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Artificial Intelligence in Pharmaceutical Research and Development

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Abstract

The field of engineering known as artificial intelligence is concerned with building intelligent machines. Artificial intelligence has being applied more and more in pharmaceutical technology over time. In 1956, a literary work used the term "artificial intelligence" for the first time. But the concept of AI has been there since 1950, when both symbolic and problem-solving methods were applied.

AI's objective is to develop intelligent modelling that supports knowledge visualisation, issue solving, and decision-making. Recent advancements in AI have had a substantial impact on a number of pharmacy-related fields, such as drug discovery, formulation development for drug administration, polypharmacology, hospital pharmacy, etc. Drug delivery formulations are made using a variety of Artificial Neural Networks (ANNs), including Deep Neural Networks (DNNs) and Recurrent Neural Networks (RNNs). Numerous drug discovery implementations (QSAR) have looked at and evaluated the efficiency of the technology in quantitative structure-property relationships (QSPR) or quantitative structure-activity relationships (QSAR). De novo design also promotes the development of considerably more modern pharmaceutical compounds with respect to desired/ideal qualities. This is a summary of artificial intelligence's inception, goals, and applications.

I. Introduction:

A branch of computer science called artificial intelligence is entirely focused on building machines that can carry out tasks that would otherwise require intelligence and human operators. A variety of well-known technologies fall under the umbrella term of artificial intelligence, including machine learning, deep learning, chatbots, non-linear grid systems, and self-modifying graph networks. Artificial intelligence (AI) has streamlined and had an impact on the pharmaceutical business in various ways, from the development of novel medications to the fight against swiftly spreading diseases. Artificial intelligence (AI) in the pharmaceutical sector refers to the application of automated algorithms to tasks that traditionally required human intelligence.

The application of artificial intelligence in the biotech and pharmaceutical industries over the past five years has transformed how researchers create new medications, treat diseases and more.

When was AI introduced?

The first attempts to characterise human thought as a symbolic system by classical philosophers in 1956 are where artificial intelligence (AI) first emerged.

The phrase "artificial intelligence" (AI) was first used in a conference at Dartmouth College in Hanover, New Hampshire, in 1956, but the discipline was not legally recognised until then.

Objectives:

- The building of automated systems that operate intelligently and advise individuals on the best course of action is involved in the development of expert systems.
- Adding human intelligence to computers8: This will allow machines to think and behave like people do, allowing them to handle challenging problems in a human-like manner. Algorithms will be used to enable automated processes and lessen the workload for human workers.
- Multi-Domain Application: AI will have applications across a wide range of implementation areas, including computer science, cognitive science, statistics, psychology, engineering, ethics, the natural sciences, healthcare, space technology, logic, languages, and more.
- Applications in Computer Science: AI supports the creation of a variety of techniques to tackle a variety of difficult problems in the field of computer science. These tools consist of Search and Optimisation, Logic, Control Theory, Language Analysis, Neural Networks, Classifiers, Statistical

Learning Methods, and Probabilistic Methods for Uncertain Reasoning.

Advantages:

Medical applications: In general, using AI software, clinicians can assess patients' illnesses as well as the side effects and other health risks associated with the medication. Trainee surgeons can learn new skills by employing AI software like various artificial surgery simulators (for example, gastrointestinal simulation, heart simulation, brain simulation, etc.).

Disadvantages:

i) Expensive: The implementation of AI is costly. Complex machine design, maintenance, and repair can be done extremely affordably. Building only one AI system takes a large amount of time from the R&D department. AI machine software requires periodic updates. Reinstallations and computer recovery are time- and money-consuming processes.
ii) No human reproduction: Robots equipped with AI technology have the capacity to think like humans and to remain detached, giving them an advantage in correctly doing the work at hand and doing so without passing judgement. Robots cannot provide inaccurate information or form opinions on unresolved issues.
iii) Experience doesn't improve anything: Experience can increase human resources. Contrarily, AI-powered technology cannot benefit from practise. They are unable to differentiate between individuals who put in hard work and those who don't.
iv) Lack of originality: AI-powered robots are not sensitive or emotional. Humans have the ability to hear, see, feel, and think. They are able to think and be creative simultaneously. These functionalities cannot be offered by using machines.
v) Joblessness: The widespread use of AI technology across all sectors could result in large job losses. Given the unfavourable unemployment rate, human workers may experience a decline in productivity and originality.

