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1D-Convnet Model for Detection of Antidepressant Drugs

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***Abstract*—A drug is a substance or mixture of materials to be used in determining the diagnosis, preventing, reducing, eliminating, curing disease or symptoms of disease, bodily or spiritual injury or disorder in humans or animals, including to beautify the body or parts of the human body. Problems begin to arise when a patient is wrong in consuming the target drug used, which is not by the type of disease suffered. For example, suppose a person suffers from a psychological disorder that requires taking different types of drugs, if it turns out that the type of drug consumed is not by the disease, it is very dangerous. This problem is certainly very dangerous because it can cause death for those who consume it. Currently, many researchers are using the deep learning Convolutional Neural Network (CNN) model for drug detection problems. The CNN model has a higher level, namely 1D-Convolutional Neural Network (1D-Convnet) which is still rarely used for drug detection problems. So, the purpose of this study was to detect the classification of Atypical antidepressants and SSRIs antidepressants using a deep learning model of the 1D-Convolutional Network (1D-Convnet) type. The results obtained using this model are 98.3% with the most influential parameter, namely dropout. The proposed research model also produces higher accuracy than the Naive Bayes supervised learning model.**

Keywords—1D-Convnet, Antidepressant, Drugs, Deep Learning

I. INTRODUCTION

A drug is a substance or mixture of materials to be utilized in deciding the determination, anticipating, lessening, killing, curing infection or indications of illness, damage, or physical or otherworldly clutter in people or creatures, counting to decorate the body or parts of the human body. [1]. Drugs also have several types, including generic drugs, patent drugs, and branded generic drugs [1]. Problems begin to arise when a patient is wrong in consuming the target drug used, which is not in accordance with the type of disease suffered. For example, suppose a person suffers from a psychological disorder that requires taking different types of drugs, if it turns out that the type of drug consumed is not in accordance with the disease, it is very dangerous. This problem is certainly very dangerous because it can cause death for those who consume it. Of course, these problems can be overcome by applying intelligent learning techniques based on machine algorithms to determine what drugs should be used.

Several studies related to determining the target drug users have been carried out by other researchers, such as in predicting the problem of drug-target interactions using the KronRLS-MKL model [2]. In another study discussing the prediction of drug-target interactions, a problem was to identify new protein-ligand interactions from previous information based on deep learning [3]. The authors created DDR, a modern strategy that makes strides DTI expectation precision. DDR is based on the utilize of heterogeneous charts containing known DTIs with numerous similitudes between drugs and a few similitudes between target proteins [4].

Another study discussed the prediction of drug-target interactions and food-drug constituent interactions with a deep learning approach which resulted in an accuracy of 92% [5]. The same problem is using the Artificial Neural Network (ANN) model [6]. Other analysts proposed the Bayesian Positioning Forecast of Drug-Target Intelligent (BRDTI). This strategy is based on the Bayesian Personalized Positioning (BPR) network factorization which has demonstrated to be an great approach for different inclination learning [7]. This model has never been used for DTI prediction before [7].

Other studies predict new interactions that have not been discovered with other problems to be addressed, namely class imbalance which has the potential to reduce predictive performance [8]. Another study focused on predicting interactions between drugs and target by playing a role in drug discovery [9]. Another study aims to focus on a machine learning approach and provide a comprehensive understanding of the prediction of drug-target interactions [10].

Other studies discuss several machine learning methods such as support vector machines, decision trees, naive Bayesian, KNN, and ANN which are used to predict drug-target interactions [11]. Another paper proposed an algorithm for predicting drug-target interactions called regulated logistic matrix factorization (NRLMF) [12]. Another study described the prediction of target drug interactions using the maximum coverage approach [13]. Related studies also predict drug-target interactions by presenting the SimBoost method which functions for continuous (non-binary) prediction [14]. In a study studying the BI-LSTM model in a problem predicting interactions between drugs used [15].

In another study discussing drug sentiment analysis which has become very significant in today's classification of drugs based on their effectiveness, the analysis was carried out through user reviews which can help potential future consumers in gaining knowledge and making better decisions about certain drugs [16]. Another author developed a High Alert Drugs (HAD) screening protocol with a machine learning model using the Gradient Boosting Classifier and screening parameters to identify the incidence of High Alert Drugs (HAD) prescribing

errors from outpatient and inpatient drug prescriptions at Maharaj Nakhon Chiang Mai Hospital in 2018 [17].

