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# Drug Discovery using Machine Learning Techniques in Healthcare

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**ABSTRACT:** The application of machine learning (ML) will become more widespread in the healthcare industry as a result of the increasing complexity and volume of data. Payers and providers of medical care and corporations in the life sciences industry are already utilizing ML in a variety of forms. The most common kinds of applications include making diagnoses and treatment recommendations, encouraging patient participation and adherence, and performing administrative duties. Even though machine learning can perform healthcare activities as well as or even better than humans in many cases, implementation issues will delay the large-scale automation of healthcare professional occupations for a considerable amount of time. Concerns regarding the ethical implications of applying machine learning in medical settings are also brought up.

**KEYWORDS:** Machine learning; Healthcare; Industry 4.0; Drug discovery;

## I. INTRODUCTION

The influence of machine learning can be seen in domains as disparate as information technology, agriculture, insurance, the financial industry, and even marketing. Because of this, our way of life is undergoing significant change[1]. Machine learning is having one of the most prominent effects in medicine. Machine learning is being used in the healthcare industry in a way similar to combining the processing power of millions of human minds to speed up and rethink things like diagnosis and medicine[2]. We will have to change the way we live now, but as a result, the average human lifespan will go up. Using algorithms that are based on ml has made it easier to come up with new medicines[3,4]. People have a lot of complaints about the healthcare industry, and one of the most common is that there aren't enough drugs on the market to treat the growing number of illnesses. Those who believe in conspiracies say that this is happening because pharmaceutical companies don't want to risk losing their patents and would rather focus on selling off their old stock[5]. They would tell you that there are waitlists for treatment. It costs an average of \$2.6 billion to research and develop a brand-new drug. The vast majority of this money is spent in the early stages of development, which can take a long time before treatments are shown to the right people for approval. After testing more than 10,000 different chemical compounds for a single treatment, the number of compounds will be cut down to ten or twenty, more tests will be done, and one or two compounds will be shown to be the most effective. In addition to the diseases these systems are meant to treat, their research is also done on thousands of different compounds[6-8]. This is done so that new ways of making drugs can be found. This is a hard and time-consuming process that gives wrong results and wastes a lot of time. In their search for a new blood pressure drug, scientists have ruled out the use of thousands of different chemicals. They may have accidentally thrown away a possible cure for a life-threatening illness like cancer, malaria, AIDS, or another disease. We can only hope that machine learning will change this industry by making drug development faster and cheaper. This could lead to better medicines being sold on the market in the long run. Everyone would come out ahead in this situation[9]. One of the biggest drug companies in the world, Pfizer, is working with IBM Watson, a computer program that uses machine learning to find the next generation of treatments. Other giants in the pharmaceutical industry are using these methods, which are on the verge of bringing in a new era of innovation in how new drugs are found[10].

## II. LITERATURE SURVEY

Multiple myeloma (MM), the second most common form of blood cancer, has been linked to a number of severe side effects, some of which include anaemia, high calcium levels, kidney failure, and damage to the bones[11]. Even though more and more effective medicines are being developed, the clinical prognosis of this incurable illness is still very

different depending on the patient and the MM. This is because there is currently no treatment available for the disease. In order for patients to have a high quality of life and a long lifespan, they need to be willing to cooperate with the individualized intervention that is being administered. Patients who have recently been given a diagnosis of multiple myeloma are in need of accurate prognostic indicators in order to facilitate the development of an effective treatment plan for the disease[12-15].

It is very early in the process of creating diagnostic tools for lymphoid neoplasms that make use of artificial intelligence (AI)[16]. Medical professionals can use diagnostic tools such as these in order to assist them in determining what is wrong with lymphoma patients by examining tissue samples taken from those patients. People who have chronic lymphocytic leukaemia (CLL) often inquire with their physicians about whether their condition has progressed into accelerated chronic lymphocytic leukaemia (aCLL) or changed into diffuse large B-cell lymphoma. This is a common diagnostic question (Richter transformation, or RT). It may be challenging to diagnose CLL, aCLL, and RT solely based on the outward manifestations of these diseases[17-20]. We used diagnostic criteria that had previously been established to construct four biomarkers that could be used to track the progression or transformation of CLL using artificial intelligence. These biomarkers were developed by using the cytologic (nuclear size and nuclear intensity) and architectural (distance from cell to nearest neighbor) characteristics of the cells[21].

