**Benefits of AI Assisted Drug Development and Delivery**

IS 601: Management Information Systems

Final Term Paper

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**Abstract**

This paper is a review of how the development of Artificial Intelligent technology is progressing at an unprecedented pace and the pharmaceutical industry is one particular field in which employment of AI for quick drug development and production is worth exploring. AI technology is proven to save time along with resources, prevent high-risks, and optimize returns. The digital transformation of all patient records, and increasing technological advances allow health care providers to quickly interact with databases, detect diseases early and identify the drug that can serve as the best target for patient care. AI can be employed by pharmaceutical companies throughout the various steps of the drug development cycle, from identifying the target of a particular drug, determining the effectiveness of an active compound, selecting best drug candidates for an illness, as well as recruiting patients for clinical trials. AI algorithms can be designed to maximize drug effectiveness, and reduce the risk of failure, making it a dependable technology for future drug research and delivery.

**Introduction**

Artificial Intelligence (AI) has begun to integrate its application with the pharmaceutical industry as a front-runner beneficiary in different sectors of society. The conventional process of drug development is an expensive and time consuming high-risk, high-return industry. It takes an average of 10 years and $2.6 billion to produce one new drug, according to the Biomedical Journal of Scientific & Technical Research. Several methods to reduce the risk of failure when designing new medicines are now being considered by several pharmaceutical companies. The use of AI in this sector would decrease the expense, resources and development time. The standard identification and validation of new drug targets has been focused on trial and error, leaving more space for error and treatment failure. AI-assisted drug discovery makes it easier to identify drug targets, to scan for good molecules from data libraries built over time, to recommend chemical modifications, to identify repurposing candidates, and design drugs *de novo* . Nevertheless, it also has a range of obstacles to conquer. AI has had the greatest effect in providing feedback on best patient targets for clinical trials, but it is not yet completely incorporated in all phases of the cycle of drug development. Every technology has some drawbacks, the same is true for AI in medicine, as it is not used as the primary treatment method in all healthcare facilities. AI needs to be qualified correctly and must be able to handle significant tasks.

AI research and its training can be adapted depending on the area in which it is applied, making it a great tool for businesses to extend their research, use it to make decisions to improve their business and increase customer loyalty. Employing AI in research for new drugs enables pharmaceutical companies to continue producing more effective treatments, with lower costs, and higher returns. Since AI is trained on data and facts collected from customers, in the case of pharmacology the data is in the form of patient records and illnesses, as well as treatments prescribed which are stored in health care databases. Employing this data to produce medicine which can cure human illnesses, reduce risks or side effects and eliminate health problems is the best way to achieve customer satisfaction.

**3. Literature Review**

**3.1 AI in the drug development cycle to optimize returns.**

Artificial Intelligence (AI) is predicted to tackle modern problems with modern solutions through its ability to make predictions like humans. Until now, AI has been employed in medicine for purposes such as biochemical modeling, bioinformatics, and predictive toxicology, but it’s full potential in pharmacology has yet to be attained (Henstock , 2019). According to a study conducted by researchers at Tufts Center for the Study of Drug Development, the most common use of AI in medicine is to recruit patients for clinical studies (Lamberti et al., 2019). It is valid to infer that some use of AI was for purposes other than clinical studies such as research and quality control in the industry but not to the fullest extent. AI employs machine learning for its ability to deliver results for any particular problem, and machine learning relies on vast amounts of data collected in the form of big data for processing inputs. The rapid advances in the field of database systems and machine learning algorithms as well as their applications enables experts to not only view massive amounts of medical data but also convert data into useful information and stimulate the decision making process at an inconceivable speed. Any drug manufacturing company can integrate these algorithms into almost every step of the business process to speed up the design and manufacturing steps of the desired product.

