

GEFA: A Novel Early Fusion Method for Enhancing Drug-Target Affinity Prediction Accuracy

Mr.K.Naresh¹., T.Sravanthi²

*1 Assistant Professor, Department of CSE, Malla Reddy College of Engineering for Women.,
Maisammaguda., Medchal., TS, India
2, B.Tech CSE (19RG1A0554),
Malla Reddy College of Engineering for Women., Maisammaguda., Medchal., TS, India*

Article Info

Received: 30-06-2022

Revised: 18-08-2022

Accepted: 29-08-2022

ABSTRACT

Aiming to improve the accuracy of CNN-based doctor recommendation systems, this research contrasts XGBoost (XGB) with CNNs. College-Related Materials: In this research, the accuracy was evaluated using two deep learning models: XGBoost (XGB) and CNN. The sample size was N=10, and the power was 80%. A significance score of ($p=0.144$) ($p<0.05$) indicates that the statistical analysis did not find a significant difference between the two groups studied in this study. Compared to XGB's 88.19% accuracy rating, CNN's is far higher at 90.15 percent. Lastly, we compare the XGBoost method to a medical recommendation system that uses Convolutional Neural Networks (CNNs). When it comes to online doctor recommendations, CNN is obviously the superior algorithm when compared to XGBoost.

Keywords: Innovative Convolutional Neural Network, XGBoost, Health and Wellness, Machine Learning, Healthcare sector, Online physician referral.

INTRODUCTION

Websites that provide both medical consultations and services are becoming more popular. They are useful and alleviate a problem with medical supply shortages, which is common in less developed or remote areas. Possible incorrect diagnoses as a result of biased reporting, variations in physician quality, long response times, and

incompatible data formats are all issues. With a doctor recommendation system in place, patients' relations with their physicians are expected to undergo significant changes [1]. With the help of healthcare recommendation systems powered by technology, patients may get personalized medical recommendations. It

gathers information about the patient's symptoms and health history, then uses sophisticated algorithms and machine learning techniques to sift through mountains of data in order to provide informed recommendations [2]. The healthcare industry is severely lacking an accurate and dependable system that can suggest physicians and other specialists. By using the doctor recommendation system, patients are given a greater opportunity to find their ideal doctor among the vast medical sector. When consumers can use the doctor referral system to get in touch with competent medical experts, it improves their health and wellbeing. There are several applications for doctor recommendation systems in healthcare, such as research, patient education, referral management, clinical decision support, treatment recommendations, and disease diagnosis [3].

Doctor referral systems have long been the subject of heated debate among academics. There is a wealth of literature in this field; 195 papers in Google Scholar and 175 in IEEE Explore attest to that. Convolutional neural networks (CNNs) have been investigated by the doctor recommendation system. In order to provide patients with personalized recommendations, medical recommendation systems may use machine learning algorithms to filter through vast amounts of patient data, such as symptoms, medical histories, and more. Healthcare providers may help enhance patient-provider matching by making recommendations based on data trends and correlations. [4]. Furthermore, neural networks reliant on optimization for useful outputs were used in

this study. Research advancement relied heavily on the implementation of a mining-based strategy to medical treatment prescription [5]. The model was used to forecast the pharmacological dose. An approach to healthcare system development was proposed in [6]. There would be a dramatic shift in healthcare if referral systems included each patient's individual medical history, treatment choices, and other factors [7]. Incorporating wellness and health criteria into the doctor recommendation system will greatly benefit patients. Giving individuals more say in their healthcare choices, the doctor recommendation system suggests hospitals and physicians that would be the best matches for each person's requirements.

By continuously learning and improving, a healthcare recommendation system powered by machine learning algorithms can ensure that the ideas it offers are relevant and up-to-date. Patients may report more happiness and better health outcomes if they are matched with healthcare professionals who are a good fit for their unique needs. Patients may find qualified doctors to consult with online using the website's referral system. Efficiency gains, cost reductions, and happy patients could be in store for us with the doctor recommendation system. [10] A medical recommendation system that prioritizes wellness might enhance patients' healthcare costs and overall quality of life. The potential for efficiency benefits was under-considered in earlier studies that attempted to forecast the physician referral system's accuracy. The goal of this research is to identify the most qualified medical

professional from a group of applicants by using deep learning techniques.

