Journal of Positive Sciences (JPS) **eISSN: 2582-9351, https://positive-sciences.com** **JPS. 2021 Aug; 1(5): 10-14**

Article info
Received on: 20.07.2021
Accepted on: 30.08.2021
Published on: 31.08.2021
doi: https://doi.org/10.52688/ASP67564

Research Article

Drugs designing using artificial intelligence based pharmaceutical systems

Sajid Hamed Reshak [1, *]

[1] Al kunooze University College, Iraq

[*] sajid.h@kunoozu.edu.iq

ABSTRACT

In the field of Artificial Neural Networks (ANNs), computer algorithms and comparable to the structure of the brain's neurons are used for modelling and pattern recognition. What the brain does with all of its experiences is learn. When one views the brain as a biological neuron, one finds inputs coming in from a variety of external resources, such as the visual cortex, the hippocampus, and the thalamus, and the cell processes those inputs, performing a nonlinear operation before producing a conclusion. Adaptive biological neurons serve as the ANNs' analogues, which mimic the biological nervous system. In contrast to statistical modelling, ANNs are simple and versatile and don't need a defined experimental design. They may use partial or historical data to map functions. ANNs are excellent pattern and classification recognizers, as well as having the capacity to make choices while using imprecise input data. The applications of ANNs to many fields, including pharmaceutical research, engineering, psychology, and medicinal chemistry, are well documented. Applied neural network technique has several potential applications in the pharmaceutical sciences. We shall describe several instances of ANNs in drug discovery in this article.

Keywords: Drugs, machine learning, ANN, FFNN, optimization

INTRODUCTION

The effectiveness of neural networks (NNs) has increased to the point that they can no longer be confused with artificial intelligence (AI). NNs find rules from samples much as the other ML algorithms for artificial intelligence do. According to some researchers, the closer one gets to solving a given problem using NNs, the more it mimics the process of approximating a mathematical formula. If there are NNs with simple design, then NNs with complex architecture may approximate a large number of functions. The basic concept of NNs is simple to comprehend, but the complex specifics of NNs are difficult to grasp (as previously described in [1-4]).

Additionally, drug discovery relationships may be defined using formulae, and this has led to the use of NNs in the process. Both discrete and continuous dependent variables may be modelled using NNs, and the resulting models may be qualitative or quantitative. Because of the significant capabilities of NNs, NNs always outperform other models (as previously reviewed in [1, 4, 5]). NNs allow many different methods of representing ligands, receptors, and receptor-ligand interactions, as seen from the viewpoint of independent variables that characterise molecules. To help with ligand-based drug design, de novo drug design, and receptor-based drug design, the group covers a lot of ground. As a medicinal chemist, I always keep in mind the significance of molecular structures while determining characteristics of compounds. In a similar vein, when constructing in silico models for drug development, the quality of the models depends on how molecular structures are represented. The traditional approach to structure representation has utilised molecular descriptors and fingerprints. However, the information is processed data and not just raw data on structures. Preprocessing before the analysis may result in molecular descriptors and fingerprints that do not precisely and completely describe structures. But even while these many types of NNs, such as genetic NNs, self-organizing maps, and radial basis function NNs, are capable of processing raw molecular information, they are inadequate for tackling complex molecular structures. This allows the models based on NNs to evaluate the rules directly and comprehensively because of the development of recurrent neural networks (RNNs), convolutional neural networks (CNNs), and molecular graph-based neural networks (MGNNs). Tools have been created by using basic NNs as building blocks, which have been refined to include NNs with advanced architectures and various components. Neural networks are the most fundamental elements that may be further merged to form new independent variables or final outputs. This makes RNNs excellent at handling consecutive inputs, such as a reduced molecular input line entry specification (SMILES). Various ANNs are employed in CNNs to merge different nearby variables into new variables that serve different purposes. The concept of CNNs is similar to MGNNs, however the implementations of MGNNs are designed to account for non-Euclidean input. Please see the previous list of components, which

