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OPTIMIZING DRUG DOSAGE AND HALF-LIFE PREDICTION FOR ADHD TREATMENT IN ADULTS AND CHILDREN USING BIG DATA ANALYTICAL BASED DEEP LEARNING APPROACH

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Abstract

Attention Deficit Hyperactivity Disorder (ADHD), a common neuro-developmental condition affects both adults and children. Choosing the right medication dose level, considering individual variability and drug half-life, is an important part of treating ADHD. In this article, we propose a thorough strategy for optimizing medication dose levels for treating ADHD utilizing a Deep Convolve NeuroNet (DCNN) with cutting-edge feature extraction and data pre-processing methods. Our database contains clinical records of individuals with ADHD, together with information on their age, gender and drug response. Using the Map-Reduce method, we can arrange the data displayed in the datasets. After the pre-processed data has been extracted, linear discriminant analysis (LDA) is used to find pertinent information, minimize dimensionality and facilitate classification. Finding the most important factors is one of the biggest obstacles in selecting the right medicine dose. Our model is more effective because of the use of Correlation-based Feature Selection (CFS), which chooses the most informative properties. We employ a DCNN architecture trained to predict the optimal drug dosage level for each patient. This deep learning approach is well-suited for handling complex relationships in the data, enabling accurate and personalized dosage recommendations. We aim to provide healthcare professionals with a valuable tool for tailoring drug dosages to individual patients, enhancing treatment efficacy and minimizing side effects.

Keywords: Attention Deficit/Hyperactivity Disorder (ADHD), Dosage Level & Half-Life Period of Drug, Deep Convolve NeuroNet (DCNN).

1. Introduction

Children with ADHD have a persistent behavioral condition. Attention deficiency and overactivity are the symptoms of ADHD condition. 5% of children and 2.5% of adults suffer from ADHD, a hereditary behavioral condition of childhood. ADHD sufferers struggle to focus on mundane chores, which hurt their performance in school and with others. The patient's therapy benefits from an early diagnosis of ADHD. Psychological interviews and observations are used to diagnose ADHD [1]. A large number of family practitioners admitted in a survey lacked the information necessary to identify ADHD. In a study of 400 primary care doctors, 44% said that the diagnostic criteria for ADHD were unclear, 72% said that diagnosing the disorder in children was simpler than in adults and 75% said that the diagnostic criteria for ADHD were poor or moderately accurate [2]. Common indicators of ADHD in youngsters include academic underachievement, problematic peer interactions and emotional deregulation, which get worse with age. Addictions to drugs and alcohol, as well as traffic-related problems, are more common in persons with ADHD than in non-ADHD control events and pregnancies in teens by adolescence and young adulthood. Behavioural signs of ADHD and cognitive deficiencies are problematic for the affected individuals, their loved ones and society. Education, interpersonal interactions, self-esteem and quality of life issues are common among people with ADHD [3]. Executive impairments are present when patients have ADHD in a total of cognitive areas, with visuospatial and verbal memory, inhibitions, vigilance, organizing and reward regulation. These deficiencies are supported by anomalous results from both functional and structural brain imaging investigations, primarily in expansive brain structures such as the frontostriatal, frontoparietal and ventral attention networks [4].

While the neurobehavioral disorder ADHD condition first appears in childhood, it lasts throughout adolescence in 40%–50% of instances and the signs persist into adulthood. Learning problems, conduct disorder (CD), oppositional defiant disorder (ODD), anxiety and depression are the most frequent psychiatric and other comorbidities among children and adults with ADHD. ADHD persistence into adulthood is predicted by the severity of the disorder and the existence of mental comorbidities, particularly ODD and CD [5]. Without the diagnosis that is disclosed, some children with disorders experience significant challenges as children and are given little care or assistance. Others who had better coping skills owing to greater intelligence or supportive families might reveal problems due to increased demands (studying, receiving a promotion at work, having children) or when their coping mechanisms would run out [6]. Contrary to the hypothesis of a neurodevelopmental origin, the prevalence of diagnosed adults increases the possibility that a full clinical image of ADHD can manifest at various stages of development. Studies show that most adults with ADHD symptoms did not have them as children, according to current longitudinal epidemiological research [7]. In this work, we forecast drug dosage and half-life for treating ADHD in both adults and children.