So, this study aims to detect the classification of Atypical antidepressant drugs and antidepressant SSRIs using the deep learning 1D Convolutional Neural Network (1D Convnet) algorithm.

II. RESEARCH METHOD

Fig. 1 is the flow of this research process.

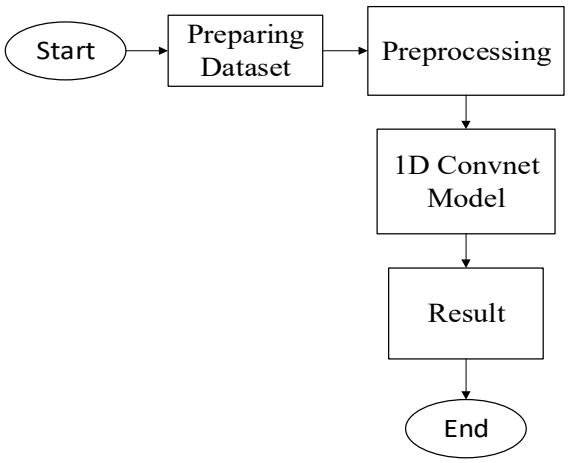

Fig. 1 Design Process

A. Dataset

In this study, data were collected through the National Library of Medicine [18]. The types of drugs used are for the category of atypical antidepressants and SSRIs as many as 502 kinds of drugs with different doses. Atypical is a treatment for major depressive disorder, while SSRIs are a treatment for depression by increasing serotonin levels in the brain.

B. Preprocessing

In this process, the dataset is separated into training and testing. Then the dataset will be converted into lowercase form and remove irrelevant symbols such as (,.”?/!*). Table 1 is an example of the results obtained after the preprocessing process is complete. In this preprocessing, stemming and tokenization processes are carried out. The goal of this preprocessing is that the dataset which was previously in the form of many sentences is converted into a vector-matrix form that functions for detection using the 1D-Convnet model.

TABLE I. PREPROCESSING RESULT

Drugs Name	Category
[trazodone, hydrochloride]	Atypical
[amfebutamone, bupropion, hcl]	Atypical
[bupropion, hcl]	Atypical
[amfebutamone, hydrochloride]	Atypical
[citalopram, hydrobromide]	SSRIs
[paroxetine]	SSRIs
[sertraline]	SSRIs
[fluoxetine, succinamic, acid]	SSRIs

C. 1D-Convnet Model

After the dataset has been preprocessed, the next step is to implement the 1D Convolutional Neural Network (1D-Convnet) model using several parameters. The 1D-Convnet model is a derivative of the Convolutional Network model. This network is one of the deep learning models which can handle long and varied input sequences [19]. In this model, there is a network that inserts a one-dimensional convolution layer and a dynamic k-max-pooling layer. The convolution layer applies a one-dimensional filter in each feature row in the sentence matrix [19].

. Step 1D-Convnet comprises of 1D convolution layer, Bunch Normalization, and pooling layer [20]. Fig. 2 shows up the concept of 1D convolution layer and max-pooling layer. The layer degree of the convolution layer is set to 32, and 128 layers are utilized in include up to. Hence, 128 yields each containing 97 128−32+1) components are delivered when a single outline spectrogram (128 container frequencies) is nourished into a 1D convolution layer. Following, a ReLU (Rectified Linear Unit) actuation work is connected [21]. Hence, a max-polling of measure 97 is connected to each yield which may be a agent esteem. Dropout is additionally connected with a esteem of 0.5 at the conclusion of Convnet to maintain a strategic distance from overfitting.