[*]**Corresponding author**
Sajid Hamed Reshak,
Al kunooze University College, Iraq
e-mail: sajid.h@kunoozu.edu.iq

are currently being updated. To some degree, the updated NNs will have a memory, and other ANNs may be used to control, read, and write the inner variables of NNs. On the other hand, the complex inner architecture of such NNs provides the NNs with more adaptability. For example, consider CNN. With the dynamic k-max pooling, CNNs have the capability to cope with consecutive inputs and are helped with the global average pooling. Modeling functions may be increased when the outputs of a single NN are assigned as fresh inputs rather than as final outcomes. A first NN (a word node or a phrase node) may be configured as an encoder, which uses its associated inputs to generate new representations and the new representations can be utilised by a second NN (a concept node or a statistic node) for qualitative or quantitative purposes. The most significant thing about the new representation is that it can be understood by the latter NN, which means that it is possible to generate new molecules from it. Adversarial autoencoders and variational autoencoders both include the introduction of an adversarial mechanism and reparameterization, and use this to make the process of encoding and decoding unique. Two critical components of generative adversarial networks (GANs) are: encoders and decoders, as well as the ability to be configured as generators and discriminators. The architecture of NNs has been built, and models that are more practical may be trained using techniques that are more practical. In application settings where there are restricted sample sizes, learning transfer and one-shot learning are well-suited. As dynamic processes, models may be taught to produce SMILES sequences according to individual characteristics, and reinforcement learning offers the ideal way to accomplish this. Traditional qualitative or quantitative activities may be completed using the NN-based technologies described, which take molecules' raw information and link in various ways, providing a large array of options for drug development [6].

RELIABILITY OF AI ON PHARMA FEDILDS

The three most essential things in training excellent models are well designed architectures, optimal hyperparameters, and correct samples. the samples are typically prepared before training, whereas rigorous validations are done on the first two variables; the weights and biases of NNs are modified based on the provided data. Including additional data for a model results in a model that is better able to react to new samples, allowing the model to be effectively generalised. When many samples are available, molecular models may be relied on to predict solubility and toxicity. Additional variables may provide a significant challenge for those who work with big datasets, such as medicinal chemists, in the process of searching for novel active molecules. With numerous samples of a target accessible, it indicates that further study and rigorous intellectual property will need more space. This needs to be verified in practise whether model-based NNs can identify compounds of interest. Another recent paper compares models built using neural networks (NNs) and other machine learning methods and brings into focus the conflict between dependability and novelty. Models shown to be worse at predicting newer samples used in research were matched against several ML models, however models built using NNs were not significantly better than their ML counterparts. With well-designed architectures and adjusted hyperparameters, effective NNs are not expected to increase much in performance. The most practical option is to provide samples of people who have no familiarity with the product. On the other hand, while there are models intended for dealing with samples that are restricted, their performance is unclear. Consider for example, models that have a one-shot learning process were shown to be unsuitable for virtual screening tasks [7]. Docking findings may also help in resolving the conflict. To some degree, the docking techniques may restrict the potential of these models. From medicinal chemists' perspectives, NNs offer excellent drug-likeness selection tools for clinical research, but in practise it is important to demonstrate that NNs are also useful in other creative endeavours, like virtual screening and target prediction. Silico modelling is commonplace, but applications in the actual world are restricted. While models have grown rapidly, some nuances have been found to enhance them. Another important impact of hyperparameters, dataset quality, and SMILES sequence variety have also been highlighted. On the other hand, medicinal chemists may still be unclear as to which model to use. To ease misunderstanding, comparisons are available to conventional activities [8] and de novo chemical synthesis [9]. Metric evaluations strive to anticipate, not depict, model values, and a model's usefulness in real-world activities is what medical chemists want. With reference to de novo molecule creation, a reasonable model would be: While the models are simple to implement, produced compounds may not be stable or accessible to react with other molecules. Researching an actual issue in drug development is more essential than testing in silico, since drug discovery is almost always a difficult process. This is excellent news, since models based solely on basic algorithms have been verified and shown to be effective. Using NN-based models, active drugs were identified that targeted nuclear receptors [10] and kinases [11]. At the same time, anticancer peptides were developed by utilising RNNs [12]. NNs provide an effective model in these situations. New chemical entities and automated drug discovery NNs appear to be used to assist in drug development at the moment, although models that use NNs are capable of doing drug discovery on their own. While most of these devices only operate as they are intended, automatic systems for synthesis, analysis, and biological testing have emerged as a trend in the business. In conjunction with machine learning, such gadgets could decide what they should do on their own, leading to a "automatic design-make-test cycle," which is a feedback loop. While it is true that ML (machine learning) was able to construct the loop effectively, four previously unknown responses were found in the process. Additionally, in the area of drug development, NNs (specifically neural networks) have shown their capacity at several phases, including the design of novel compounds and the design of synthetic routes. As well, the process of learning via reinforcement may also be dynamic, making it possible for models based on NNs to learn and create new medicines. Specifically, NNs are able to use both abstract information and intuitive representations such as words and pictures; furthermore, they have a distinct advantage over other ML algorithms because of this feature. It is fair to believe that NNs may be better incorporated into the drug discovery automatic feedback loop on the basis of their many benefits.

