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Internet of Nanothings (IoNT) and Machine Learning (ML) – Innovations in drug discovery and Healthcare system

R Senthil Prabhu [1, *], D SabithaAnanthi, D Umamaheswari [1] and S Rajasoundarya [2]

[1] *Department of Pharmaceutics, College of Pharmacy, Madurai Medical College, Madurai-20. Affiliated to The Tamilnadu Dr.M.G.R. Medical University, Chennai-32, Tamilnadu.*
[2] *Department of Computer science, University of Texas, El Paso, USA*

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Abstract

The IoNT offers a medium to connect various nanodevices with the help of high speed networks. Using this technology nanodevices can be deployed along with other advanced technologies such as cloud computing, big data and ML. Many tedious tasks can be taken over by linked inanimate objects and better availability of information using IoNT-ML. This technology has shown great promise in improving efficiencies across numerous pharmaceutical and healthcare industries with high quality and vast datasets. It has the potential to foster innovation while simultaneously improving productivity and delivering better outcomes across the value chain. IoNT-ML can significantly improve the value proportion of pharmaceutical companies by driving innovation and the creation of new business models. This technology can be implemented in almost every aspect of the pharmaceutical industry, right from the drug discovery and development to manufacturing and marketing. This review discusses the principle of ML and its various applications in healthcare sector.

Keywords: Internet of Nanothings; Machine Learning; Artificial Intelligence; Applications

1. Introduction

Machine learning (ML) is a branch of artificial intelligence (AI) and computer science which focuses on the use of data and algorithms to imitate the way that humans learn, gradually improving its accuracy. Machine learning is an application of AI that provides systems the ability to automatically learn and improve from experience without being explicitly programmed.ML comprises of designing efficient and accurate prediction algorithms [1]. The IoT is a collective of sensors networks, data collectors and transmitters that send data from multiple entry points through the cloud into a centralized location. Once all this data has been brought together in one place, advanced algorithms, artificial intelligence processes such as ML, deep learning (DL) or artificial neural networks (ANN) analyse the data without human input and spot trends, patterns and anomalous data points by comparing historical data with the real-time data [2]. This enables the IoT to be self-sufficient, without the need for human interaction, unless the system alerts an operator to a problem which it finds through its analyses. The Internet of Nanothings (IoNT) is a miniaturized version of these systems which employ very small sensors and data network hubs to transmit data over long distances [3]. This interlinking of IoNT and ML provide enormous applications in the healthcare sector and the pharmaceutical industry. Due to furtherance in machine learning and artificial intelligence, several classifiers and clustering algorithms like K-nearest, Decision Tree, Random Forest, Support Vector Machine (SVM), Naive Bayes [4] were accustomed to treat and

*Corresponding author: R Senthil Prabhu
Department of Pharmaceutics, College of Pharmacy, Madurai Medical College, Madurai-20.Affiliated to The Tamilnadu Dr.M.G.R. Medical University, Chennai-32, Tamilnadu.

develop the dosage forms for the health problems like liver cancer, chronic kidney, breast cancer, diabetes, and heart syndrome [5]. The Machine Learning has broader applications in various fields [6] as shown in the figure 1:

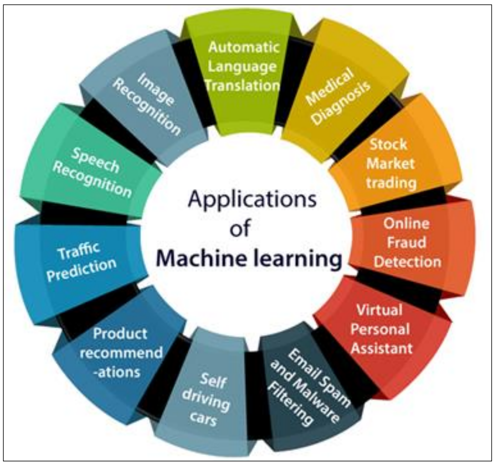

Figure 1 General applications of Machine Learning

2. Principle of Machine Learning

Machine learning can be divided into three main categories, namely, supervised learning, unsupervised learning, and reinforcement learning.