The following sectors are organized throughout the remainder of the paper: Section 2 presents relevant work, Section 3 discusses categorization, Section 4 displays the findings as well as discussion and Section 5 provides the paper's conclusion.

2. Literature review

2.1 The Role of Healthcare Providers in ADHD Medication Management

The study [8] was to determine the degree of knowledge, understanding, perspective and outlook among Indonesian community members, educators in primary schools, medical learners, general practitioners, physicians and psychologists about ADHD and its relationship with various relevant factors. The degree of knowledge/understanding, perspective and attitude towards ADHD in every participant category were evaluated using a cross-sectional survey with accurate questionnaires. The research [9] was to investigate parents' opinions on how the staff and medical processes in Danish hospital clinics impact their daily lives as parents of children with ADHD. The main data-gathering techniques were participant interviews and observation. From the clinics of somatic and mental hospitals, fifteen families with children who had ADHD were enrolled. The study [10] looked at how healthcare provider (HCP) subgroups screen and treat ADHD. The poll examined problems with adult ADHD diagnosis and treatment as well as HCP perspectives of elements affecting patient decision-making about medication. For neurological specialists and nurse practitioners, expertise in diagnosing or treating ADHD in adults was necessary (5 patients/month; for psychiatrists and PCPs, ten patients/month). The study [11] used the 2016 National Survey of Children's Health (NSCH) to determine the nationwide incidence of ADHD and its treatment amongst U.S. children 2 to 17 years old. The NSCH is a cross-sectional national questionnaire of parents that asks them about their children's health before the 2016 gathering of data. The factors to consider involved whether children had ADHD at the time, whether the diagnosis had been made in the past and if the child had received medication or behavioral therapy for ADHD. The study [12] focused on children and adolescents with ADHD who can benefit from a variety of psychosocial therapies involving organizational training applications, behavioral peer interventions, behavioral classroom management and behavioral parent training. However, there is a substantial gap in investigation and exercise, making it difficult to apply evidence-based methods in communities and educational contexts. They explore possible study paths that promote the transition from the present, fragmented structure of caring to a multi-systemic strategy utilizing a life course framework for the implementation of ADHD therapy. The study [13] found that ADHD is a common neuro-developmental disorder in children and adolescents that lasts into adulthood. The patient's primary care physician was the one to diagnose ADHD and start a course of action with them. While it reduces the main signs of ADHD, guidelines advise using psychostimulant medication as the first-line treatment in the administration strategy. Numerous methylphenidate and amphetamine formulas have been developed, giving patients various possibilities to suit their unique lifestyle requirements.