***Corresponding author**
Sajid Hamed Reshak,
Al kunooze University College, Iraq
e-mail: sajid.h@kunoozu.edu.iq

RESULTS AND DISCUSSIONS

Using of paramedical data illustrating the amount of materials (chemical materials) required for designing drugs and the events taking place if such amounts hiked. Deep neural network i.e. Long short term Memory neural network (LSTM) is used for predicting the drugs error due to imbalance in the mixing components (raw materials). Long short term Memory neural network (LSTM) is made according to the structure (configurations) given in Table 1.

Table 1: structure of LSTM model

Layer	Information
Sequential CNN	Main model type
Conv2D	First layer with 32 filters and (3,3) kernel size and "linear" activation
LeakyReLU	Second layer with alpha transfer function
MaxPooling2D	Third layer with (2, 2) kernel size
Conv2D	Fourth layer with 64 filters and (3,3) kernel size and "linear" activation
LeakyReLU	Fifth layer with alpha transfer function
MaxPooling2D	Sixth layer with pool size is (2, 2)
Conv2D	Seventh layer with 128 filters and (3,3) kernel size and "linear" activation
LeakyReLU	Eighth layer with alpha transfer function
MaxPooling2D	Ninth layer with pool size is (2, 2)
Flatten	Tenth layer
Dense	Eleventh layer with 128 filters
LeakyReLU	Twelfth layer alpha transfer function
Dense	Last layer with 3 filters

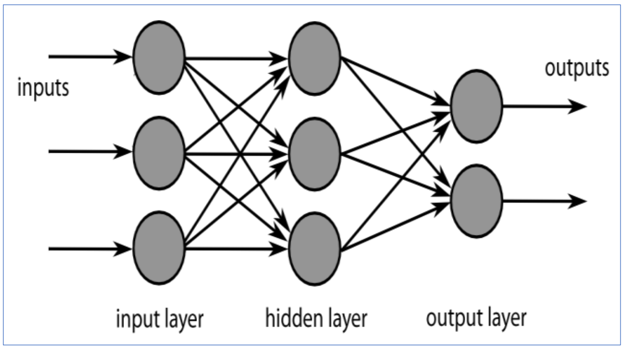

Figure 1: Layering structure of the neural network

The layers of the Long short term Memory neural network (LSTM) is illustrated in Table 1. The input layer is considered to intake the input data so that the size of this layer must be the same as the input size of the data. LSTM had been trained with 20 epochs and the training results of this model is given in Figure 2. Results of the Accuracy versus the epoch number is given in Table 2.

*Corresponding author
Sajid Hamed Reshak,
Al kunooze University College, Iraq
e-mail: sajid.h@kunoozu.edu.iq

Journal of Positive Sciences (JPS) eISSN: 2582-9351, https://positive-sciences.com Published by: Ve Technology Pvt. Ltd

Table 2: Accuracy per epoch of LSTM model.