In terms of drug research, unsupervised machine learning algorithms can process relevant data, cluster related data, interpret the information and produce an output about disease diagnoses so a chemical compound and its target can be isolated. Deep learning, a subfield of machine learning can be employed to process various forms of experimental data, to find potential molecular compounds with a desired target and produce effective results (Mak & Pichika, 2019). The same process when performed manually by humans could take months or even years of reading published work, planning, sorting to just get through the first step of collecting relevant data, lengthening the time required for a company to bring one drug to the market significantly.

The discovery of new drugs is crucial when diseases evolve at a faster pace than researchers can provide a cure. Machine learning combined with data mining makes assessing various new compounds for potential effects on target cells easier, compared to testing every compound in the lab. In the drug discovery process, finding hits is important to determine which compound out of the millions available, is able to produce chemical activity with a given target (Mak & Pichika, 2019). The end goal is to pick out a lead agent for modification to maximize therapeutic benefits and define a specific structure-activity relationship. These initial steps can be tedious since they are based on trial and error, but having a database system which stores information about the structure of each compound and scans it against targets and their binding sites quickly to make a decision on effective compounds can reduce the laborious work. It is believed that with proper establishment of AI methods, it is possible to minimize failures in clinical trials from new drugs and establish a much cheaper drug development process (Mak & Pichika, 2019).

Additionally, the method of employing AI can be flexible and does not need to be secluded to new compound discovery but also drug repurposing. In this process databases containing drugs that have been repurposed get combined with databases of open chemicals and open drugs to find the required chemical for a cure (Mohanty, 2020). These are the methods currently being employed by the researchers to test for a quick cure for symptoms of Covid-19, and to effectively deliver medications to the world population quickly and efficiently reducing failures during the clinical trials phase. Drug repurposing is especially efficient for diseases that impact similar biological processes, and allows companies to tackle recurring issues such as flu and antibiotic resistance, by giving insight on modifications required to create an effective drug.

Scientists believe that machine learning offers the option of reverse synthesis of molecules for conditions like cancer, allowing scientists to come up with treatment chemicals through use of information about biological processes and chemicals involved (Liang et al., 2020). According to research published by Guangdong Medical University, using the vast data collected in clinics for cancer patients and processing them via machine learning models can provide insights on the drug sensitivity of patients to various drugs that are predicted to be resistant to certain forms of cancer with high mutation state of cancer cell genome. AI could be used to understand how cancer cells mutate, gaining resistance over time using large data sets on highly resistant cancer forms, allowing scientists to alter drug treatments accordingly (Liang et al., 2020). In this manner AI can give more accurate information allowing the drug industry to keep up and produce treatments that are based on the ever changing nature of biological processes.

**3.2 AI saves time and resources, prevents risks and optimizes returns**

Recent developments in AI, can take advantage of the massive, digitized data across the medical sector accelerating the ability to uncover hidden patterns and make predictions (Agrawal 2018; Wu et al., 2020). Also, AI does not require laid out instructions to make predictions; it learns the patterns by reviewing a massive number of examples and training. Accordingly, AI is predicted to generate massive changes in business practices, innovation, and decision-making in the future. AI has already disrupted many industries such as automobile, manufacturing, and healthcare (Dixon et al., 2020). With the rapid adoption of AI in the pharmaceutical industry in recent years, it is obvious that AI has the potential to significantly change the drug development process (Ekins et al., 2019). Without prior knowledge, machine learning can quickly discern patterns from existing drug molecules that have known antibacterial activities and then identify new promising drug molecules out of a database of molecule libraries in just a few days. However, AI’s success in antibiotics may not translate into finding other types of drugs. In essence, machine learning can find both true and false correlations (Marcus and Davis, 2019). While prior IT infrastructure systems can also find some relationship to make predictions, AI can do this faster and at a much lower cost, which shifts the competitive advantage towards using AI to make even more predictions than before (Agrawal et al., 2018). As with all new technologies, it is critical to understand the conditions under which AI should be applied to innovation and when it should not be applied.