2.2 ADHD UsingMachine Learning Approaches

The article [14] used a number of rating scales that were created by specialists to diagnose ADHD. The structural, functional and drug-related aspects of the ADHD brain were studied using MRI patterns. The purpose of the research was to create several machine learning models for precise forecasting of this illness. A large portion of machine learning research has focused on developing models for classification, among which support vector machine (SVM) and artificial neural network (ANN) have been shown to provide the most accurate analysis. Using a genetic programming-based approach, a more accurate prediction framework has been created with excellent correlation coefficient (CC) values, specificity and sensitivity. The study [15] used deep learning models and resting-state functional magnetic resonance imaging (rs-fMRI) data to offer an automated technique for diagnosing ADHD. In contrast to conventional approaches, this research developed a 4-D CNN, a deep learning approach that utilizes granular computation. This approach can compute layer stacking to achieve coarse granularity and it was trained based on derivative variations in entropy. To assist the community of children who are impacted, investigators need to create acceptable techniques for predicting ADHD and dyslexia. Based on this, several machine learning (ML) techniques were utilizing a variety of online datasets to improve the categorization and accuracy of predictions. Achieving clinical acceptance with these current methodologies poses particular research hurdles such as dataset privacy, a suitable classifier model, excellent feature and optimizer selection, hyperparameter selection and over-fitting issues [16]. The work [17] created a balanced class label and they used oversampling and undersampling techniques. Using logistic regression (LR) and p-values (0.05), we were able to identify the relevant predictors for ADHD in youngsters. For predicting the outcome of children with ADHD, random forest (RF), eight ML-based classifiers, 1-dimensional convolution neural network (1D CNN), decision tree (DT), xg boost, support vector machine (SVM), multilayer perceptron (MLP), naive Bayes (NB) and k-nearest neighborhood (KNN) were used. The article [18] extracted volumetric characteristics using the brain's gray matter (GM) volume areas identified by the cortical thickness-based (CT) and automated anatomical labeling (AAL3) attributes identified by the atlas of distress. Utilizing ensemble feature selection (EFS) and techniques with a minimum of repetition and maximum of relevance, a collection of important features was chosen. The logistic regression, radial-based SVM (RBSVM), linear SVM, K-nearest neighbors and random forest classifiers were utilized to train the decision models. The study [19] begins with an adaptive feature recalibration (AFR)-based multi-resolution convolutional neural network (MRCNN) feature extraction component was used. The AFR can enhance the value of the features extracted by predicting the connections among the features, while the MRCNN can extract high and low-frequency characteristics.

3. Classification

In this section, we discuss ADHD treatment in adults and children, the prediction of drug dosage and half-life using deep learning. Figure 1 shows the flow of the proposed method.

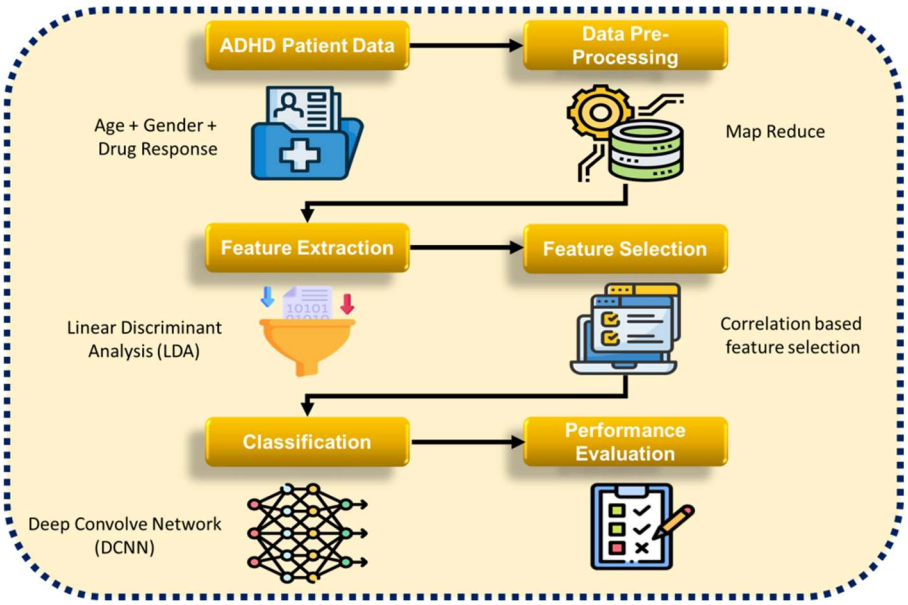

Figure 1: Proposed method's flow diagram

3.1 Data collection

The methodology involves generating a synthetic dataset for ADHD medications, specifically Adderall XR and Concerta. It defines various parameters, including age groups, genders, and drug attributes and simulates 2000 patient entries. For each drug, a set of dosage rules is established, which recommend specific dosages based on age groups. This synthetic dataset allows for the creation of patient profiles with associated drug dosage guidelines, making it conducive for researching the connection between patient characteristics and medication dosages in the realm of ADHD treatment.

