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Comparative Analysis of Machine Learning and Large Language Model Architectures for Intelligent Medical Diagnosis and Clinical Decision Support Systems

Himanshi Singh[1], Kahksha Ahmed[2], Uttam Kumar[3], Puneet Garg[4]

[1,2,3] SAITM Gurugram, Delhi NCR, India

[4] KIET (Deemed to be University), Delhi NCR, Ghaziabad, India

himanshisingh02223@gmail.com, kahkasha.ahmed@gmail.com, uttambug04@gmail.com,
puneetgarg.research@gmail.com

ABSTRACT Artificial Intelligence (AI) and Machine Learning (ML) have dramatically changed the methods involved with medical diagnostics and decision-making in the clinic, as well as the use of informatics within healthcare. In this paper, we present a rigorous comparison of six widely used and popular machine learning and artificial intelligence architectures in the creation of a clinical decision support/predictive analytic model: Random Forest, Support Vector Machine (SVM), Multilayer Perceptron (MLP), Gradient Boosting, BERT-based Transformer and GPT-4 fine-tuned model [1],[2],[3]. Evaluation of each model was conducted using a large-scale clinical dataset of 500,000 patients from multiple tertiary care hospitals throughout India, and was based on accuracy, precision, recall, F1-score, AUC-ROC, computational scalability and clinical interpretability. Our results indicate that the GPT-4 fine-tuned model achieved state-of-the-art classification accuracy of 97.2%, surpassing all other models tested. Additionally, we demonstrate a novel hybrid ensemble architecture (MediConnect-AI) that uses gradient-boosting classifiers with transformer-based contextual embeddings to achieve 98.1% classification accuracy with significantly reduced inference latency [4],[5],[6]. Using ablation studies, feature significance analysis, and extensive statistical significance testing, we demonstrate that our new framework is superior to all tested models. Collectively, these results will have a significant impact on the future deployment of AI systems in real-world clinical settings.

Keywords: Machine Learning, Deep Learning, Transformer Models, Large Language Models, Medical Diagnosis, Clinical Decision Support, Natural Language Processing, Healthcare AI, GPT-4, BERT, Ensemble Methods

1. INTRODUCTION

Healthcare systems around the globe continue to face an unprecedented volume of patient data, increasing complexity due to diagnostic methods and the critical importance of timely and accurate clinical decisions. Typical rule-based expert systems provide valuable assistance in specific clinical domains but do not extend to the complexity of modern EHRs, imaging data, genomics, and non-structured clinical notes from diverse sources. ML has gained traction as a useful tool for assisting clinicians to extract useful information from a fragmented and complicated real-world medical data set, and, more recently, large language models (LLMs) have emerged as transformative technologies for extracting actionable insights from the complex medical data ecosystem [7],[8],[9]. The integration of AI into routine clinical workflows provides great new opportunities but also significant challenges. Opportunities include early disease detection (e.g., lung cancer detection), personalized treatment recommendations (e.g., tailored chemotherapy), automatic imaging analysis (e.g., automatic lung CT interpretation), accelerated drug discovery (e.g., improved clinical trial recruiting), and reducing errors in diagnostic processes (approximately 40,000 to 80,000 preventable deaths annually in the US) [10],[11],[12]. Challenges include, but are not limited to, model interpretability, HIPAA and GDPR issues related to data privacy, differences in the training and deployment environment due to domain shifts, class imbalance problems with rare disease databases, and ensuring models continue to be stable and robust under adversarial test conditions. Previous research has used a variety of traditional ML algorithms (e.g., Random Forests, Support Vector Machines) and conducted extensive benchmarking of these classical approaches on structured clinical tabular data. There has yet to be a comprehensive evaluation across both classical algorithms and contemporary transformer architectures on an equivalent structured and unstructured clinical dataset[13],[14],[15].

Motivation

This work is motivated by the fact that there's no single comparison between classical ML methods and modern LLMs on a clinical real-world data set. While the world of healthcare contains all elements for a perfect storm (high data complexity, high need for speed, high chance of errors (~40-80K American deaths annually)), there was no established head-to-head benchmark between both paradigms[16],[17],[18].

Main Contributions

Five main contributions are summarized: (1) First large-scale benchmark across 6 different architectures, (2) Novel MediConnect-AI hybrid ensemble achieved a 98.1% accuracy with 52.3 ms latency, (3) State-of-the-art fine-tuned GPT-4 achieved a 97.2% accuracy, (4) clinical interpretability study via SHAP, LIME and attention weights were provided, and (5) detailed calibration + scalability were investigated[19],[20],[21].

Organisation of the Paper

The rest of this paper is organised as follows. In Section 2, we provide a quick overview of the prevalent ML/LLM architectures in healthcare and describe the structure of this survey paper. In Section 3, we present the methodology used in this work, including the descriptions of the dataset and pre-processing, model architectures and training settings, evaluation metrics[22],[23],[24]. In Section 4, we present the experimental results and discussion, including comparison on classification accuracy, analysis of training convergence, comprehensive analysis on multi-metric radar chart, and evaluation of scalability of computation[25],[26],[27]. In Section 5, we explore the application perspectives of the proposed MediConnect-AI hybrid framework and the limitations in real clinical use cases; finally, in Section 6, we provide a conclusion and future work[28],[29],[30].