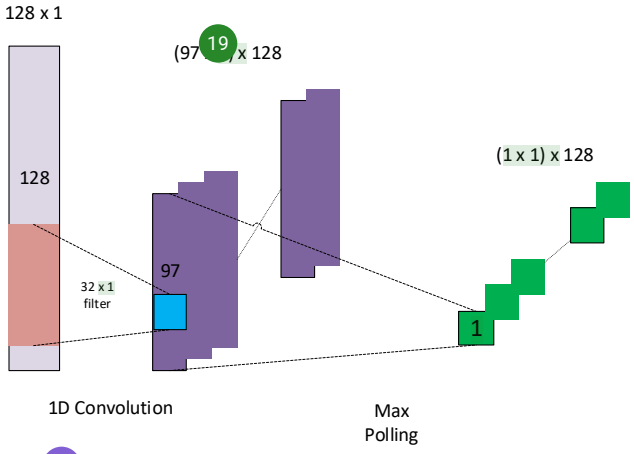

Fig. 2 1D-Convnet Structure for frame feature extraction [19]

The 1D Convolutional Network model, has several common layers, such as fully connected, max polling, and convolutional. This study uses a combination of the three layers. Fig. 3 is the layer on 1D-Convnet.

A convolutional layer is a layer that performs spatial convolution between input and filter. The filter contains the weights which are the components of the layer being considered. Max surveying could be a layer that takes input tests to create yield with littler measurements by selecting the most extreme esteem component. Completely associated is the layer that interfaces the yield of the volume layer to the ultimate yield. They permit meeting of choices at higher levels. [22].

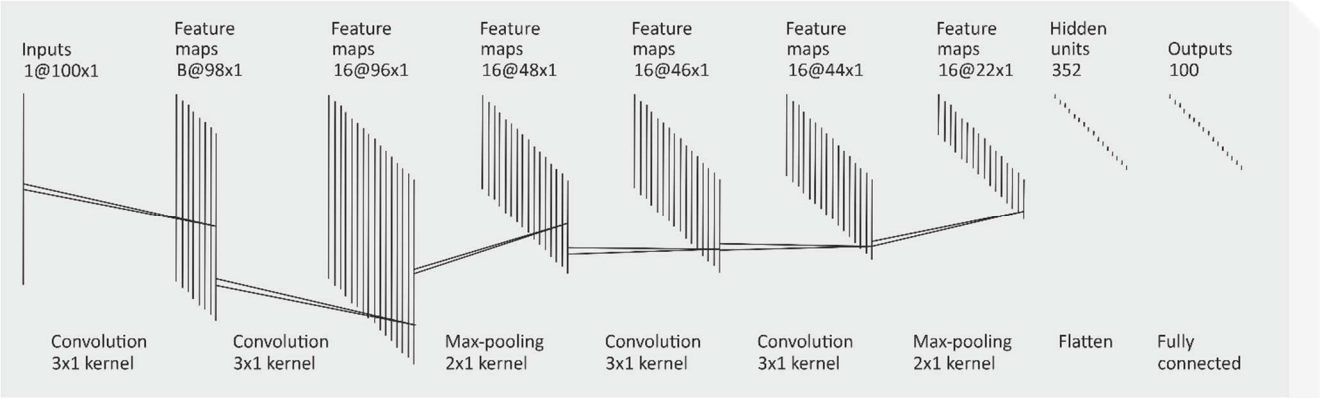

Fig. 3 1D-Convnet: Each 1D-Convnet block consists of 4 convolution layers, 2 max-pooling layers, and 1 fully connected layer

The output value of the 1D-Convnet layer with the input (N, Cin, L) and output (N, Cout, Lout) sizes in formula (1) [23].

$$out\left(N_i, Cout_j\right) = bias\left(Cout_j\right) + \sum_{k=0}^{Cin-1} weight\left(Cout_j, k\right) * input\left(N_i, k\right) \quad (1)$$

Where Ni is the size of batch I, Cout j is the jth channel, L is the length of the signal sequence (if the input is an image, width and tallness ought to be utilized rather than length). At that point the length of the yield flag arrangement can be calculated utilizing equation (2) [23].

$$L_{out} = \frac{L_{in} + 2\ x\ padding - dilation\ x\ (kernelsize - 1) - 1}{stride} + 1 \quad (2)$$

Where strides is a cross-correlation step. Padding is the number of zero padding on both sides. Dilation is the distance between kernel elements. Kernel size is the convolution size of the kernel. For max-pooling 1D, the output value with size input (N,C,L) and output (N,C,Lout) can be seen in formula (3) [23].

$$out\left(N_i, Cout_j\right)_{m=0,\ldots,kernel\ size-1}^{max} input(Ni, Cj, stridex + m) \quad (3)$$

Where Ni is the I-th input, Cj is the jth channel. kernel size is the window size to take max. Stride is a step from the window. Padding is the number of zeros to be added on both sides. Dilation is a parameter that controls the step of an element in the window.

