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ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL INDUSTRY: A REVIEW

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Abstract:

Artificial Intelligence (AI) focuses in producing intelligent modelling, which helps in imagining knowledge, cracking problems and decision making. Recently, AI plays an important role in various fields of pharmacy like drug discovery, drug delivery formulation development, polypharmacology, hospital pharmacy, etc. In drug discovery and drug delivery formulation development, various Artificial Neural Networks (ANNs) like Deep Neural Networks (DNNs) or Recurrent Neural Networks (RNNs) are being employed. Several implementations of drug discovery have currently been analysed and supported the power of the technology in quantitative structure-property relationship (QSPR) or quantitative structure-activity relationship (QSAR). In addition, de novo design promotes the invention of significantly newer drug molecules with regard to desired/optimal qualities. In the current review article, the uses of AI in pharmacy, especially in drug discovery, drug delivery formulation development, polypharmacology and hospital pharmacy are discussed.

Key words: *Artificial intelligence, Artificial neural network, Drug discovery, Drug delivery research*

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INTRODUCTION:

Artificial Intelligence (AI) is a stream of science related to intelligent machine learning, mainly intelligent computer programs, which provides results in the similar way to human attention process [1]. This process generally comprises obtaining data, developing efficient systems for the uses of obtained data, illustrating definite or approximate conclusions and self-corrections/adjustments [2]. In general, AI is used for analyzing the machine learning to imitate the cognitive tasks of individuals. AI technology is exercised to perform more accurate analyses as well as to attain useful interpretation [3]. In this perspective, various useful statistical models as well as computational intelligence are combined in the AI technology [4]. The progress and innovation of AI applications are often associated to the fear of unemployment threat. However, almost all advancements in the applications of AI technology are being celebrated on account of the confidence, which enormously contributes its efficacy to the industry. Recently, AI technology becomes a very fundamental part of industry for the useful applications in many technical and research fields.The emergent initiative of accepting the applications of AI technology in pharmacy including drug discovery, drug delivery formulation development and other healthcare applications have already been shifted from hype to hope[5-6] .The uses of AI models also make possible to predict the in vivo responses, pharmacokinetic parameters of the therapeutics, suitable dosing, etc. [7] .According to the importance of pharmacokinetic prediction of drugs, the uses of in silico models facilitate their effectiveness and inexpensiveness in the drug research[8]. There are two key classes of AI technology developments [9]. The first one comprises the conventional computing methodologies including expert systems, which are capable of simulating the human experiences and illustrating the conclusions. from the principles, like expert systems[10] .The second one comprises the systems, which can model the mode of brain functioning employing the artificial neural networks (ANNs). In specific, various ANNs like deep neural networks (DNNs) or recurrent neural networks (RNNs) control the evolutions of AI technology. In Merck Kaggle[11] and NIH Tox21 challenge,[12] DNN issues show the greater predictivity than the baseline machine learning methodologies[13]. The machine learning employs suitable statistical methodologies with the capability to learn with or devoid of being unequivocally programmed[14]. In addition, de novo design promotes the invention of newer drug molecules with regard to optimal or desired qualities. In the current review article, the uses of AI in pharmacy, especially in drug discovery, drug delivery formulation development, polypharmacology and hospital pharmacy are discussed.

CLASSIFICATION OF AI:

AI can be classified into two different ways: according to calibre and their presence [15-16]. According to their ability, AI can be categorized as: i) Artificial Narrow Intelligence (ANI) or Weak AI: It performs a narrow range task, i.e., facial identification, steering a car, practicing chess, traffic signalling, etc. ii) Artificial General Intelligence (AGI) or Strong AI: It performs all the things as humans and also known as human level AI. It can simplify human intellectual abilities and able to do unfamiliar task. iii) Artificial Super Intelligence (ASI): It is smarter than humans and has much more activity than humans drawing, mathematics, space, etc. According to their presence and not yet present, AI can be classified as follows: i) Type 1: It is used for narrow purpose applications, which cannot use past experiences as it has no memory system. It is known as reactive machine. There are some examples of this memory, such as a IBM chess program, which can recognize the checkers on the chess playing board and capable of making predictions. ii) Type 2: It has limited memory system, which can apply the previous experiences for solving different problems. In automatic vehicles, this system is capable of making decisions there are some recorded observations, which are used to record further actions, but these records are not stored permanently. iii) Type 3: It is based upon "Theory of Mind". It means that the decisions that human beings make are impinged by their individual thinking, intentions and desires. This system is non-existing AI. iv). Type 4: It has self-awareness, i.e., the sense of self and consciousness. This system is also non-existing AI.