Classification of AI:

AI can be categorised in two ways: by quality and by presence.
According to its capabilities, AI can be categorised as follows:
i) Artificial Narrow Intelligence (ANI) or Weak AI: It is capable of performing a limited range of tasks, such as traffic signalling, chess practise, face recognition, and auto steering.
ii) Artificial General Intelligence (AGI) or Strong AI: It is also known as human-level AI and performs all things that humans do. It can execute novel tasks and streamline human cognitive processes.
iii) Artificial Super Intelligence (ASI): It is smarter than people and performs a much wider range of tasks than people, including space exploration, mathematics, and sketching.
The following categories of AI can be made depending on their existence and absence:
i) Type 1: It is employed for specialised applications without a memory system that cannot make use of prior knowledge. Reactive machine is the term used to describe it.
Examples of this memory include an IBM chess programme that can identify checkers on a chess board and anticipate outcomes.
ii) Type 2: It has a constrained memory system and can draw on prior knowledge to address a range of issues. In automatic automobiles, this system is capable of making decisions. Although some recorded observations are utilised to document subsequent activities, these records are not kept indefinitely. Things as mathematics, space exploration, and sketching.
iii) Type 3: is predicated on the "Theory of Mind." It means that people's individual thoughts, intentions, and desires have an impact on their decisions. This AI system doesn't exist.
iv) Type 4: It has a sense of self and consciousness, or self-awareness. This AI system doesn't exist either.

Application of artificial intelligence in the pharmaceutical industries:

1. Research development.
2. Drug Creation.
3. Diagnosis.
4. Disease prevention.
5. Epidemic forecast.
6. Remote observation.
7. Manufacturing.
8. Marketing.
9. Rare diseases and personalized medicine.
10. Processing biomedical and clinical data.
11. Identifying clinical trial candidates.

R&D:

Pharma businesses all over the world are accelerating the drug discovery process with the help of cutting-edge machine learning algorithms

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and AI-powered tools. These clever technologies can be used to solve issues with complicated biological networks because they are made to find nuanced patterns in vast datasets.

Drug creation:
The use of AI has the potential to boost research and development. AI is capable of a wide range of tasks, including developing and recognising new chemicals as well as verifying and finding target-based medications.

Diagnosis:
Doctors can gather, process, and analyse vast amounts of patient healthcare data using cutting-edge machine learning technologies. Healthcare providers all across the world are using ML technology to safely store sensitive patient data on the cloud or other centralised storage systems.

Disease prevention:
Pharmaceutical companies can use AI to develop medicines for uncommon ailments as well as widespread illnesses like Parkinson's and Alzheimer's. Pharmaceutical companies typically do not devote their time and resources in this field since the return on investment (ROI) on creating solutions for rare diseases is frequently very low compared to the time and money necessary to generate medications to treat uncommon disorders.

Epidemic forecast:
Today, a lot of pharmaceutical companies and healthcare organisations use AI and ML to monitor and forecast epidemic outbreaks globally. These programmes gather data from numerous web resources, examine the effects of various geological, environmental, and biological aspects on population health in various places, and make an effort to make linkages between these elements and earlier epidemic outbreaks. Such AI/ML models are especially helpful for underdeveloped countries that lack the financial and medical infrastructure required to control an epidemic outbreak.

Manufacturing:
Pharma companies can utilise AI in their production processes to raise productivity, efficiency, and speed up the development of life-saving drugs. AI may be used to manage and enhance every aspect of the manufacturing process., including:

- Quality control,
- Predictive upkeep.
- Waste minimization.
- Process automation;
- Design optimization.

Marketing:
Pharma marketing companies employ AI to investigate and develop unique marketing strategies that guarantee high sales and brand recognition.

Remote observation:
It represents a milestone in the pharmaceutical and healthcare industries. Many pharmaceutical companies have already developed technologies that remotely monitor patients with critical illnesses using AI algorithms.

AI in hospital pharmacy:
In hospital pharmacy-based health care systems, AI is applied in a variety of ways, such as structuring dose forms for specific patients, selecting the best or most practical administration techniques, and establishing treatment protocols.

