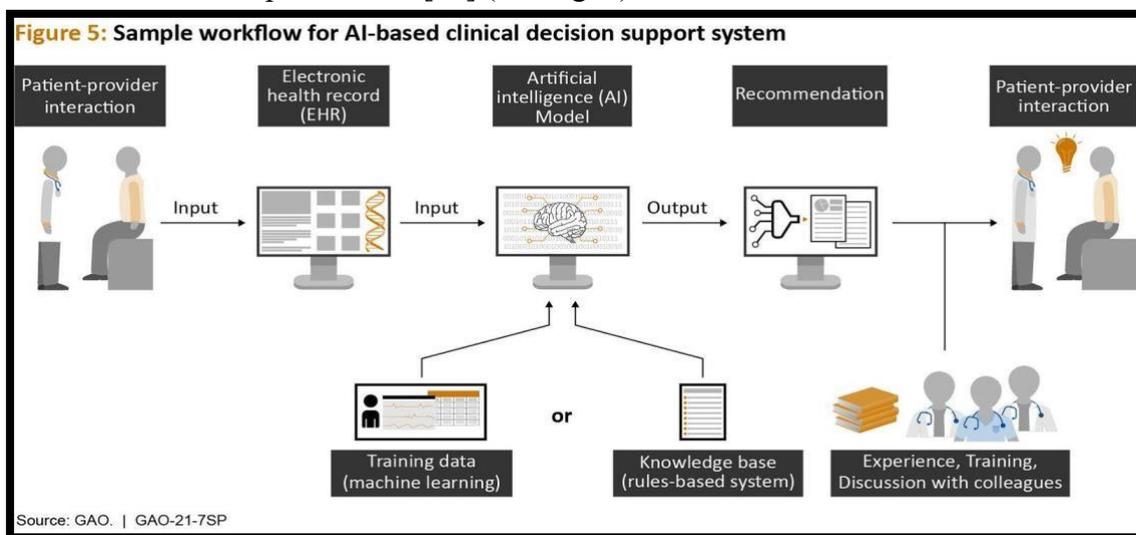
6. AI in Clinical Decision Support Systems (CDSSs)

Primary care is a key part of healthcare, serving as the first point of contact for patients and managing large, diverse populations. Primary Care Physicians (PCPs) often handle patients with multiple chronic conditions and complex medication regimens, making accurate health records and up-to-date clinical knowledge essential [34].

Clinical Decision Support Systems (CDSSs) were promoted in the U.S. in 2007 to be integrated with Electronic Health Records (EHRs). By 2017, over 40% of hospitals had advanced CDSSs. These systems help providers with diagnosis, treatment planning, prescribing, and monitoring medications, often using alerts. CDSSs improve adherence to clinical guidelines, enhance preventive care, increase patient safety, and reduce

adverse drug events. They can also tailor recommendations to individual patient needs [34]. Studies show that CDSSs can increase the number of patients receiving recommended care by about 6%. However, their effect on overall morbidity and mortality is not yet clear. PCPs may still face challenges when coordinating care with specialists due to differences between CDSS advice, specialist recommendations, and outdated HER data [34].

AI, particularly Machine Learning (ML) and Deep Learning (DL), has strengthened CDSS capabilities. ML algorithms— supervised, unsupervised, and reinforcement learning—analyze large datasets to make predictions and improve over time. DL, a subset of ML, uses layered feedback to produce more accurate and reliable results. These AI-based CDSSs help manage the growing amount of healthcare data, support evidence-based decisions, and enhance patient care [34] (see Fig. 7).

Fig No.7: AI in clinical decision support system

AI and ML are now essential in healthcare, improving clinical decision-making, patient safety, and overall efficiency, making them indispensable tools in modern medical practice [34].

Artificial Intelligence (AI) Tools and Software in the Pharmaceutical Industry

The pharmaceutical sector is increasingly adopting Artificial Intelligence (AI) tools and software to improve efficiency, accuracy, and innovation across multiple areas, including drug discovery, clinical trials, pharmacovigilance, personalized medicine, and marketing. These AI-driven technologies leverage machine learning (ML), natural language processing (NLP), and advanced data analytics to automate and streamline complex workflows. In the realm of drug discovery and development, AI plays a crucial role in predicting interactions between drug molecules and biological targets, thereby accelerating the identification of viable drug candidates. For example, platforms such as Nuclear Wisdom can forecast molecular binding and efficacy, significantly shortening timelines and reducing costs in the early phases of drug development.[35]