Epoch Number	Accuracy
1	32
2	41
3	44
4	48
5	51
6	53
7	56
8	59
9	66
10	74
11	84
12	88
13	89
14	92
15	93
16	96
17	97
18	97.54
19	97.989
20	98.23

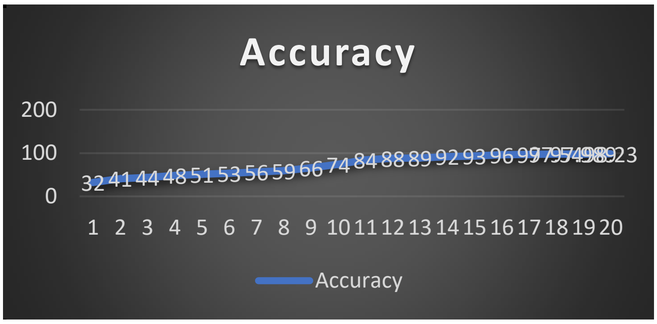

Figure 1: Machine learning methods popularity

CONCLUSION

It seems that pharmaceutical chemists have fallen behind when it comes to the changing nature of NN models. Virtual drug discovery presents fresh concepts and models, however it is difficult to choose the appropriate application of the latest models. The results of computational analysis do not warrant further options in silico. Moreover, remarkable practical situations are still restricted. Because these complicated jobs with few samples are typically the focus of medicinal chemists, it is possible that the primary reason is NNs' inability to cope with them. The findings may be spectacular, since the cooperation of chemists who specialise in cheminformatics and medicinal chemists is likely to reveal flaws with current models and develop more effective models, all of which could lead to remarkable outcomes. However, the collaboration will also expedite the process of NNs' integration and the 'design-make-test' cycle, thereby paving the way for the automated drug development in the future. LSTM is outperformed by producing accuracy of 98.23 percent in error prediction in the drug.

***Corresponding author**
Sajid Hamed Reshak,
Al kunooze University College, Iraq
e-mail: sajid.h@kunoozu.edu.iq

REFERENCES

[1] Carpenter KA, et al., "Deep learning and virtual drug screening", Future Med. Chem., 2018.
[2] Hornik K., "Approximation capabilities of multilayer feedforward networks", Neural Net., 1991.
[3] Gawehn E, et al., "Deep learning in drug discovery", Mol. Inform., 2016.
[4] Zhang L, "From machine learning to deep learning: progress in machine intelligence for rational drug discovery", Drug Discov. Today, 2017.
[5] Xu Y, et al, "An overview of neural networks for drug discovery and the inputs used", Expert Opin. Drug Discov., 2018.
[6] Liu R, et al., "Dissecting machine-learning prediction of molecular activity: is an applicability domain needed for quantitative structure–activity relationship models based on deep neural networks?", J. Chem. Inf. Model., 2019.
[7] Altae Tran H, et al, " Low data drug discovery with one-shot learning", ACS Cent. Sci., 2017.
[8] Zhou Y, et al., " Exploring tunable hyperparameters for deep neural networks with industrial ADME data sets", J. Chem. Inf. Model., 2019.
[9] Chen L, et al., " Hidden bias in the DUD-E dataset leads to misleading performance of deep learning in structure-based virtual screening", PLoS ONE, 2019.
[10] Bjerrum EJ, et al,"SMILES enumeration as data augmentation for neural network modeling of molecules", ArXiv E-prints, 2017.
[11] Wu Z, Ramsundar, et al., " MoleculeNet: a benchmark for molecular machine learning", Chem. Sci., 2018.
[12] Brown N, "GuacaMol: benchmarking models for de novo molecular design", J. Chem. Inf. Model., 2019.

***Corresponding author**
Sajid Hamed Reshak,
Al kunooze University College, Iraq
e-mail: sajid.h@kunoozu.edu.iq