D. Naïve Bayes

Naive Bayes is a simple technique for constructing classifiers: a model that assigns class labels to problem instances, represented as feature value vectors, where class labels are drawn from some finite set [24]. Naïve Bayes is also a model that is often used for text classification problems [24].

In formula (4) is a formula for calculating Naive Bayes.

$$P(Y\_j|X\_i) = \frac{P(X\_i|Y\_j)\ P(Y\_j)}{P(X\_i)} \quad (4)$$

Where P(Y_j|X_i) is the posterior probability to be searched. P(X_i|Y_j) is the likelihood, P(Y_j) is the prior probability class and P(Xi) is the prior probability predictor.

E. Detection

In this detection process using the 1D-Convnet model with the dataset first separated between training and testing. To measure the value of this process using the calculation of accuracy and loss function. The accuracy formula can be seen in formula (5), while the loss function formula can be seen in formula (6) [25].

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} \quad (5)$$

$$Loss\ (p, q) = \frac{1}{|M|}\sum_{i=1}^{i=M} -qiLogpi \quad (6)$$

Where M is the data points where qi is the correct value between 0 or 1, while pi is the SoftMax probability. TP is true positive, TN is true negative, FP is false positive, FN is false negative.

III. RESULT AND DISCUSSION

The best results were obtained through several experiments by changing the parameters on the 1D-Convnet model such as max feature, embedding dimensions, sequence length, dropout value, and epoch. So that the results obtained look like in Table II.

TABLE II. RESULT

Max Feature	Embedding Dimension	Length	Dropout	Epoch	Accuracy %	Loss
20000	128	500	0.5	8	95	0.4
5000	100	250	0.3	100	98.3	0.1
30000	200	700	0.7	100	96.6	0.3
5000	200	700	0.7	100	96.6	0.3
30000	100	250	0.3	100	96.6	0.3
5000	100	250	0.3	8	98.3	0.1

It can be seen from the results of Table II above that the highest accuracy is 98.3%. After experimenting by changing the parameters on the 1D-Convnet model, the most influential parameters are dropout and epoch. If the dropout value is below 0.5, the resulting accuracy is stable at an average of 97.6%, which means that the figure is higher when used generally. Conversely, if the dropout value is above 0.5, the resulting accuracy is stable at an average of 96%. The epoch parameter does not have a significant effect because when the epoch is worth 8 and the dropout value is 0.3, the resulting accuracy is very high.

In addition to the accuracy value, this study also uses measurements in the form of loss values, which if the loss value is getting smaller, indicates that the model used is very good at predicting a problem. In Table II, the smallest loss value is 0.1, where the accuracy is 98.3%. This indicates that the selection of parameter values and the model used is correct.

In Fig. 4 and Fig. 5 is a form of visualization of the name of the drug used based on the Atypical category and SSRIs.

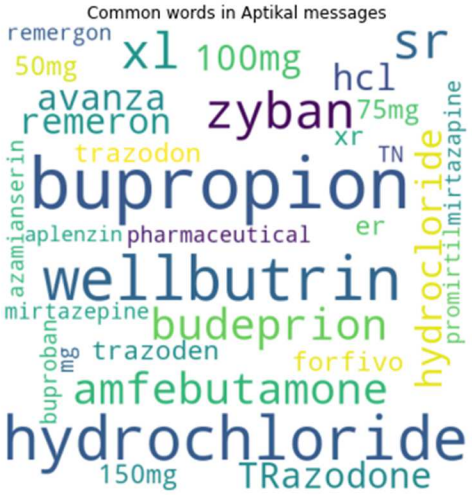

Fig. 4 Antidepressant Atypical

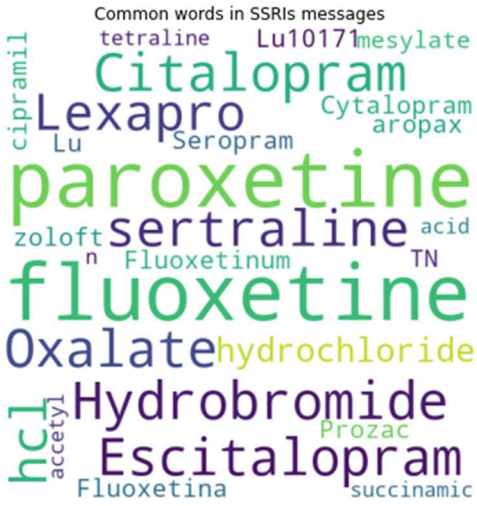

Fig. 5 Antidepressant SSRIs

Meanwhile, Fig. 6 is the distribution of the number of words based on density. It can be seen from the density results that the SSRIs class has more density and more than 1.