NEURAL NETWORKS AND ANNS:

The learning algorithm of neural networks (from input data) takes two different forms mainly. The classes of neural networks are as follows [17]. i) Unsupervised learning: Here the neural network is submitted with input data having recognised pattern. It is used for organizational purpose. The unsupervised learning algorithm uses 'Self Organizing Map' or 'Kohonen'. This is known as very useful modeling for the searching of relationships amongst the complex data sets. ii) Supervised learning: This kind of neural network is illustrated with the sequences of harmonizing inputs and outputs. It is used for learning relationship connection between the inputs and the outputs. It shows its usefulness in formulation to measure the cause and effects linking between input-output. It is the most frequently employed ANNs and is entirely linked with the back propagation learning rule. This learning algorithm is known as the outstanding methodology for the prediction as well as classification jobs. A simple mathematical processing unit called neuron is the main part of the neural network. Every input possesses an associated weight having relative importance and calculates the weighted sum of all the inputs as output. This output is then forwarded to another neuron after being modified by a transformation function. The whole processing is called a perceptron (a feed-forward system). A neural network having many neurons is organized into network architectures. The most famous and prosperous network is multilayer perceptron network. In this network system, the identical neurons are arranged in such a way that in one layer, the outputs are presented and in the subsequent layer, the inputs are presented. There are one or more secret layers, which can be introduced between the input and output layers. In theory, amount of secret layers can be attached according to solitary need. In practice, multiple layers are needed in case of applications with extensive nonlinear behaviour.

ANN is one of the computational modellings figured from hundreds of single units of artificial neurones associated with the constituents comprising the neural structure, which are known as processing elements as they participate in information processing [18]. ANN methodology presents a potential modelling procedure, in particular for the data sets of non-linear links commonly encountered in the pharmaceutical research [19-21]. For the model specification analyses, ANNs don't necessitate acquaintance of the data source. However, they frequently have many weightages that should be analyzed. They also necessitate larger training sets. Additionally, ANNs can mix as well as add in both the literature and the investigational data to resolve the problems. Recently, ANN models are being hybridized with other kinds of simpler models[22]. For example, a recently proposed combination of neural networks and logistic regression allow the generation of hybrid linear/ nonlinear classification surfaces and the identification of possible strong interactions that may exist between the attributes (also known as covariates in the Logistic Regression literature which define the classification problem. All these hybrid models perform reasonably well for a given set of databases. The prospective uses of ANNs in pharmacy are wideranged from the data analyses via the modeling of pharmaceutical quality control[23]. ANNs are also proved functional for the uses in the drug designing, especially in molecular modeling and QSAR[24]. It is also used in formulation optimization processes for dosage form designing and in biopharmaceutical analyses, such as pharmacokinetic modeling, pharmacodynamic modeling, in vitro-in vivo correlation analysis, etc.[25]

FUZZY LOGIC AND NEUROFUZZY LOGIC:

According to the conventional logic, proposal may be true or false. The hypothesis behind the logic lies either in or totally outside the "true" set. When the hypothesis lies within the "true" set, the membership function is denoted as "1" and when the hypothesis lies outside the "true" set, the membership function is denoted as "0". The basic concept of fuzzy logic is promoted by Lotfi Zadeh in the 1960s[26]. In contrast to the conventional logic, the fuzzy logic is not limited to be 0 or 1. However, any continuous value in-between these limits can be taken here. When 20°C temperature is taken as "comfortable", according to the conventional logic temperature of 19 or 21°C, which remain outside this set, are "uncomfortable". But, according to fuzzy logic, 17°C may obtain a membership of 0.4 in the "hot" set as well as 0.6 in the "cold" set. This logic is very useful in process control. For the automated circulations by the arteries and venous, the automated system based on fuzzy logic for drug releasing has been framed and analysed [27]. Fuzzy hemodynamic management modules have already been employed for the assessment of the condition of patients to report the regulation of the arterial as well as pulmonary pressures. This can be used to monitor the cardiac output of patients. The fuzzy logic-based automated system offers a comparative faster reaction and more effectual haemodynamic control. In addition, the uses of supervisory-fuzzy rule-dependent adaptive control system is considered as a potential way for controlling the multiple drug hemodynamic process [28]. When the fuzzy logic system is strongly combined with a neural network, it is called as neurofuzzy logic system. Here, the capability of neural networks of learning from data and the ability of fuzzy logic of expressing complex concepts intuitively are combined properly. It has data mining capability. The neurofuzzy logic also presents neural network having 2 extra layers for the fuzzification of inputs as well as defuzzification of outputs. In a research, the simulation of probucol absorption via the lipid formulations has been studied by means of neurofuzzy networkings[29] According to the outcome of the research, the probucol releasing rate from the lipid formulations was found to be significantly lesser in comparison with that of the self-emulsifying formulations. The adaptive neurofuzzy network model together with in vitro-in vivo correlation tool demonstrated the competent predictive presentation and the prospective for the development of complex relationships as well as interpolates the pharmacokinetic constraints.