In cancer research AI has proven to take the lead on optimizing returns through quick implementation of large data to pave a path to discovery of effective treatments, as well as reduce the overall cost and time of generating new drugs each time cells mutate and become resistant (Liang et al., 2020). Organizations looking to maximize profit and produce best products and reduce the cost in resources, human labor, capital etc., would need to keep up with the change in nature of customer requirements, and implement technologies that are up to date with changes in the industry which employs their products.

The COVID-19 pandemic has unveiled a pressing issue on the industry, which is the need to develop effective drugs swiftly. But developing a new drug is easier said than done. While currently there is no decisive treatment for this disease, the pharmaceutical industry is assisting governments to address the COVID-19 needs that are yet to be met, from research and development measures on potential treatment strategies to balancing the supply chain of medications in the time of crisis. Additionally, according to WHO, pharmaceutical sectors are struggling to maintain natural market flow; as the recent pandemic affects access to essential medicines at an affordable price, which is the main goal of every pharmaceutical system.

The techniques which work on the fundamentals of artificial intelligence provide great benefits in the several phases of drug development, such as identifying targets molecules, modelling of molecules, and improving their molecular properties. It also plays a pivotal role in designing clinical trials for patients, hence, optimizes the strategy for making decisions (Wu et al., 2007). “Open Targets” is a new application designed to study the relationship between drug targets with diseases and the way genes are linked to diseases.

**3.3 Digitization of patient records enabled training of AI algorithms making patient treatment easier.**

The digitization of patient records opens up rich opportunities for medical practitioners, search capabilities to access and process patient data instantly, automatic reminders to prevent prescription errors, enhanced exchange of knowledge through the medical staff, and increased clarity by providing both accurate and legible recording of the condition of the patient.

A Harvard Business Review study, showed how Paschalidis and his team in Australia worked on a project in 2017 in which they used electronic health records (EHRs) and machine learning to predict hospitalizations for diabetes and heart disease. Using this approach, the group found that with an accuracy rate of up to 82 percent, they could predict hospitalizations around a year in advance.

A successful research on Electronic Medical Records (EMRs) was a great achievement in Digitization for healthcare, they were mainly implemented as a digital health tool in hospitals to enhance patient care, but over the past decade, research works have introduced EMR data in clinical trials and omics studies to improve translational potential in drug production. An EMR is a digitized record of a medical incident recorded in a medical setting either before or after a meeting by a medical professional. For example, part of an EMR could be the results of a blood test performed at a hospital. The EMR also contains clinical notes made by the doctor during a routine check-up at a nearby clinic.

In a position paper entitled, "The coming age of artificial intelligence in medicine," summarized the results of a panel discussion conducted at an AI in Medicine (AIM) conference in 2007 in the Netherlands (Patel et al., 2009) . The authors focus on the maturity and effect of AI research on the field of medicine and have so far attempted to describe the influence of AI in medicine. The authors conclude that one indicator of AI's progress in medicine is that Target techniques are becoming more integrated and not clearly evident as such within applications. The question being asked has changed from "does the system operate?" to "does it also support the system? This, according to the authors, suggests that in clinical practice, AIM-based solutions are being implemented (Patel et al., 2009). According to the authors, machine learning research is becoming more important for the future due to the prevalence of Electronic Medical Records (EMR), medicine is now a data-rich quantitative area and such research is important to make sense of this data and to establish discovery-support systems that support the work of a human doctor (Patel et al., 2009).

# **4. AI Risks and Limitations**

While AI has an extensive potential to help redefine the pharmaceutical industry, the adoption itself is not as easy as it may seem. For many pharmaceutical companies, AI still seems like a “black box” because of its newness and esoteric nature. According to Dr. Robert Mittendorff of Northwest Venture Partners in a Topbots article, one significant challenge to AI is the lack of a collection of data sets which would help in training the system to carry out operations. Also, the needed IT infrastructure is not available in the companies. This is because most IT applications and infrastructure currently in use at the laboratories were not developed with Artificial Intelligence in mind. AI technology is expensive, so companies have to allocate more capital to upgrade their system.