MATERIALS AND METHODS

The project's training and testing were conducted at the Saveetha Institute of Medical and Technical Sciences' Computer Science Engineering Department. Twenty samples were used in this experiment to test the Novel CNN classifier. We ran the statistical analysis for this study using IBM SPSS version 26, software developed by IBM. Considering the elements listed below: We calculated the sample size for each group using the G Power calculator, taking into account the following parameters: 80% pre-test power, 0.95 alpha error, 0.05 threshold, and 95% confidence level.

An 8 GB RAM, 1 TB storage, AMD Ryzen 5 5500U, and Radeon Graphics 2.10 GHz laptop running Windows 11 was used for all of our research and testing. This study examines the Doctor recommendation system using data gathered from kaggle.com [8]. The data used by the system for doctor recommendation likewise originated from this location and was stored in.csv format [8]. Each tactic's efficacy was determined by conducting separate T-test examinations.

CONVOLUTIONAL NEURAL NETWORK

When it comes to image processing and recognition, convolutional neural networks (CNNs) are the deep learning algorithms of choice. Doctor recommendation systems may leverage new convolutional neural networks (CNNs) to sift through patient

evaluations, medical records, and doctors' profiles for pertinent information, which can then be used to provide individualized recommendations for patients. New Convolutional Neural Network (CNN) algorithms may be able to learn to recognize correlations and patterns in data by examining input across many levels. It is possible to utilize these correlations and patterns to make predictions or suggestions. Systems that connect patients with physicians can potentially function more efficiently and effectively using this technology. One big problem with multilayer perceptrons is that, being fully linked networks, the input will likewise have a lot of weight. Using multilayer perceptrons, novel convolutional neural networks (CNNs) may be trained. As a result of this limitation, multilayer perceptrons can only have a certain number of layers and neurons within each layer. Absolute values of the effective parameters are often less than 1 since the activation function needs to adjust neuronal output. The input and output of each neuron must also be in harmony. To get the values down via back propagation, you have to multiply a bunch of integers by one [11].

Pseudocode for Convolutional Neural Networks

Step 1: Bring in the data and read it out..

Step 2: Load required libraries.

Step 3: carry out data preprocessing.

Step 4: Sorting datasets into different categories.

Step 5: Get all three layers—the convolutional, pooling, and fully connected—finished.

Step 6: Put the taught data through its paces.

Step 7: Find out how precise.

XGBoost

A gradient descent architecture is used by the XGBoost ensemble tree strategy to enhance low-performing learners. One way to find XGboost is to check the membership list of the Distributed Machine Learning Community (DMLC). When it comes to tree-based model-operating, lightning-fast machine learning algorithms that aim for best-in-class accuracy while optimizing CPU utilization, XGBoost is head and shoulders above the competition. The XGBoost algorithm, developed by Tianqi Chen and made famous by Kaggle, has been generating quite a stir at the last hackathons. A popular and open-source machine learning technique, Extreme Gradient Boosting (or XGBoost for short) is renowned for its speed and efficiency. This tree-based parallelized algorithm is ideal for massive datasets including both structured and unstructured data, and it is both scalable and efficient [12]. Notable applications that rely on it include recommendation systems, computer vision, and (NLP) because to its efficiency and versatility.[13]. An XGBoost-powered doctor recommendation system excels at providing patients with personalized, expert advice [14]. Healthcare may be tailored to each patient's unique needs and circumstances with more accurate and relevant recommendations [15].

Algorithm

Step 1: Bringing in the required library files.

Step 2: Make sure you load the dataset..

Step3: The dataset should undergo preprocessing, which include cleaning and transforming the data.

Step 4: To begin, do exploratory data analysis after showcasing the data.

Step 5: Make a distinction between the "train" and "test" sets of data.

Step 6: Confirm the information.

Step 7: For data training and testing, use an innovative XGBoost.

Step 8: Be exacting.

STATISTICAL ANALYSIS

The Doctor's Recommendation is evaluated and executed using Python, with accuracy values provided by important features. For statistical assessments of the Python compiler's output, we use IBM SPSS version 26 software in conjunction with the Python Google Collab tool [16]. The review, rating, and ID are treated as separate entities. Interdependent model output parameters are the accuracy variables. The XGB and CNN algorithms were compared using an independent t-test.

RESULT

As shown in Table 1, the results of a Google Collaborative Run were used to compare the accuracy of a CNN-based doctor recommendation system with that of an XGBoost algorithm. Twenty participants made up the sample. The XGBoost algorithm has little chance against CNN when it comes to accuracy.