3.2. Data pre-processing using Map Reduce

The MapReduce structure is a system that facilitates the processing of massive data by distributing the data as discrete subsets from clusters and offers optimistic results. To prevent major problems, the enormous volume of information is divided into subgroups and its relationships must be confirmed, while result set aggregation produces structured data. Depending on their size and data linkages, the data should be grouped. The data processing might be combined to create a cluster if it requires another data output as its input. The cluster might be created depending on the processing needs of the data clusters. This technique is utilized for distributing datasets over several clusters, known as filtering, executed by the function of a map and for producing computing results with the aid of aggregation, which is the operation of reducing. The handling of unrelated data elements uses the map, join and reduce method. The outcomes of this technique are mixed up. The following two major phases are used by the MapReduce algorithm:

- Map phase
- Reduce phase

3.2.1 Map Phase

The Map function is used as the initial stage in the MapReduce algorithm implementation. It splits the supplied datasets into a number of small pieces. The necessary computation is carried out on each subunit.

3.2.2. Reduce phase

It requests a set of sorted key-value pairs from the map function that does a reduction operation. Here, the output values from the map phase are combined. This step is in charge of consolidating the whole dataset and the reducer stage computes the weight parameter. It combines advantages from the map stage and produces a single output result.

3.3 Feature extraction using linear discriminant analysis (LDA)

To reduce dimensionality, linear discriminant analysis (LDA) was employed. LDA maintains potential discriminative data while reducing dimensionality. It seeks to identify the boundaries close to the groups of classes and projects the line of data points in a way that keeps the clusters formed as far apart as feasible, using every cluster having a reasonably close proximity to a given centroid. There are two methods for reducing dimensions. The first one is feature extraction and the second one is feature selection. To reduce dimensionality, LDA employs a method called feature extraction. By obtaining fresh independent variables, LDA distinguishes the majority of groups of the variable that depends.

If we consider two classes and $\mu_1 \& \mu_2$, their mean of the samples used to extract the features can be expressed numerically as

$$\omega = T_{\omega}^{-1}(\mu_1 - \mu_2) \quad (1)$$

Where, $\omega$is the biggest eigenvalue of the eigenvector that corresponds to $T_{\omega}^{-1}T_a$.

Here, $T_{\omega} = T_1 + T_2$ (2)

T_1 and T_2 are the scatter matrices for classes 1 and 2. Additionally, the calculation for T_a is,

$$T_a = \frac{1}{D}\sum_{j=1}^{D} \left(\mu_j - \mu\right)\left(\mu_j - \mu\right)^S \quad (3)$$

Here, S is a threshold.

3.4 Feature selection using Correlation-based Feature selection (CFS)

Multivariate filters for CFS alleviate the disadvantage of univariate filters for information acquisition, which is that they consider interactions among characteristics. CFS assesses a subset of characteristics' value by taking into account the degree of duplication among them as well as the unique ability to predict each feature. The estimation of the correlations amongst the characteristics, as well as the inter-correlations between them, is done using correlation coefficients. When features and classes are correlated, the relevance of a collection of characteristics increases and when inter-correlation is correlated, it decreases. With the goal of increasing model performance and decreasing computational complexity, it is important to minimize the dataset's dimensionality while keeping the most valuable characteristics. Equation (4) is the formula provided for CFS.

$$q_{yd} = \frac{l\,\underline{q_{yj}}}{\sqrt{l+l(l-1)\underline{q_{jj}}}} \tag{4}$$

where q_{ye} is the relationship among the cumulative feature subsets and the class variable, l is the number of features in a subset, q_{yj} is the mean of the correlations among the variable of the class and the subset characteristics and q_{jj} is the average correlation between the characteristics of the subgroup.

3.5 Deep Convolve NeuroNet (DCNN)

The spatial organization of the inputs is utilized by a subtype of neural network called DCNN. Convolutional and pooling layers are alternated in the usual framework for DCNN models, with the pooling layers coming after the convolutional layers. Figure 2 depicts the structure of DCNN. Using stochastic gradient descent (SGD) backpropagation, DCNNs are trained to discover biases and weights that reduce the loss functions and map random inputs to desired outputs as feasible.