- Maintaining medical records: It might be challenging to keep track of patients' medical records. By implementing the AI system, data collecting, storage, normalisation, and tracking are made simple. Quickly extracting medical records is made possible by Google's Deep Mind health effort. This project will help deliver quicker and better healthcare as a result. This project aids in enhancing eye treatment at Moor Fields Eye Hospital NHS.
- Creating a treatment plan: AI technology can be used to create efficient treatment plans.When a patient's health deteriorates to the point where selecting an acceptable treatment plan becomes difficult, the AI system is needed to maintain control. All previous data, reports, clinical expertise, etc. are taken into consideration in the treatment plan that this technology offers. A initiative by IBM Watson has been launched to help oncologists.
- The analysis of X-ray pictures, radiology reports, ECHOs, ECGs, and other data to locate and identify diseases and other disorders is one repetitive task that AI technology assists with.
- A "cognitive assistant" with high analytical and logical abilities is IBM's Medical Sieve algorithm. A medical start-up is necessary to improve patient conditions by combining deep learning with medical data. There is a specialist computer programme for every body part that is used in specific disease scenarios. Deep learning can be applied to almost all imaging analyses, including X-ray, CT scan, ECHO, and ECG.

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- Health support and medication aid: In recent years, it has been discovered that the use of AI technology is efficient for both health support services and medication assistance. Molly, a startup's virtual nurse, hears a warm voice and sees a friendly face. Its goal is to assist people in managing their own treatment and to support patients with chronic diseases in-between medical sessions. Ai Cure, a smartphone webcam app, monitors patients and assists them in managing their illnesses.
- Because AI in the health care system can collect and compare data from social awareness algorithms, people benefit from it. A patient's medical history, treatment history profile going back to their infancy, habits, and way of life are only a few of the enormous data collected in the healthcare system.

AI in Clinical Trial Design:

- Clinical trials take about 6-7 years to complete and include a substantial monetary investment in order to determine the efficacy and safety of a medicinal product in humans for a specific disease condition. Only one out of every ten compounds that undergo these trials, however, receive successful clearance, which represents a significant loss for the industry. These failures may be the result of bad infrastructure, poor technical requirements, and poor patient selection. With the use of AI, these problems can be minimised thanks to the abundance of digital medical data that is already available.

- One-third of the time required for a clinical trial is spent enrolling people. The enrollment of suitable participants can prevent the 86% of clinical trials that fail that would otherwise occur from occurring. By applying patient-specific genome-exposome profile analysis, AI can help in the selection of only a certain diseased population for enrollment in Phase II and III of clinical trials. This analysis can aid in the early prediction of the available therapeutic targets in the patients selected. The early identification of lead molecules that would pass clinical trials while taking into account the chosen patient population is aided by preclinical discovery of molecules as well as early lead compound prediction before the start of clinical trials using other aspects of AI, such as predictive ML and other reasoning techniques.

- The failure of 30% of clinical studies is attributed to patient dropout, which increases the need for recruiting in order to complete the trial and results in a time and money loss. This can be prevented by closely monitoring the patients and assisting them in adhering to the intended clinical trial protocol. In a Phase II experiment, AiCure developed mobile software that monitored individuals with schizophrenia's routine medication intake. This boosted patient adherence by 25% and ensured the clinical trial's successful conclusion.

AI based advanced applications:
AI-based nanorobots for drug delivery:

Integrated circuits, sensors, a power source, and a safe data backup are the key components of nanorobots, which are maintained by computational technologies like AI. They are programmed to avoid collisions, identify targets, find and attach to them, and then excrete from the body. Nano/microrobot advancements enable them to go to the intended spot based on physiological variables, such as pH, increasing effectiveness and minimising systemic negative effects. Considerations like dose adjustment, sustained release, and control release must be taken into account when developing implantable nanorobots for the controlled delivery of drugs and genes, and the release of the drugs requires automation managed by AI tools like NNs, fuzzy logic, and integrators. Implants with microchips are used for both programmed release and to locate the implant in the body.