Moreover, the success of AI depends solely on the availability of an extensive amount of data because the system uses them for subsequent training and learning. Access to data from various database providers can lead to extra costs, and the data needs to be of high quality to ensure accurate result prediction. Despite all these limitations, AI is already redefining the industry. In a few years from now, artificial intelligence would be a basic, every day, technology.

With digitization of health records there is a feasibility issue with Data mining in EMRs, established machine learning tools can, however, help solve these bottlenecks in EMR mining to unlock new drug development approaches. When incorporating EMRs into healthcare provider networks, there are concerns with implementation and process disruptions. Funding, necessary staff, and up-to-date digital technology are required for implementation. This implementation will only benefit institutions and geographic regions with ample resources. However, implementation is not financially viable for many smaller-scale practices. For regions where institutions do not have access to technologies that allow EMRs to be manufactured, stored, and shared. Although researchers are still working on it to eliminate the gap and build a bridge between small and large providers of healthcare. In addition, to complete record documents, the workflow is disrupted when clinicians and other medical professionals need to change their workflow according to EHR. In the medical community, EHRs are notorious burdens to professionals, they need to type constantly on their computer rather than caring for their patients. The Healthcare Industry is not able to see long-term benefits, rather they use EHRs for financial and administrative purposes. Although there are no global guidelines on what can be included in an EHR, billing codes are mostly used for administrative purposes.

In target recognition, the AI algorithm may have difficulty differentiating between possible positive and negative biological effects on the course of the disease or predicts the drug targets that scientists know will probably have major side effects. The best way to assist the machine is by selecting a method to filter out particular groups of drugs or goals here. While this is a necessary step for the AI system to understand, biologists find that certain drug goals are poor choices. However, this phase of human refinement is critical for helping the AI system learn and thus guaranteeing the best science performance. Artificial intelligence's role, whether applied to identifying targets, developing new drugs, or repurposing old ones, is to enhance, not substitute, the abilities of scientists. In deciding the data to be used in machine learning and in providing expert assessment of the outcomes, scientists play important roles, both for additional precision and nuance. Since scientific evidence may be contradictory examples as in animal models.AI systems are often not yet sophisticated enough to pick up on such context, but yes they are definitely in the developing phase.

# **5. Implications in the Society**

Drug development partly depends on biomedical data. There are a lot of complex interactions between molecules, so to get some meaningful output; AI is needed.One of the reasons for the high cost of drugs is because of the many false starts, which could occur at any of the development process stages through to clinical trials. Artificial intelligence is changing several aspects of our lives and deploying solutions that address both simple and complex problems. Research has shown that artificial intelligence can improve the efficiency of the drug development process and collaboration of pharmaceutical industry giants with AI-powered drug discovery firms. (Ekins et al., 2019).

In the field of digitization in AI to help deliver effective cancer care, individual full genome data could be a regular practice to be used as part of EHRs. Furthermore, Open EHR is also a forum that puts together industry standards, clinical models, and applications intended for healthcare data science solutions. In terms of the nationwide systematization of digital medical documents and the high standard of EHRs, Estonia is one of the world's leading countries. By the end of 2014, Estonia had consolidated access to EHRs through a single portal, enabling more than 99% of the population to display their own medical records. This is an excellent figure.

EMRs have been a vital source of data in advancing healthcare in the past decade. EMRs are particularly desirable in the sense of AI because there is a large amount of rich and variable types of data that can not be manually processed. EMRs have exciting potential for impactful medical applications in the field of biomedical science, but only if actionable biomedical conclusions can be reliably extracted.