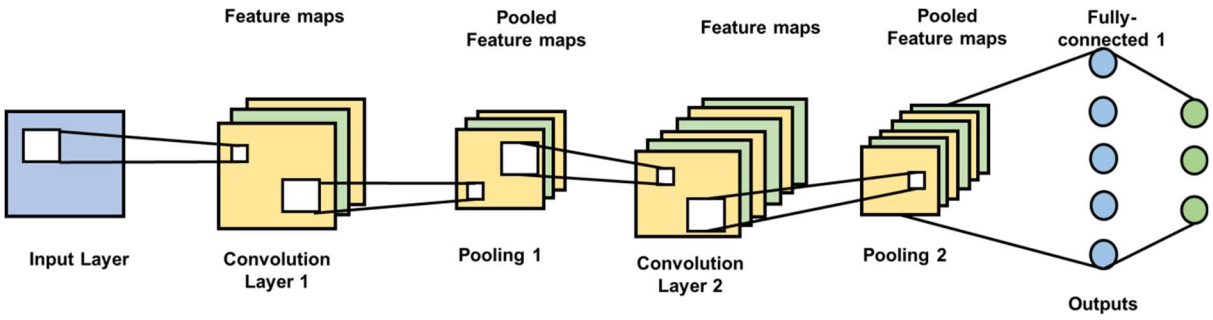

Figure 2: Architecture of DCNN

In order to extract local features from the input, a collection of learnable kernels or filters make up the convolutional layer. A feature map is produced by computing every kernel. A small part of the input, known as the reception field, is accessible to the elements of the feature map. The frequency

of a new feature map is created by applying it to the input filter, calculating the resultant dot product and adding non-linearity to the model using a non-linear activation function. Every unit on every feature map has equal weight. Sharing weights results in smaller constraints and the capacity to recognize the same characteristic irrespective of where it appears in the inputs.

These include sigmoid, tanh and ReLU, among other nonlinear functions for activation. ReLU $[e(w) = max\ (0, w)]$ is chosen, nevertheless, as it allows for training to proceed more quickly than the others. This feature map's output size is dependent on the length and stride of the filter, therefore when convolving the size of the input image (GXG) above a filter that is the size of (EXE), the stride of (T), the resulting size of output (XxX) is determined by

$$X = \lfloor \frac{G-E}{T} \rfloor + 1 \quad (5)$$

The preceding feature maps' density is lowered by the layer of down-sampling or pooling. Invariability to a little distortion or change is produced via pooling. The inputs are divided into disconnected areas with a size of (QXQ) by pooling, which results in one output from every region. Max or average-based pooling is possible. The output size will be determined by the following formula if an input of size (XxX) is sent to the pooling layer:

$$O = \lfloor \frac{X}{Q} \rfloor \quad (6)$$

DCNNs have at least one linked upper layer that resembles neural networks and is designed for the inputs to be extracted as overall attributes. Units between these layers are related to every concealed unit in the layer above them. In the very final layer, a classifier using softmax calculates the posterior likelihood of every class labeling over L classes, as shown by Equation (7).

$$z_k = \frac{expexp\ (-y_s)}{\sum_{i=1}^{L} exp(y_i)} \quad (7)$$

In this approach, a structural hyperparameter (∧) that captures the following information about the design of the DCNN architecture is used to specify our learning method for the DCNN (λ):

$$\lambda = \left(\left(\lambda_1^j, \lambda_2^j, \lambda_3^j, \lambda_4^j \right)_{j=1,N_d}, \left(\lambda_1^i \right)_{i=1,M_e} \right) \quad (8)$$

where $\lambda \in \Psi$ specifies each hyperparameter's domain, (N_d) shows the number of layers in a convolutional and (M_e) the number of connected layers (i.e., the depth = N_d+M_e). There are four hyperparameters that need to be determined before building any convolutional layer. For instance, for the layer of convolutional j: λ_1^j the number of filters, λ_2^j the size of the filter and λ_3^jspecifies the sizes and locations of the pools. If λ_3^jequivalent to one, this means the convolutional layer is shown by no pooling layer j. A pooling layer follows the convolutional layer j and the value $\lambda i3$ determines the size of the area of pooling$\lambda_4^j$is stride step. $\lambda_5^j$is the quantity of totally linked units in layer i. We also use $k(\Lambda,\ S_{SQ},\ S_U)$to consider the validity loss (e.g., classification error)