AI in combination drug delivery and synergism/antagonism prediction:

Because they can have a synergistic effect for a speedy recovery, many medication combinations are approved and marketed to treat complex diseases including TB and cancer. For example, cancer therapy requires six to seven drugs as a combination therapy, which makes the process laborious. The selection of precise and potential drugs for combination requires high-throughput screening of a sizable number of drugs. Drug combinations can be screened and the total dosing regimen can be improved using ANNs, logistic regression, and network-based modelling. Rashid et al. used a framework for quadratic phenotype optimisation to identify the best possible treatment regimen for bortezomib-resistant multiple myeloma using 114 FDA-approved medications. The best two-drug combination suggested by this model was decitabine (Dec) and mitomycin C (MitoC), and the best three-drug combination was Dec, MitoC, and mechlorethamine.

If supported by data on the synergism or antagonistic effects of medications delivered simultaneously, combination drug administration may be more effective. 'Mater regulator genes' were effectively utilised by the Master Regulator Inference Algorithm to predict 56% synergism. For the same purpose, other techniques like RF and Network-based Laplacian regularised least square synergistic drug combination can also be utilised.

For the purpose of predicting synergistic anticancer medication combinations, Li et al. created a synergistic drug combination model employing RF. The authors successfully predicted 28 synergistic anticancer combinations using this model, which was built using gene expression patterns and different networks. They have listed three of these pairings, while the others could possibly be significant. Similar to this, Mason et al. used ML to estimate potential synergistic antimalarial combos based on a data set of 1540 antimalarial medication molecules using a technique known as the Combination Synergy Estimation.

AI emergence in nanomedicine:

In order to diagnose, treat, and monitor complicated diseases like HIV, cancer, malaria, asthma, and numerous inflammatory conditions, nanomedicines combine drugs and nanotechnology. Because they have improved treatment effectiveness, nanoparticle-modified drug delivery has recently grown in significance in the therapeutics and diagnostics fields. Many issues in formulation development could be solved by combining AI and nanotechnology.

A methotrexate nanosuspension was created computationally by analysing the energy produced during the interaction between the drug molecules and keeping an eye on any circumstances that would cause the formulation to aggregate. The assessment of drug encapsulation within the dendrimer and the determination of drug-dendrimer interactions can both be aided by coarse-grained simulation and chemical computation. In addition, the effect of surface chemistry on the internalisation of nanoparticles into cells can be investigated using tools like LAMMPS and GROMACS 4.

The creation of silicasomes—a mix of irinotecan-loaded multifunctional mesoporous silica nanoparticles and the tumor-penetrating peptide iRGD—was aided by AI. Because iRGD enhances the transcytosis of silicasomes, with improved treatment outcomes and enhanced overall survival, this boosted the uptake of silicasomes three to fourfold.

Future of Artificial Intelligence: Self-driving car technology is already being used by businesses like Google and Uber. AI will significantly impact the field of automated transportation by assisting drivers with disabilities and reducing accidents. More advanced AI systems may replace humans as well as assist in dangerous industry occupations. AI systems can forecast climate change utilising environmental technology and data sciences. AI systems that are efficient and timely will handle about 80% of customer care tasks. Artificial intelligence (AI) systems' symptom recognition and medical data processing capabilities will facilitate the management of personalised health. By interacting with a robotic system, cyborg technology can help patients make the most of artificial prosthesis for a higher quality of life. With the advancement of space technology, AI is now able to analyse the orbital routes of successful launches and make recommendations for future activities. Regarding the pharmaceutical industry, AI is the future, yet the technology is already present. Artificial intelligence may reduce expenses, provide novel, efficient therapies, and most importantly, it can help save lives. Therefore, biotech companies should start utilising the benefits of AI as soon as possible.

In terms of compound design, the breadth and expansion provided by AI and machine learning will allow us to access a lot bigger chemical space, providing us a much wider and more diversified spectrum of chemicals, improving our ability to choose the finest drug discovery compounds. The software will also assist businesses in identifying potential individuals for clinical trials and identify any issues with medications' efficacy and safety far earlier. Therefore, the sector stands to gain significantly from adopting AI and machine learning technologies. It can be effectively used to build a solid, long-lasting pipeline of novel medications. We could produce medications more quickly and cheaply by utilising the capabilities of contemporary supercomputers and machine learning.

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