### III. GAINING A BETTER UNDERSTANDING OF DISEASES AND THEIR SYMPTOMS

BenevolentBio, a company based in London, has developed an advanced SI that uses machine learning to sift through massive amounts of data on various illnesses, symptoms, and causes of mortality and other topics[22]. Machine learning models are trained with data from patient records, clinical trials, research publications, and prescription data to generate a comprehensive study of the correlations between symptoms and diseases and the medications recommended to treat them. The information can be put to use by researchers so that they can investigate the connection between patient data and illnesses. This data helps researchers track potential pandemics and understand why certain diseases are more prevalent in certain cultures and demographics[23-25]. Additionally, it streamlines the process of discovering new therapies and detecting new illnesses. These days, hospitals are technologically advanced facilities, replete with high-tech equipment and trained staff who understand how to use it. The slow but steady adoption of automation across the healthcare industry paves the way for a future in which accurate and prompt diagnoses will be possible. The process of diagnosing illnesses could be completed more quickly and accurately if machine learning were utilized[26-30].

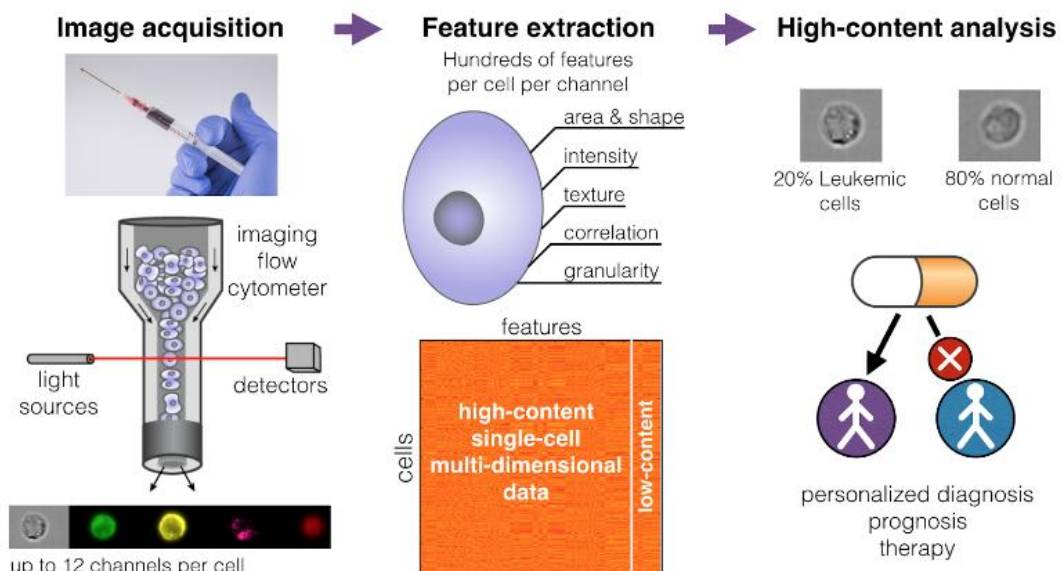


Fig. 1. Personalised diagnosis of high content single cell

Imaging flow cytometry also referred to as IFC, is a method that can take multichannel pictures of hundreds of thousands of single cells in just a few minutes. This can be accomplished in the process of flow cytometry. The implementation of deep learning algorithms at IFC is helping to foster the growth of a paradigm shift away from low-information-content analysis and toward high-information-content investigation. We are anticipating a massive variety of applications, any one of which may be modified for use in clinical settings[31].



IFC is currently utilised more frequently in research as opposed to actual clinical practice at this point in time. Because it is susceptible to variation, manual adjustment, and interpretation, we believe that the data analysis will prove to be the most challenging obstacle to overcome. It's possible that solutions can be found through the use of machine learning techniques. Additionally, standardization of the IFC is required, and as part of this requirement, standard operating procedures and standardised hardware performance quality control should be included. Additionally, there is a need for standardisation to take place[32-35]. Utilizing fluorescent markers is a common clinical technique used to determine the total number of different white blood cells (WBC) that are present in human blood. This can be done in several different ways. WBC counts are beneficial diagnostic tools for physicians because they can provide insight into a wide variety of illnesses. We present a novel method for recognizing WBC that is based on machine learning, does not require the use of labels and does not require any special training. We will develop a method that utilizes open-source software and will seamlessly combine the recorded images from the instruments with machine learning. FlowML will make it possible to identify WBC in a quick, cost-effective, and highly accurate manner, while simultaneously preserving the availability of marker channels to address other biological challenges. In addition, FlowML will keep marker channels open so that they can be used to address other biological problems. It is possible to perform a WBC count in clinical settings that do not require labeling, and this is sometimes done.

The majority of the approximately 50 petabytes of data that are generated by hospitals each year is made up of medical pictures and meta-data. The hospitals themselves produce this data. Sadly, they do not possess the resources that are required in order to collect and evaluate all of this information. When data was collected, it was not uncommon for the information to be misplaced or stored in a data centre that the hospital had constructed on its own initiative. The situation has undergone a significant shift as a direct consequence of the proliferation of machine learning. With the assistance of advanced machine learning algorithms, it is now possible to examine all of the medical data accumulated over the years to gain new perspectives. This can be done in order to gain new insights. The information that was gained is being put to use to enhance our understanding of the human condition and to broaden our knowledge of a number of different diseases[36].