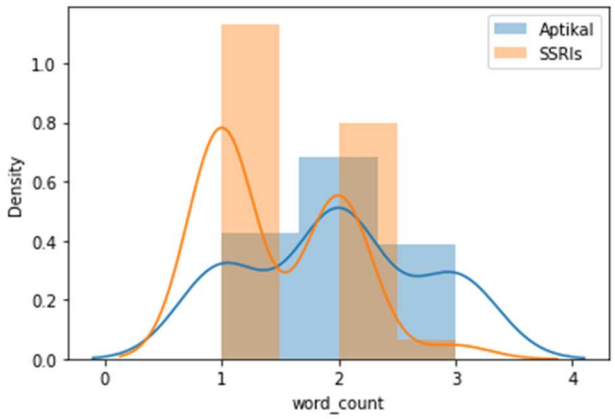

Fig. 6 Word Count Density

Fig. 7 is the result of a comparison of the 1D-Convnet model using the Naive Bayes model.

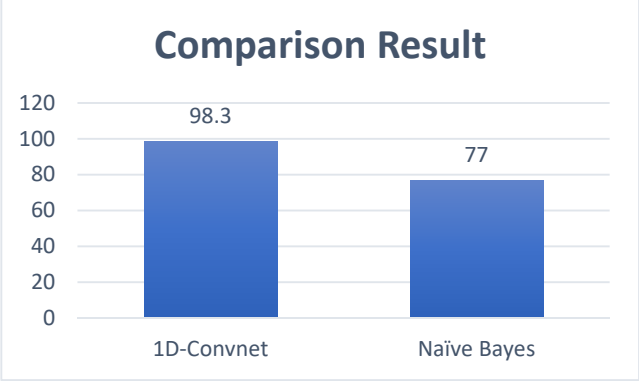

Fig. 7 Comparison Result

Seen from Fig. 7 that the proposed research model has higher accuracy results than supervised learning models such as Naïve Bayes. The results of the difference in accuracy can reach 21%. Judging from the value of the difference in accuracy is so large, of course in the selection of learning models for the detection of drugs used must be done properly.

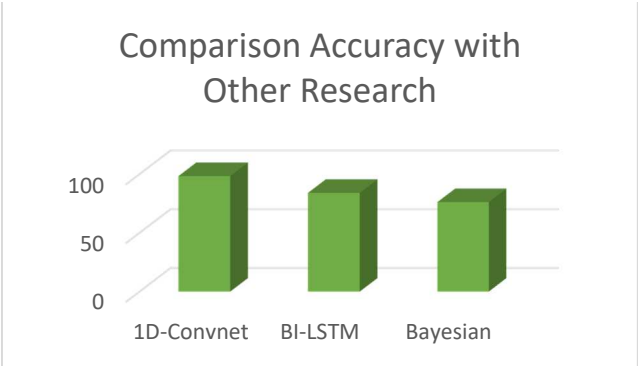

Fig. 8 Comparison with Other Research

Fig. 8 is a comparison with other models in previous studies. The results obtained for the proposed research model are still far superior to about 20% compared to other models.

The results also show that the model using the deep learning approach results in accuracy for text classification problems much better than the unsupervised learning model.

IV. CONCLUSION

Conclusion in this study include, the 1D-Convnet model was successful in detecting classifications related to the category of Atypical antidepressants and SSRIs. Parameters in the 1D-Convnet model have an influence on the accuracy results. The most influential parameter is the dropout value. The highest accuracy produced is 98.3% with a dropout value of 0.3. The 1D-Convnet deep learning model also produces higher accuracy than the supervised learning Naive Bayes model with a difference of 21%.

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