AI Applications in Clinical Research, Pharmacovigilance, Marketing, and Personalized Medicine
Artificial Intelligence (AI) is increasingly revolutionizing clinical research by enhancing participant recruitment and enabling real-time monitoring of clinical trials. These capabilities contribute to improved safety, efficiency, and higher trial success rates. Platforms like IBM Watson Health exemplify this by assisting in the design of intelligent clinical trials, predicting potential device or protocol failures, and thus enhancing the overall reliability of research outcomes.[35]
In pharmacovigilance, AI plays a pivotal role by processing extensive datasets sourced from electronic health records, clinical documentation, and even social media platforms to identify adverse drug reactions (ADRs). Tools such as Aegis AI utilize machine learning and natural language processing to detect and categorize safety signals early, allowing for quicker and more accurate response to potential drug-related risks.[35]
AI is also transforming pharmaceutical marketing and sales through predictive analytics. By analyzing customer behaviors and interaction data, AI helps refine engagement strategies. For instance, Salesforce Einstein integrates AI capabilities into customer relationship management (CRM), providing predictive insights that improve sales performance and enhance customer service, often via intelligent chatbots.[35]

Another significant area of AI impact is personalized medicine, where AI models analyze diverse data inputs—including genomic profiles, clinical records, and lifestyle factors—to develop individualized treatment plans. Platforms like Tempus use AI to interpret genomic and clinical data, supporting oncologists in tailoring therapies that are most likely to yield positive patient outcomes. Similarly, IBM Watson leverages AI to assess patient-specific variables and suggest optimal treatment strategies, especially in oncology. In addition, it enhances pharmacovigilance by analyzing vast volumes of structured and unstructured data, including scientific literature and real-world evidence, to identify emerging drug safety concerns more efficiently than traditional approaches.[35]

The Role of IBM Watson in the Pharmaceutical Industry

IBM Watson, an advanced AI system, has made a substantial impact across several domains within the pharmaceutical sector, driven by its robust natural language processing and machine learning capabilities.[35] In drug discovery, IBM Watson accelerates early-stage research by mining vast databases of scientific publications, biological data, and medical literature to uncover novel drug targets and anticipate drug-drug interactions. This data-driven approach significantly reduces the time and cost associated with bringing new therapies to market.[35]

In the optimization of clinical trials, Watson analyzes patient data from Electronic Health Records (EHRs) to match suitable candidates with ongoing studies. It also assists in designing more effective protocols and enables continuous monitoring of trial progress, enhancing the accuracy of efficacy and safety evaluations.[35]

IBM Watson also excels in personalized medicine. By integrating genomic data, medical history, and lifestyle information, it supports clinicians in crafting tailored treatment regimens—most notably in oncology—where precision therapies are critical for patient outcomes.[35]

Moreover, in pharmacovigilance, IBM Watson offers a comprehensive solution for ADR detection by extracting insights from both structured sources (such as medical databases) and unstructured content (such as social media and public health records). This capability not only boosts early risk identification but also helps ensure regulatory compliance and enhances overall drug safety.[35] Collectively, these applications underscore IBM Watson's transformative influence on pharmaceutical practices by enhancing innovation, streamlining operations, advancing personalized care, and ultimately improving public health outcomes.[35]

Future Prospects

AI and ML are expected to reshape the pharmacy field by enhancing processes from early drug discovery to individualized treatment. These technologies will speed up the identification of new drug candidates, lower research costs, and support the rapid repositioning of existing drugs. In pharmacovigilance, AI will enable early detection of potential adverse reactions, improving medication safety. Clinical trials will become more efficient through AI-assisted patient recruitment, continuous digital monitoring, and the growing use of virtual trial platforms. Predictive models will improve understanding of drug response and support precision medicine by tailoring therapies to a patient's genetic and clinical profile. Additionally, AI-driven clinical decision support tools will strengthen diagnostic accuracy and promote evidence-based prescribing. Collectively, these advancements will lead to more reliable, efficient, and patient-focused pharmaceutical care, guiding the profession toward a fully data-integrated healthcare system.

Summary:
Artificial Intelligence (AI) and Machine Learning (ML) are transforming the pharmacy sector by introducing smarter, data-driven solutions. These technologies are being used in drug discovery, personalized medicine, clinical trials, disease prediction, and pharmacy automation. AI helps in analyzing large datasets quickly, identifying potential drug candidates, and predicting treatment outcomes more accurately. ML algorithms also support pharmacists in decision-making, detecting drug interactions, and improving patient care. Overall, the current trends show that AI and ML are making pharmacy more efficient, precise, and patient-focused.

Conclusion:

The integration of Artificial Intelligence (AI) and Machine Learning (ML) in pharmacy is revolutionizing the field by enhancing drug discovery, optimizing personalized medicine, and streamlining clinical and operational processes. These technologies enable faster, more accurate predictions, reducing the time and cost of drug development while improving patient outcomes. From AIdriven diagnostics to automated

pharmaceutical manufacturing and real-time patient monitoring, the applications are vast and rapidly evolving. As AI and ML continue to advance, their role in pharmacy will become even more central, fostering a future of smarter, safer, and more efficient healthcare delivery.

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