acquired after training a model Λ with the training set (S_{SQ}) and the validation set and assess it (S_U). Our framework's goal is to maximize the interaction of organizational hyperparameters$\lambda *$, which minimizes the classification error by designing the architecture for a given dataset in the manner described below:

$$\lambda^* = argmin\ k\left(\Lambda, S_{SQ}, S_U\right) \tag{9}$$

4. Result and discussion

In this section, we detail the drug dosage and half-life prediction for ADHD treatment in adults and children. Using an Intel Core i7 computer with 40 GB of RAM, the DCNN runs. Python was used to implement our suggested model once it had been trained on an NVIDIA GTX 1070 GPU. The performance evaluation parameters are accuracy, precision, recall and F1-score. The existing methods of Random Forest (RF) [20], K-Nearest Neighbour (KNN) [20], and Support Vector Machine (SVM) [20] are used in this study.

$$Accuracy \rightarrow \frac{TP}{TP+FP+FN+T} \tag{10}$$

$$Precision \rightarrow \frac{TP}{TP+FP} \tag{11}$$

$$Recall \rightarrow \frac{TP}{TP+F} \tag{12}$$

$$F1-score \rightarrow 2 * \frac{(Precision \times Recall)}{(Precision+Recal\ )} \tag{13}$$

4.1 Classification result

4.1.1 ROC curves and AUC scores

Comparing the area under the curve (AUC), receiver operating characteristic (ROC) and classification accuracy (CA) of each classifier for response to therapy and classification accuracy of various techniques. Figures 3 and 4 present the proposed method DCNN's ROC curves and AUC score for each class.