PRINCIPAL COMPONENT ANALYSIS (PCA) :

PCA is another AI based model for decreasing the dataset-dimensionality by preserving as much 'variability' (i.e., statistical information) as possible and at the same time, PCA modelling minimizes the loss of information. PCA modelling translates into searching newer variables, which are linear functions of those in the original dataset by generating newer uncorrelated variables so that maximize the variance, successively.Searching of such newer variables, the principal components reduce the resolving of an eigenvector or eigenvalue problem[.30-31] PCA can be based on either the covariance matrix or the correlation matrix and the main applications of PCA are descriptive in nature, rather than the inferential uses. Recent years, PCA is well-known for using as a 'hypothesis generating' AI tool generating a useful statistical mechanic's frame for modelling of biological systems without the requirement for strong a priori theoretical assumptions, which makes PCA of paramount significance for drug discovery research by a systemic perspective overcoming too narrow reductionist approaches [32].

ADVANTAGES OF AI TECHNOLOGY:

The potential advantages of AI technology are as follows: [33]

i) Error minimization: AI assists to decrease the errors and increase the accuracy with more precision. Intelligent robots are made of resistant metal bodies and capable of tolerating the aggressive atmospheric space, therefore, they are sent to explore space. ii) Difficult exploration: AI exhibits its usefulness in the mining sector. It is also used in the fuel exploration sector. AI systems are capable of investigating the ocean by defeating the errors caused by humans. iii) Daily application: AI is very useful for our daily acts and deeds. For examples, GPS system is broadly used in long drives. Installation of AI in Androids helps to predict what an individual is going to type. It also helps in correction of spelling mistakes. iv) Digital assistants: Now-a-days, the advanced organizations are using AI systems like 'avatar' (models of digital assistants) for the reduction of human needs. The 'avatar' can follow the right logical decisions as these are totally emotionless. Human emotions and moods disturb the efficiency of judgement and this problem can be overcome by the uses of machine intelligence v) Repetitive tasks: In general, human beings can perform single task at a time. In contrast to the human beings, machines are capable of performing multi-tasking jobs and can analyze more rapidly in comparison to the human beings. Various machine parameters, i.e., speed and time can be adjusted according to their requirements. vi) Medical uses:In general, the physicians can assess the condition of patients and analyze the adverse effects and other health risks associated with the medication with the help of AI program. Trainee surgeons can gather knowledge by the applications of AI programs like various artificial surgery simulators (for examples, gastrointestinal simulation, heart simulation, brain simulation, etc. vii) No breaks: Unlike human beings who have the capacity of working for 8 h/day with breaks, the machines are programmed in such a way that these are capable of performing the work in a continuous manner for long hours devoid of any kinds of confusions and boredom. viii) Increase technological growth rate: AI technology is widely used in most of the advanced technological innovations worldwide. It is capable of producing different computational modelling programs and aims for the invention of the newer molecules. AI technology is also being used in the development of drug delivery formulations. ix) No risk: In case of working at the risky zone like fire stations, there are huge chances of causing harm to the personnel engaged. For the machine learning programs, if some mishap happens then broken parts can be repairable. x) Acts as aids: AI technology has played a different function by serving children as well as elders on a 24x7 basis. It can perform as teaching and learning sources for all. xi) Limitless functions: Machines are not restricted to any boundaries. The emotionless machines can do everything more efficiently and, also produce more accurately than the human beings.

CONCLUSION:

During past few years, a considerable amount of increasing interest towards the uses of AI technology has been identified for analyzing as well as interpreting some important fields of pharmacy like drug discovery, dosage form designing, polypharmacology, hospital pharmacy, etc., as the AI technological approaches believe like human beings imagining knowledge, cracking problems and decision making. The uses of automated workflows and databases for the effective analyses employing AI approaches have been proved useful. As a result of the uses of AI approaches, the designing of the new hypotheses, strategies, prediction and analyses of various associated factors can easily be done with the facility of less time consumption and inexpensiveness.

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