For example, in 2016, a team of researchers from the United Kingdom analyzed a large number of eye scans to develop a system capable of accurately identifying a variety of eye diseases. The finished product was a diagnostic tool with an accuracy rate of 94 percent when attempting to identify the condition. This tool is currently being implemented as a primary treatment to direct patients to the appropriate department. When it comes to medicine, experience is the best teacher, and if a doctor has encountered a specific issue more than once, they are more likely to be able to identify it in the future. This task can be finished by a machine in hours, whereas it may take a human doctor their entire career to go through enough eye scans to fully comprehend this part of the human anatomy. A machine can finish this task in a matter of hours. It is also possible to use these technologies to process the data obtained from CAT scans, MRI scans, and data obtained from other types of scans. It is truly incredible to think that such a significant amount of progress has been made in such a short period[37].

Machine learning is also being used in the healthcare industry to reliably forecast the likelihood of miscarriage, stillbirth, and other pregnancy-related issues. This is accomplished by analysing data from thousands of pregnancies, both successful and unsuccessful, and generating a set of probabilities based on that data. The utilization of data allows for the successful completion of this task.

These systems can analyze anything from the results of an HSG to a woman's age, weight, and medical history, as well as any previous births or miscarriages the woman may have experienced. When you input information about a new patient into this system, it has the potential to provide a set of recommendations that are based on the outcomes of previous patients. This will increase the likelihood of a healthy baby and mother, as well as a successful birth.

#### IV. VIRTUAL ASSISTANTS

In addition to this, machine learning is currently being utilised in the process of bettering healthcare delivery systems. Because of this, there is no longer a need for ongoing assistance from specialists, which paves the way for a future in which a virtual assistant will provide assistance[38-42].

##### a. **Transcription**

Virtual assistants equipped with machine learning capabilities can be taught to transcribe conversations that take place between medical professionals and their patients. When working with software of this kind, you won't have to depend in any way on specific dictation or prompting words at all. Before being presented to the attending physician for review and signature, the clinical note has been accurately formatted and transcribed in its entirety. The attending physician then reviews the document. After that, it is included in the patient's existing electronic medical records, which are now being kept electronically.

As an illustration, Robin Healthcare has created a medical transcription assistant that goes by the name of Robin. This assistant uses machine learning in order to transcribe pertinent clinical information based on a conversation that is taking place in real-time between a doctor and a patient. The conversation is taking place between the doctor and the patient. For doctors to make use of this transcription tool, they must install speaker systems in the examination rooms where they see patients. The noises that are produced by the device are transcribed by an algorithm that is built into the device itself while the clinicians are engaged in interaction with the patients.

**b. The Application of Electronic Medical Assistants in Order to Facilitate Improvements in Patient Health**

The elderly, patients who suffer from chronic conditions, and people who live in remote areas with limited access to healthcare are the groups that stand to benefit the most from the use of virtual assistants. They are also the groups that are most likely to benefit from the use of virtual assistants. Patients may feel less embarrassed and be more honest with a virtual assistant rather than a human assistant because they are afraid of being judged by the human assistant. Virtual assistants are also less likely to make patients feel like they are being watched. This is an additional factor that should not be overlooked.

**c. During Recuperation and Discharge, Patients have Access to the Assistance of a Virtual Nurse**

According to the Harvard Business Review, by 2026, the utilization of virtual nursing assistants will result in cost savings in the healthcare industry, equaling twenty billion dollars. In order to accomplish this goal, the amount of time that registered nurses are required to spend providing care for their patients will be decreased.

In addition to the financial benefit, there are additional advantages to utilising the services of virtual nurses. It is not uncommon for there to be an insufficient number of nursing staff members compared to the number of duties expected of them, which places the patients' health in jeopardy. When a nurse's workload is higher than the level that is recommended, the risk of an adverse event occurring to a patient increases by approximately 30 percent. This is because a nurse's ability to pay attention to each patient is diminished when their workload is too high. The strain that is placed on human workers is alleviated by virtual nurses' ability to automate laborious tasks.

Patients recovering from surgery may choose to have a virtual nurse monitor them to ensure that they do not experience any further deterioration in their condition. It can take patients' vital signs, provide answers to questions posed by patients, and schedule appointments with medical professionals. Because virtual nurses possess the communication skills necessary to empathize with patients, they are available around the clock, seven days a week, and twenty-four hours a day. They can determine when something has gone wrong with the healing process and immediately inform the doctors of this fact because they are based on algorithms for machine learning. Within virtual nursing, one of the most common specialties is that of the discharge nurse. There is a problem with avoidable readmissions in many hospitals, which could be avoided if improvements were made to the discharge procedure. These readmissions could be avoided in many cases.