2.1 Supervised Learning

It uses an algorithm that requires external help. It is based on the same principles as a standard fitting procedure. It tries to find the unknown function that connects known inputs to unknown outputs. This desired result for unknown domains is estimated based on the extrapolation of patterns found in the labelled training data [7].These algorithms include two main categories: (a) classification (discrete modelling) and (b) regression (continuous modelling). Both categories are predictive modelling techniques; the only difference is their target variables [8][9].

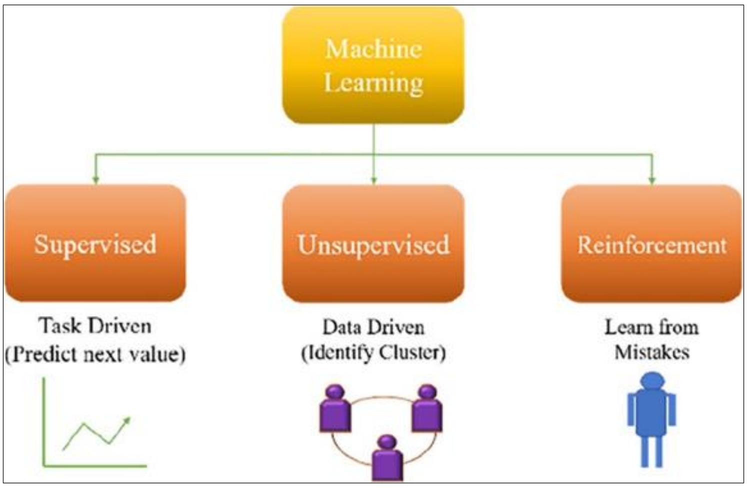

Figure 2 Principle of Machine Learning

2.2 Unsupervised learning

This is an ML algorithm that learns some characteristics of input information. After providing anew database, it utilizes formerly learned characteristics for the identification of the class of data. It is mostly preferred for feature reduction also for clustering. Unsupervised learning further categorized into clustering (k-means [10], hierarchical and fuzzy-c-means) and dimensionality reduction (Principle Component Analysis PCA, Independent component analysis ICA and Singular value decomposition SVD).

2.3 Reinforcement learning

It is based on decision concept learning. In this learning, actions are based as per the decision taken so that the results become more valuable at the output or desired favourable condition [11]. However, the learner doesn't have prior information of data. After providing the situation, it learns to decide which action to be taken according to the given situation. The present and future situation is affected by the learner's decision i.e. action taken [12].

3. Applications of IoNT-ML

ML, the most fundamental form of AI, has started infiltrating the medical field, and it seems that machines can play a crucial role in improving our health. A study of over 50 executives in the healthcare sector by TechEmergence revealed that by 2025 AI will be adopted on a broader scale. The improvement of data technologies, including storage size, computational power, and data transfer speeds has enabled the widespread adoption of ML in healthcare field [13].

3.1 Improving Medical Diagnosis

The idea behind ML in pharmaceutical field is not to replace the doctor but to enhance his/her medical expertise. AI programs take the entire knowledge that a physician has, which is everything they learned in medical school and while training besides their experience in treating patients, and scales it to unprecedented levels. In the realm of image processing, most techniques rely fundamentally on DL and specifically in ANNs. Modern techniques utilize improvements to ANNs in the form of convolutional neural networks (CNNs) to boost performance when classifying images [14]. Object detection in medical images are performed by using some form of CNNs [15]. Cerebral microbleeds were detected from susceptibility weighted MRI scans. 3D CNNs were used and also replaced the candidate detection stage with a CNN, proposing a two stage approach. The improved results with 3D CNN were obtained when compared to various classical and 2D CNN approaches [16]. Modernizing Medicine, a program that collates data from 3,700 providers and 14 million patient visits, is easily able to diagnose a rare condition, scroll through the available treatment options, and write a prescription within seconds. This saves time, which translates to greater efficiency and lowered costs. IBM recently acquired Merge Health Care, a firm with a repository of more than 30 billion unique medical images, which will train WATSON to diagnose diseases. Radiologists in China, which is home to the highest number of lung cancer patients in the world, have started using AI programs to improve medical diagnosis in reading x-rays and CT scans and identify suspicious nodules and lesions in lung cancer patients.VFI5 is a machine learning algorithm for the diagnosis of cardiac arrhythmia [17]. Weight gain biomarkers were identified by mass spectrometry and most discriminant features were determined by a machine learning approach using Random Forest algorithm [18].