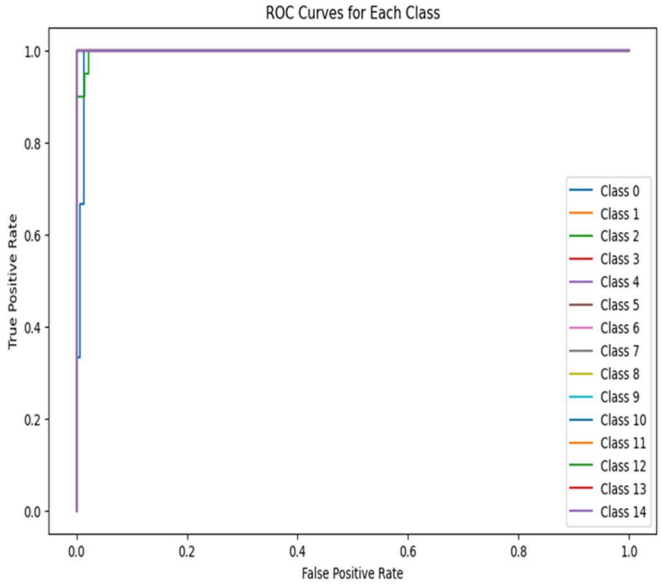

Figure 3: ROC curves for each class

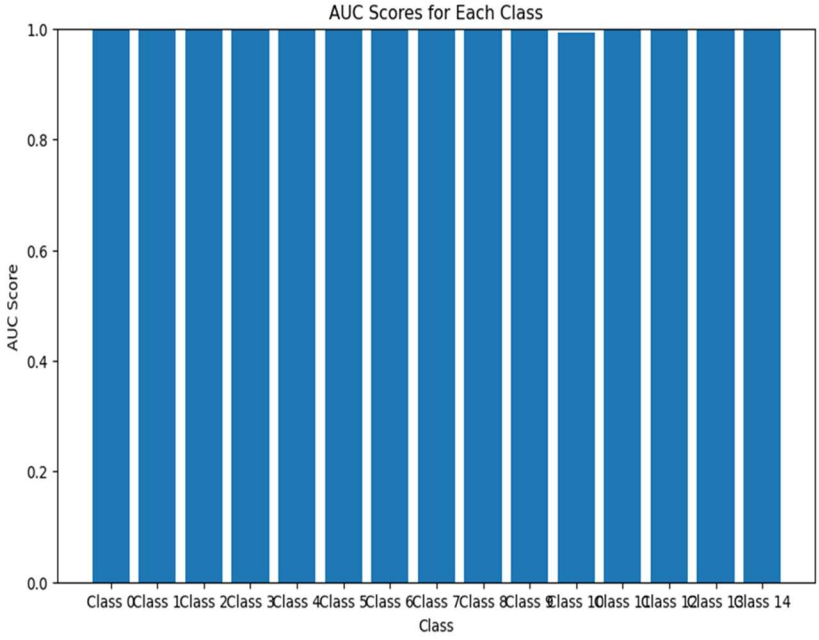

Figure 4: AUC scores for each class

4.2 Comparison with other techniques

To get the therapeutic advantages of ADHD drugs while reducing any dangers or side effects, predicting the right dosage is crucial. According to the patient's age, weight, metabolism and unique reaction, accurate dose prediction guarantees that they receive the right quantity of medication. The accuracy value is expressed in the equation (10). Figure 5 and Table 1 show the accuracy comparison of the suggested DCNN and alternative procedures. Whereas SVM, RF and

KNN succeed with 93.45%, 92.65% and 89.76% accuracy, respectively, the suggested technique of DCNN achieves 97.5% accuracy.

Table 1: Outcomes of proposed and existing methods

Methods	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)
SVM [20]	93.45	89.32	90.63	91.8
RF [20]	92.65	90.14	87.73	88.7
KNN [20]	89.76	92.78	93.8	89.53
DCNN [Proposed]	97.5	98	97	97

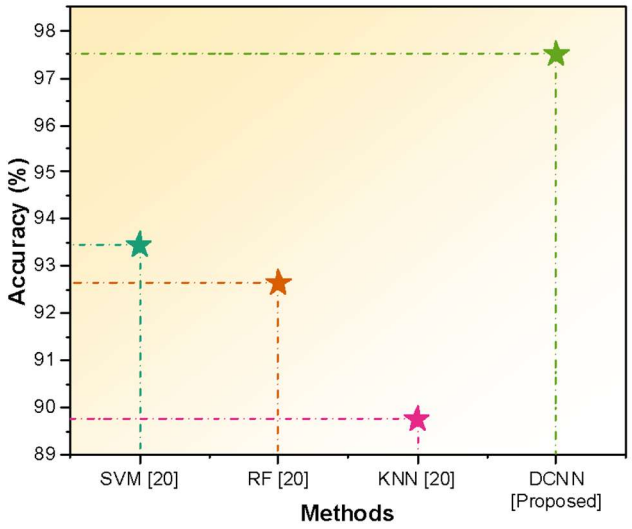

Figure 5: Accuracy comparison of the DCNN with existing methods

When estimating the precise dosage of medication a patient needs, precision in drug dosage prediction refers to the consistency and accuracy of the calculation. This precision is attained by accounting for individual elements, including age, weight, metabolism and the patient's particular reaction to the medicine. Figure 6 depicts the precision comparison of the suggested DCNN and existing methods. Whereas SVM, RF and KNN succeed with 89.32%, 90.14% and 92.78% precision, accordingly, the proposed method DCNN reaches 98% precision. The precision value is represented in equation (11).