Pharmaceutical companies are encouraged to maintain drug monitoring to track, assess, and avoid adverse drug effects that cause medical and financial pressures after a drug is subjected to clinical trials and is approved for market launch. By constantly mining EHR narratives, such surveillance can be achieved cheaply and effectively. This initiative encouraged further work to build even more robust ML techniques for the extraction of ADEs from oncology EMRs and reflects the overall trend towards CRF, SVM, and random forest models in the pharmacovigilance space.

It is believed that the best way for AI to become smarter, to be accepted by scientists, and thus to have an effect is to have this technology built by interdisciplinary teams while they test theories in the laboratory to make the systems more capable of learning. Through checking their predictions and assumptions, allowing certain feedback loops to strengthen the algorithms would also increase results in artificial intelligence.

Moreover, patient privacy is a major concern when it comes to data collection and research in Pharmaceutical research. Data provenance is important for ensuring data quality and promoting trust (Heidelberg et al., 2020). It is the key to prevent misuse of patient’s information for purposes such as fraud and ensure safety of the public. In order to ensure safety of all persons and increase trust in company products, every patient should be forewarned about the data that their medical institutions are sharing with companies, and should be able to have a say in which places can collect their personal data and how it may be used, with their right to deny all use of their health records if they wish. Patients should also receive full transparency on how their personal information will be used and its benefits should be accessible to them. These guidelines would ensure that AI uses data that is approved of by patients, and addresses the ethical concerns that follow the expansion of such technologies.

Through making predictions in more novel areas of biology and chemistry, artificial intelligence will further extend the drug research field. By following ethical guidelines, a company can gain their consumer’s trust and satisfaction of patients and doctors who use their products. AI can help to recognize relevant information faster by extracting text from scientific papers and to connect biomedical entities, such as medicines and proteins, often with simple databases and medical texts making it more reliable than ever before.

**6. Future Work**

Although it is not an easy task to predict the future of AI in drugs, its implementation paves a path for a more efficient drug research process. It also needs a lot of work in terms of expanding data sets, and training AI with the correct data, it is certain in coming years it will be possible to perfect AI for a more widespread use in pharmacology. From our research, it is evident that the areas of improvement from which big pharma can benefit the most is an expansion of databases for individual business processes and more accurate predictive capabilities of AI.

With an exponential growth in database systems and technology in recent years, there also remains a lot of grey space in terms of government regulations to monitor the ethics of public data collection and distribution, making it difficult to trust the systems and their decisions without involving a human in the process. It is quite possible that with increasing regulations and protocols these decision-making systems wouldn’t need human intervention at all. Until then AI will only be employed for tasks such as clinical trial recruitment, and collection and processing of data for collecting information. Full AI-based pharmaceutical research and development process is still a distant yet attainable goal.

**7. Conclusion**

While there are many ways in which AI can be used within the pharmaceutical industry to improve the ways doctors work, it can also improve the sector, to promote a far better health experience and system. The advancement of AI serves as a solution to reduce challenges faced by pharmaceutical companies, impacting the drug development process along with the overall lifecycle of the product, which could explain the increase in the number of start-ups in this sector (Chan et al., 2019). The healthcare sector is facing numerous challenges, such as the increased cost of drugs and therapies and society needs significant changes in this area. Using the latest AI-based technologies will hasten the time for the products to come to the market, improve the quality of products and the overall safety of the production process, and provide better utilization of available resources along with being cost-effective ( Jämsä-Jounela, 2007).

The most significant worry regarding the adoption of the technology is the job losses that would follow, and the strict regulations needed for the implementation of AI. However, these systems are intended only to simply the job and not to completely replace humans (T.H. Davenport and R. Ronanki, 2018).AI can also aid quick decision-making, which leads to faster manufacturing of higher quality products. AI can also contribute to establishing the safety and efficacy of the product in clinical trials,as well as ensuring proper positioning and costing in the market through comprehensive market analysis and prediction. Although There are no drugs currently on the market developed with AI-based approaches and specific challenges remain with regards to the implementation of this technology, it is likely that it will become an invaluable tool in the pharmaceutical industry in the near future.

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