3.2 Better Patient Care

Physicians often have a difficult time keeping track of signals from test results, charts, and other metrics. The task of integrating and monitoring all of these data for a huge number of patients while making real-time decisions is also equally difficult. Medline(R), EBM Reviews, Embase, Psych Info, and Cochrane Databases were focusing on human studies that used ML to directly address a clinical problem [19].Recently a team from MIT's Computer Science and Artificial Intelligence Laboratory (CSAIL) created a program called ICU Intervene that takes massive amounts of intensive care unit (ICU) data and finds possible treatments for various symptoms. The AI system makes real-time predictions with the knowledge from past ICU cases to make recommendations for critical care besides explaining the reasons behind the decisions. This machine learning program could help physicians in the ICU, which is a high-demand, high-stress environment [20].

3.3 Predicting the Next Epidemic

The Malaysian start-up, Artificial Intelligence and Medical Epidemiology (AIME), has managed to give users the exact location and date of the next dengue outbreak, 3 months ahead.The program also recommends anti-dengue measures for the infected area within a 400-meter radius. The system from AIME analyzes public health data along with data from other sources like wind speed, weather, allocation's proximity to massive water bodies, previous outbreaks and anything that influences the behavior of mosquitoes responsible for carrying the disease. The outbreak of COVID-19 Coronavirus, namely SARS-CoV-2, has created a calamitous situation throughout the world. ML and Cloud Computing can be deployed very effectively to track the disease, predict growth of the epidemic and design strategies and policies to manage its spread. The ML models are built to make a good advanced prediction of the number of new cases and the dates when the pandemic might end.In a cloud based environment as in Fig 3, the government hospitals and private health-centers continuously send their positive patient count. Population density, average and median age, weather conditions, health facilities etc. are also to be integrated for enhancing the accuracy of the predictions [21]. ML methods including linear regression, linear kernel support vector machine (SVM), radial kernel SVM [22], polynomial kernel SVM, and decision tree were used to predict the spread of COVID-19 [23].

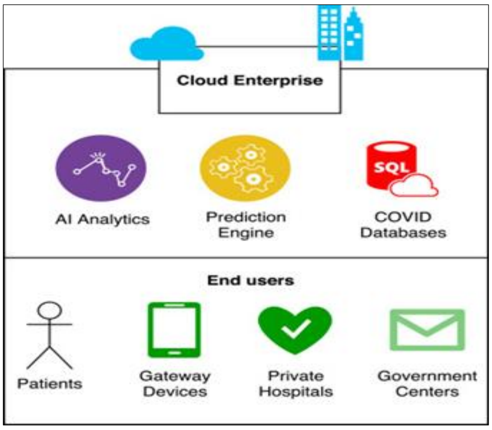

Figure 3 Cloud based AI framework for COVID-19 related analytics

3.4 Helping Farmers Fight Famine

Recently, researchers from Makerere University in Uganda teamed up with experts to start the Mcrops Project in their quest to develop a ML system that can fight cassava diseases. Using cheap smartphones, farmers can take pictures of their plants and use computer vision that can identify signs of the four important diseases responsible for demolishing cassava crop. So farmers know if they need to rip their crops or spray them. The system has been able to detect cassava diseases with 88% accuracy. Mcrops also uses the images to find out patterns in disease outbreaks, which allows officials to halt epidemics that can possibly lead to famine. The team is now planning to use the technology to study banana diseases and automate identification of crop pests.CNN classifier detects more number of diseases with high accuracy. Other classification techniques in ML like decision trees, Naive Bayes classifier may be used for disease detection in plants and in the sense of helping farmers an automatic detection of all types of diseases in crops [24][25]. The Random Forest Regression model was trained on past weather data and can forecast the attack of diseases on Mango fruit crop using past weather data and crop production which can be used to calculate disease outbreak probability [26]. Weather data from past history is used to train the machine learning model to perform more accurate wind speed predictions. It aims on forecasting the wind speed of a particular area and alerts the farmers through short message services about those forecasted disasters in order to reduce the impact of those future wind disasters on crops and agricultural fields [27]. By using Decision tree algorithm, selection of the crop based on the existing data to forecast a suitable harvest for cultivation by appropriate methods. The prediction will help to the farmers' crop choice for drought-prone areas before cultivating onto the agriculture field [28].