According to Table 2, the accuracy rates for the CNN and XGB algorithms were 96.20% and 2.02133, respectively, with a mean of

90.522% and a standard deviation of 2.74677. The CNN's standard error was 0.63920 lower than the XGB's. Independent sample t-tests reveal a statistically significant disparity in accuracy between the two approaches.

According to Table 3, the results of the independent sample tests showed that the proposed two-stage approach was much more accurate than the conventional one-stage technique. The p-value is less than 0.05 ($p=1.44$), indicating that there is no statistical difference between the two approaches.

Both the traditional approach and the suggested over-selected input were able to effectively complete the accuracy and mean accuracy computations, as seen in Figure 1. Investigating the average accuracy of XGB and CNN-based online medical recommendation systems. The suggested procedure achieved a mean accuracy of 90.28%, which was higher than the standard approach's 89.19%. The CNN and XGB accuracy levels are shown on the X-axis, while the mean accuracy plus or minus one standard deviation is shown on the Y-axis.

DISCUSSION

By using deep learning methods, the suggested method seeks to enhance the efficacy of doctor referral systems. In terms of accuracy, CNN-based classifiers outperform XGB. Compared to XGB's accuracy of 89.19%, CNN's accuracy of 90.28% is much better. The statistical analysis determined that the CNN and XGBoost algorithms are separate from one another with a p-value of 0.144 ($p<0.05$).

By incorporating medical data from Novel CNN and review text, the model is trained to provide more accurate consultation recommendations. By training CNN on review text and doctor data, we can learn to describe them using features. The augmented CNN model also incorporates the review information element into its recommendation process, in addition to the initial value of the doctors' data. The suggestion system of a medical website allows professionals to make more efficient use of public health resources. [17]. The health-based recommender system is a decision-making tool that might benefit doctors and patients alike. This technology allows clinicians to gather crucial data for treatment suggestions, improve patient care, and teach people self-management skills to reduce their risk of sickness. in [18] in This HRS must be reliable and trustworthy since the end users, the patients, rely on it. The physician recommendation system sheds light on trends and patterns in health and fitness, which helps physicians make informed judgments.

While there are many benefits to using doctor recommendation systems, people should be mindful of the risks involved. Accuracy issues, impersonal service, problems navigating complex situations, privacy worries, and reliance on technology to an unhealthy degree are all part of these downsides. By working together with real doctors, doctor recommendation systems might help patients get the best care possible. To make sure these technologies don't take the place of human doctors, it's

important to know what they can't accomplish.

CONCLUSION

This research compares the algorithms' accuracy and introduces a novel approach to medical recommendation making based on CNN. The lack of statistical significance is due to the fact that $p=0.144$ ($p<0.05$). When looking at doctor recommendation systems, the findings reveal that CNN(90.15%) performs better than XGBoost (89.19%).

DECLARATIONS

Conflict of Interest

This work is free of any conflicts of interest that the authors may have..

Author Contributions

Statisticians, writers, editors, and text processors all fall within the purview of Author SMB. Author PGR is involved with the manuscript's conception, validation of statistics, and critical review.

Acknowledgement

The author is very grateful to Saveetha University, namely the Saveetha School of Engineering and SIMATS, for facilitating the research work and providing the necessary resources.

Funding

The following group's financial backing allowed us to finish the research, and we are grateful to them.

1. InfySec, Chennai.
2. Saveetha School of Engineering.
3. Saveetha Institute of Medical and Technical Sciences.
4. Saveetha University.

REFERENCES

- [1] H. Singh, M. B. Singh, R. Sharma, J. Gat, A. K. Agrawal, and A. Pratap, "Optimized Doctor Recommendation System using Supervised Machine Learning," *Proceedings of the 24th International Conference on Distributed Computing and Networking*. 2023. doi: 10.1145/3571306.3571372.
- [2] G. Chauhan and A. Chaudhary, "Crop Recommendation System using Machine Learning Algorithms," *2021 10th International Conference on System Modeling & Advancement in Research Trends (SMART)*. 2021. doi: 10.1109/smart52563.2021.9676210.
- [3] K. S. M. Anbananthen *et al.*, "An intelligent decision support system for crop yield prediction using hybrid machine learning algorithms," *F1000Res.*, vol. 10, p. 1143, Nov. 2021.
- [4] M. L. Islam, K. Alam, A. Ansari, and K. Godambe, "Doctor Recommendation and Appointment System," *International Journal of Computer Sciences and Engineering*, vol. 7, no. 2. pp. 610–613, 2019. doi: 10.26438/ijcse/v7i2.610613.
- [5] L. Ronquillo, V. Zamudio, D.