**V. USING OLD DRUGS TO FIND NEW CURE**

In the medical field, the application of machine learning can help discover new treatments hidden within the chemical databases that are at the disposal of pharmaceutical corporations, but it can also help in the discovery of how tried-and-true medications can be used to treat current conditions.

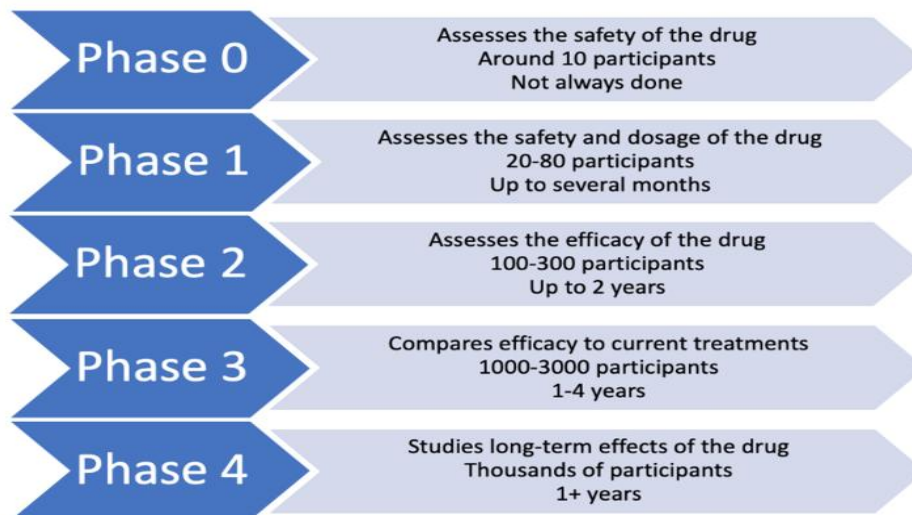


Fig. 2. Phases in Drug Discovery

One of the most common functions of pharmaceuticals is to act upon the biological processes associated with disease progression. Because tumours result from uncontrolled cell growth and replication, it is possible that components of the signalling that tells cells to grow and replicate could be used to target and restrict the growth of tumours. This would be the case due to the fact that tumors are the result of uncontrolled cell growth and replication.

During phase 0, only low doses of the treatment are administered to a select group of healthy volunteers in order to ensure that the treatment is risk-free. During the first phase of the study, patients are given



progressively higher doses of the treatment to establish the maximum amount of the drug that they can withstand before beginning to experience negative side effects. Phase 0 is the preliminary stage of the clinical trial, and it is immediately followed by phase 1, which is the concluding stage. During phase 2, researchers look into the potential negative side effects of the treatment while also attempting to establish whether or not the treatment has any positive effects. Patients who are participating in Phase 3 trials are given a random assignment that determines whether they will receive a new drug, a placebo, or a control. At any given point in time, neither the patients nor the scientists are aware of who is assigned to which group.

Daniel Cohen is an essential part of the creative method that this group developed, and he plays a pivotal role in it. He is the founder of Pharnext and serves as its Chief Executive Officer. Pharnext is a company that uses machine learning technologies in the healthcare industry to evaluate the effects of existing pharmaceuticals and combine them to develop new treatments. The authors expressed their self-assurance by claiming, in an interview with Fortune Magazine, that "with 50 medications, we can heal anything." If this company's approach is the right one, the treatment for cancer might already be tucked away in one of these countless possible combinations. Even if this method has some flaws, it is abundantly clear that machine learning is the way of the future and is propelling the industry forward at a dizzying rate. This is the case regardless of the validity of the method in question. This movement toward providing medical support virtually has also been helped along by technological factors such as the widespread availability of cellphones and internet connectivity. This is a trend that has been growing in recent years. According to ResearchAndMarkets' projections, the market for virtual medical assistants will reach \$1.73 billion by 2024. This would represent a compound annual growth rate (CAGR) of 34.6 percent between 2019 and 2024. The progression from low-content analysis to high-content analysis in IFC will be sped up by user-friendly procedures that are also robust and standardised, promoting machine learning, particularly deep learning.

## VI. CONCLUSION

Computing in the cloud also has the ability to sidestep issues that are brought on by insufficient underlying computational infrastructure. These advancements are necessary for bringing practical IFC applications into the clinic. This will make it possible for IFC to be used as a diagnostic tool and a tool for prognosis and therapy. The concept of treating diseases with different medications is not a brand-new one, but it is becoming an increasingly widespread practice. By enlisting the assistance of machine learning, Pharnext may be able to produce more of these combinations of medications at a significantly faster rate than what has been achieved in the past. Both chemotherapy and the treatment of HIV and AIDS use multiple medications combined with one another.

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