3.5 Combating Cancer

The best way to spot cancer early is through screening. DeepMind, owned by Alphabet and IBM have been using their technology to fight this threat. DeepMind has teamed up with renowned clinical partners to train its AI to plan cancer treatments by identifying regions of healthy tissue from tumours in neck and head scans. IBM's Watson can analyze images and evaluate patient notes to identify tumours accurately in up to 96% of cases. Currently, the system is being used to help diagnose lung, breast, cervical, colorectal, prostrate, gastric and ovarian cancers. Major types of ML techniques including ANNs and DTs have been used for nearly three decades in cancer detection[29]. The projects like Dialogue for Reverse Engineering Assessments and Methods (DREAM) help in bridging experiment with theory by challenging the research community with real data for predictive modeling and inferring cellular networks [30]. Different ML methods were used for Cancer susceptibility prediction of various types of cancer. Breast cancer susceptibility [31] was predicted by ANN and SVM, Multiple myeloma was predicted by SVM. Cancer recurrence was predicted by various ML methods such as BN, SVM [32], Graph based SSL algorithm for various types of cancers such as Oral cancer, cervical cancer and both colon and breast cancer respectively. Cancer survival can be predicted by ANN, Graph based SSL, SVM, BN, DT and SSL Co-training algorithm [33].

3.6 Drug Efficacy Detection

The success of personalized drugs largely depends on the ability to identify patient sub-populations, which can be facilitated with precise diagnostic tests based on biomarkers. With the huge amount of proteomics, metabolomics or genomics data, identifying the most effective biomarker is a complicated task. Huge amounts of patient Omics data are being accumulated. Unfortunately, there are no tools in place to extract the required information from the data.But with many machine learning companies rewriting the code for drug discovery, the implications will possibly be far ranging in the years to come. Benevolent AI, a leading AI company in the UK, uses ML for discovery of drugs and diagnosis of diseases. Their system recently successfully identified biomarkers in Amyotrophic Lateral Sclerosis (ALS) also known as Motor Neuron Disease (MND). The technology was used to review billions of sentences from countless scientific research papers and abstracts. Following this, they started finding direct relationships between the data and transformed them into known facts. These known facts were then curated by the system to develop many hypotheses against qualified criteria. The data might show that a particular protein upregulates a given gene which may not be directly related, propelling researchers to find drugs in an entirely different arena. Consequently, this model is able to find novel targets with data mining. The integrated pharmacogenomic data derived from 3D organoid culture models and network-based methods are used to develop an ML framework for the prediction of patient–drug responses. The biomarkers identified by this approach accurately predict the drug responses of colorectal cancer patients [34].