- Gutierrez-Hernandez, C. Lino, J. Navarro, and F. Doctor, "Towards an automatic recommendation system to well-being for elderly based on augmented reality," *2020 16th International Conference on Intelligent Environments (IE)*. 2020. doi: 10.1109/ie49459.2020.9155010.
- [6] G. Dhabal, J. Lachure, and R. Doriya, "Crop Recommendation System with Cloud Computing," *2021 Third International Conference on Inventive Research in Computing Applications (ICIRCA)*. 2021. doi: 10.1109/icirca51532.2021.9544524.
- [7] B. Ihnaini *et al.*, "A Smart Healthcare Recommendation System for Multidisciplinary Diabetes Patients with Data Fusion Based on Deep Ensemble Learning," *Comput. Intell. Neurosci.*, vol. 2021, p. 4243700, Sep. 2021.
- [8] C. Prasitpuriprecha *et al.*, "Drug-Resistant Tuberculosis Treatment Recommendation, and Multi-Class Tuberculosis Detection and Classification Using Ensemble Deep Learning-Based System," *Pharmaceuticals*, vol. 16, no. 1, Dec. 2022, doi: 10.3390/ph16010013.
- [9] I. Journal and IJSREM Journal, "Smart Farming-Crop Recommendation System," *INTERANTIONAL JOURNAL OF SCIENTIFIC RESEARCH IN ENGINEERING AND MANAGEMENT*, vol. 06, no. 11. 2022. doi: 10.55041/ijsrem16989.
- [10] Taylor & Francis Group, *Asian Medical Industries: Contemporary Perspectives on Traditional Pharmaceuticals*. Routledge, 2021.

TABLES AND FIGURES

Table 1. Convolutional Neural Network improved the accuracy of the doctor recommendation system's prediction system (90.15%) compared to XGBoost (89.19%).

Iteration No.	Convolutional Neural Network	Extreme Gradient Boosting (XGB)
1	93.46	89.25
2	93.72	89.50
3	94.44	90.00
4	95.00	90.25
5	95.33	90.59
6	97.05	90.76
7	97.92	91.01
8	98.11	92.42
9	98.33	94
10	98.64	94.91
Accuracy	90.15	89.19