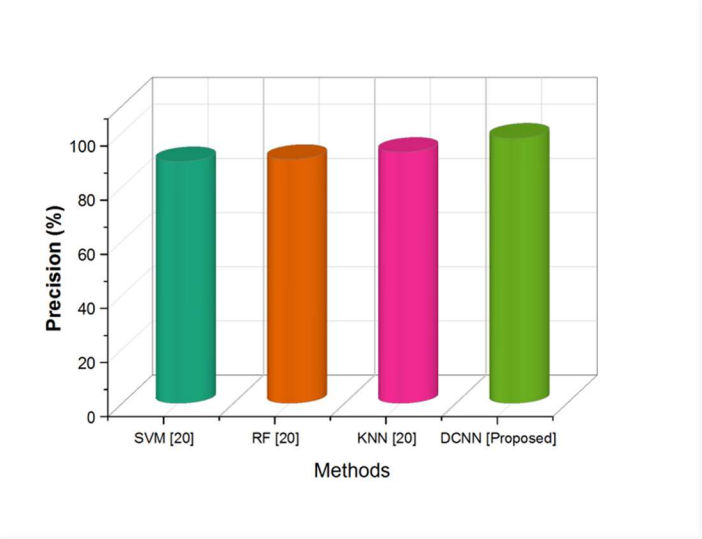

Figure 6: Precision comparison of the DCNN with existing methods

When predicting medicine dose, recall is the capacity to recall and consider pertinent patient-specific information. In drug dose estimation, high recall ensures that important data are not missed, assisting in preventing both under- and overdosing. Figure 7 denotes the recall comparison of the suggested DCNN and existing methods. SVM, RF and KNN achieve 90.63%, 87.73% and 93.8% accuracy, respectively, as a result, the suggested approach, DCNN, achieves 97% recall. Equation (12) illustrates the recall value.

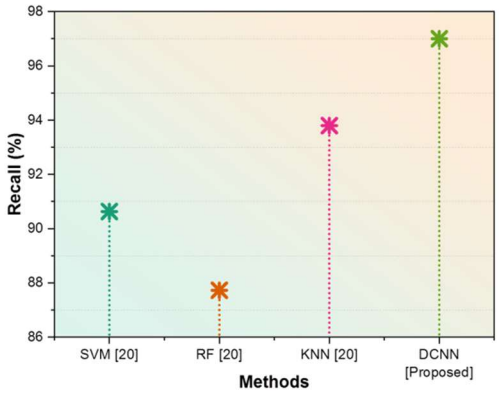

Figure 7: Recall the comparison of the DCNN with existing methods

A high F1-score indicates crucial patient-specific factors were taken into account and the dose estimate was correct. As a result, the best symptom management is achieved while the dangers of under-dose or over-dose are minimized. The F1-score comparison between the proposed DCNN and existing methods is shown in Figure 8. The proposed method, DCNN, achieves a 97% F1-

score, whereas SVM, RF and KNN manage 91.8%, 88.7% and 89.53% F1-score, respectively. Equation (13) shows the F1-score value.

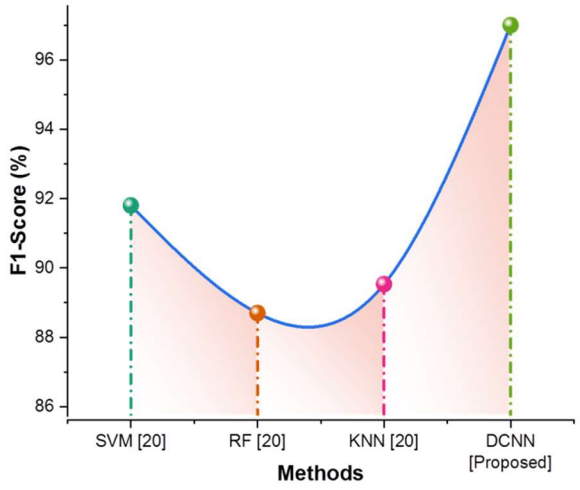

Figure 8: F1-score comparison of the DCNN with existing methods

5. Conclusion

ADHD is a general neurodevelopmental condition that affects people of all ages and presents particular difficulties for successful treatment. In this study, Deep Convolve NeuroNet (DCNN) technology, supported by sophisticated data preparation and feature extraction techniques, is used to improve medicine dose levels for treating ADHD. Our study dataset consists of clinical records of ADHD patients, which include crucial demographic data like age and gender as well as useful information on treatment response. The key contribution entails the use of a DCNN architecture that has been trained to predict the ideal medicine dose amount for each patient. The result shows the proposed method achieves high accuracy (97.5%), precision (98%), recall (97%) and F1-score (97%). Further improving medicine dose recommendations is the development of sophisticated machine learning algorithms, such as reinforcement learning methods, which promise to capture complex interactions in patient profiles.

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