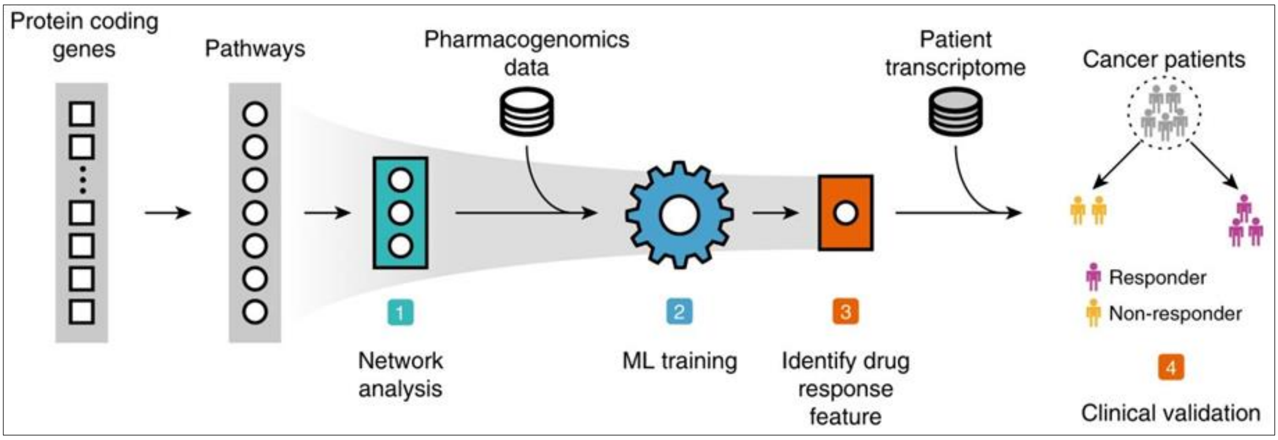

Figure 4 Overall framework for the *in silico* identification of drug-response biomarkers through network-based machine-learning (ML)

3.7 Facilitating Clinical Trial Process

The invention of IoNT, mobile and wearable have allowed people to convey important information effortlessly. This offers a way to capture relevant data from patients in a convenient and continuous way. The data captured is also precise, contextual and of high quality. Various ML approaches are available for managing large and heterogeneous sources of data, identifying intricate and occult patterns, and predicting complex outcomes. As a result, ML has value to add across the spectrum of clinical trials, from preclinical drug discovery to pre-trial planning through study execution to data management and analysis. Two broad approaches are available to improve participant retention and protocol adherence using ML-assisted methods. The first is to use ML to collect and analyze large amounts of data to identify and intervene upon participants at high risk of study non-compliance. The second approach is to use ML to decrease participant study burden and thereby improve participants' experiences [35].AiCure is a commercial entity focused on protocol adherence using facial recognition technology to ensure patients take the assigned medication. AiCure was demonstrated to be more effective than a modified directly observed therapy strategy at detecting and improving patient adherence in both a schizophrenia trial [36] and an anticoagulation trial among patients with a history of recent stroke [37]. Some commercial entities offer similar services, including Mendel.AI and Deep6AI [38]. With the improvement of data capturing technologies, the opportunity to leverage qualified data into an AI program will reduce patient risk and improve pharma's quality and time. Boston-based biopharmaceutical company, Berg Health, has started using its unique AI-based platform, Interrogative Biology, which enables them to identify biomarkers for drug discovery and keep a track on patient responses during clinical trials. They build models using the platform with the patient's own biology and monitor patient response on a biological level. Another example of machine learning in clinical trials is the ATACH-II app that provides assistance in assessing patient eligibility, pre-screening and randomization.

3.8 Revolutionize Pharmaceutical R&D

The world's leading drug companies are turning to machine learning to improve the hit and miss business of finding new drugs. GlaxoSmithKline unveiled a $43 million deal in the arena in 2017. Other pharma giants like Sanofi, Johnson & Johnson and Merck & Co are also exploring the potential of big data to aid streamline the drug discovery process [39].A fairly recent breakthrough in protein design uses generative Deep learning, more precisely, Generative Adversarial Networks (GANs) [40].

4. Conclusion

Machine learning is still in its infancy and will not be able to replace a doctor. But its ability to understand natural language like clinical notes and structured data like numbers and dates is being seen as the fourth industrial revolution, for which the pharmaceutical and healthcare industries will be the biggest beneficiaries. The ML algorithms have enabled the utilization of AI in the industry setting and in day to day life. The impact of ML methods in all areas of drug discovery and healthcare is already being felt, especially in the analysis of omics and imaging data.

Compliance with ethical standards

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Disclosure of conflict of interest

There was no conflict of interest what so ever because all the authors that appeared on the manuscript contributed significantly in making this publication processes a success.

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