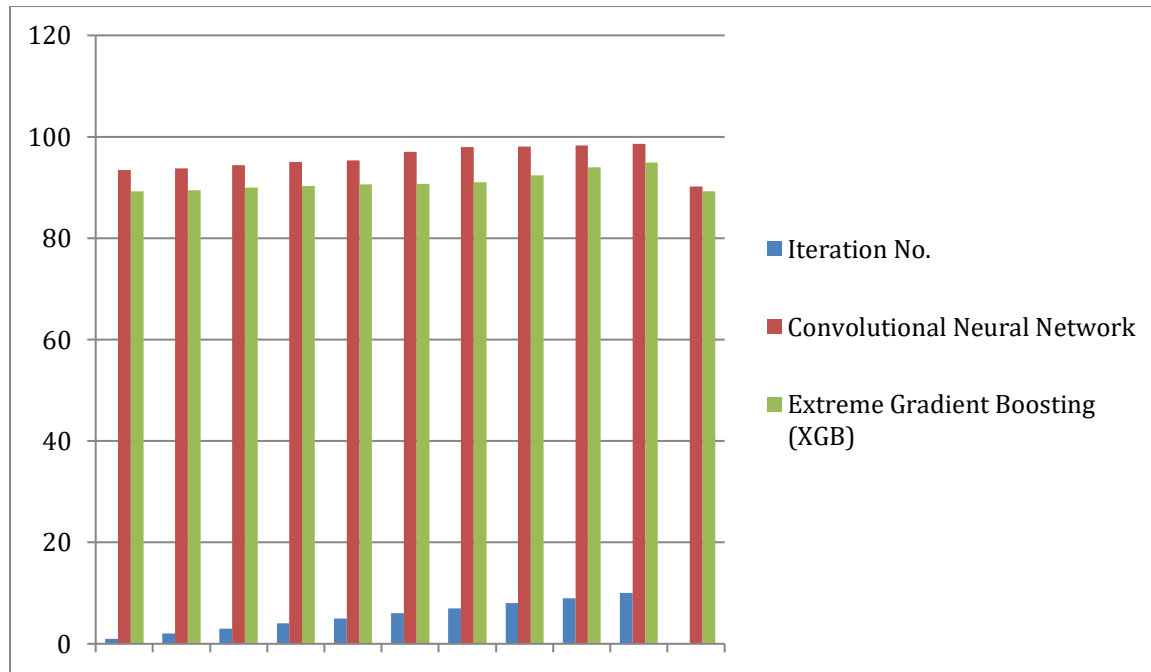


Table 2: The CNN obtained an accuracy of 89.192% with a group standard deviation of 2.02130 and an XGB standard deviation of 1.29770. Ninety-0.28% was the average for the group. The CNN's standard error was.63920 lower than the XGB's.

Group Statistics					
	GROUP NAME	N	Mean	Dispersion measure	Probability of Error
Accuracy	CNN	10	96.200	2.02130	.63920
	XGB	10	89.192	1.29770	.86861

Table 3: Based on the results of an independent sample test, the two-stage procedure that was suggested was more accurate than the gold standard one-stage methodology. There is a significant difference between the two approaches since $p < 0.05$ and ($p = 0.144$) is less than 0.05.

A Test of Independence for a Sample										
Checking for Equality of Variances using Levene's Test				T-test to determine whether means are equal						
		F	Sig.	T	Df	Notable (2-tailed)	Average Distinction	Differences in Standard Errors	Range of Percentage Determination for the Distinction	
									Lower	Upper
Accuracy	Presumed to be equal variances	.159	.695	1.526	18	.144	2.125	1.392	-.80025	5.05025
	No assumption of equal variances made			1.526	17.85	.144	2.125	1.392	-.80195	5.05195

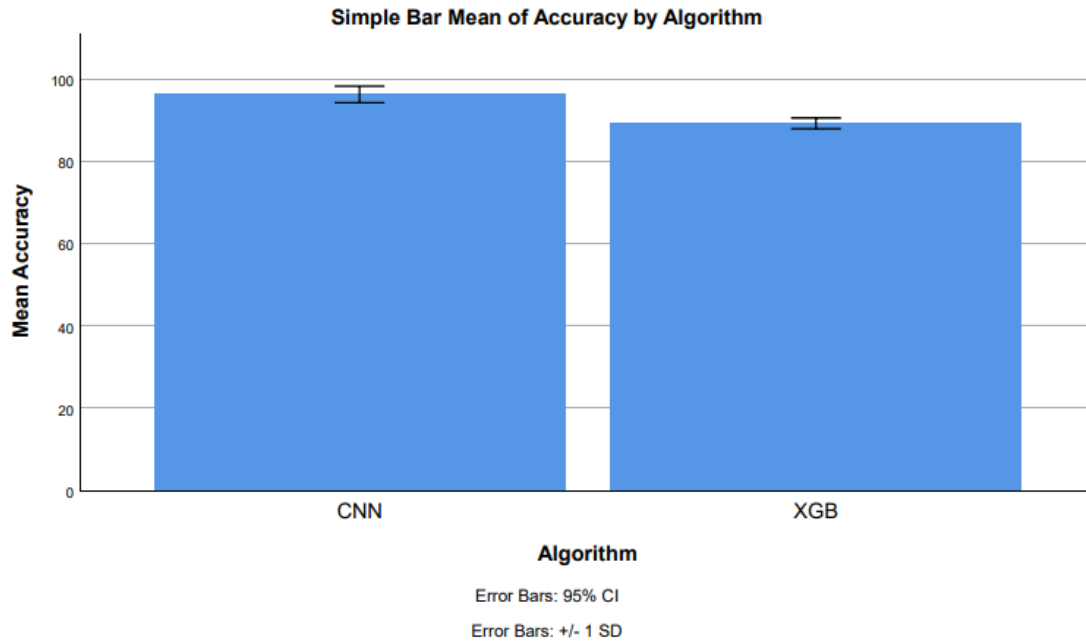


Fig. 2. Compare and contrast the online medical advice services offered by CNN and XGB. The suggested procedure achieved a mean accuracy of 90.28%, which was higher than the standard approach's 89.19%. The CNN and XGB accuracy levels are shown on the X-axis, while the mean accuracy plus or minus one standard deviation is shown on the Y-axis.