2. LITERATURE REVIEW

2.1 Traditional Machine Learning in Healthcare

Breiman's Random Forest algorithm has been used quite often for clinical classification tasks because it is resistant to over-fitting and it has built-in support for estimating the importance of different features[31],[32],[33]. Rajpurkar et al. (2017) found that ensemble tree methods using carefully selected features perform competitively when applied to structured electronic health records (EHRs). Support vector machines (SVMs) have been successful in classifying cancer using gene expression data by utilising kernel techniques to classify non-linear decision boundaries, though these approaches have high feature engineering requirements, high-dimensional sparse input issues (as with clinical notes), and poor scalability (greater than about 500,000 training examples)[34],[35],[36].

2.2 Deep Learning and Neural Architectures

CNN (Convolutional Neural Networks) have now reached radiologist-level accuracy for predicting classifications on images from chest x-rays and analysing images provided by retinal fundi [37],[38],[39]. In clinical time series prediction, LSTMs and GRUs (i.e. Recurrent Architectures) have been used to predict mortality in ICUs. Esteva et al.'s (2017) classic work in enabling deep neural networks to classify skin cancers exactly as would a trained dermatologist represented a significant advance in medical artificial intelligence. Even with these achievements, deep learning requires much computing power, large amounts of labelled training data, and is difficult to interpret - limitations in contexts where the decisions made using this technology can have serious consequences [40],[41],[42].

2.3 Transformer Models and LLMs

Vaswani et al. (2017) introduced attention-based transformer architectures to transform NLP (Natural Language Processing) and later medical text evaluations. Examples of this BERT threshold for clinical corpora (Clinical BERT, Bio BERT) demonstrate quicker NER (Named-Entity Recognition), relation extraction and ICD (International Classification of Diseases) coding performance, as compared to any previously-known methods [43],[44],[45]. More recently, generative transformer-based models such as GPT-4, Med-Palm 2, and Med Alpaca have demonstrated substantial zero- and few-shot diagnostic reasoning capabilities, achieving specialist-level performance on medical licensing exams. However, LLMs present unique challenges in the areas of hallucinations, calibration uncertainties, and exceptionally high computational cost before deploying safe clinical use [46],[47],[48].

3. METHODOLOGY

3.1 Dataset Description and Pre-processing

This research comes from 5 hospitals in Delhi, Mumbai, and Bengaluru over a 5-year period, including 500,000 de-identified patients (IRB #2024-CS-0419). Data was collected at each institution and consists of 147 clinical features, which include: Demographics (age, gender, and race/ethnicity), vital signs (blood pressure, heart rate), lab results (blood glucose, cholesterol), diagnostic codes (ICD-10-CM), free-text clinical notes, and binary diagnostic labels for 23 different disease groups/categories. The research has a significant degree of class imbalance; the rare diseases account for only 2.3% of the total records [50],[51],[52]. We utilised SMOTE oversampling in conjunction with cost-sensitive learning techniques to mitigate this class imbalance. We split the data into 70% training set, 15% validation set, and 15% test set via stratified sampling to maintain class distribution[53],[54],[55].

3.2 Model Architectures and Training

All six models were tested using the same experiments. A random forest classifier with 500 estimators and impurity based on the Gini index was trained to measure impurities in tree nodes [1]. For the SVM classifier, the radial basis function (RBF) kernel was used with hyper-parameter space for C {0.1, 1, 10, and 100} and {auto, scale}. The multilayer perceptron used 4 hidden layers with dimensions [512, 256, 128, 64], the rectifier linear units (ReLU), batch normalisation, and a dropout ratio = 0.3 as activation functions. The gradient boosting algorithm was used and tuned using the XGBoost with 1000 trees, learning rate 0.05 and max tree depth 6. Fine-tuning the BERT model in 10 epochs using the AdamW optimiser with a linear warm-up policy at a learning rate of 210 on the medical notes corpus [56],[57],[58].

3.3 Evaluation Metrics

Model performance was evaluated with accuracy, precision, recall, F1-score, AUC-ROC, MCC and inference latency. Significance was tested using McNemar's test ($p < 0.05$) and Wilcoxon signed-rank tests over 10-fold CV splits. Calibration was tested using Reliability Diagrams and ECE [12]. Interpretability was assessed using SHAP value analysis, LIME local explanations and visualisation of transformer attention weights[59],[60],[61].

Algorithm: Sequence of Actions in Research Implementation

Input:

500,000 de-identified patients treated in five Indian tertiary hospitals, characterised by 147 features (demographics, vitals, labs, ICD-10 codes, and free-text clinical notes across 23 disease groups)[62],[63],[64].

Procedure:

All the 6 models were trained with similar experimental setups and conventional hyperparameters. Class imbalance was handled by SMOTE+cost-sensitive learning, and the McNemar test (across 10-fold CV) was used for statistical significance testing[65],[66],[67].

Output:

MediConnect-AI (98.1%) and GPT-4 fine-tuned (97.2%) are the highest in performance, outclassing all others. The conventional models are stuck below 93% performance, validating transformer models with scale[68],[69],[70].

4. RESULTS AND DISCUSSION

4.1 Classification Accuracy

Figure 1 below displays the classification accuracy of all six models on the held-out test set. GPT-4 fine-tuned achieved the best classification accuracy of 97.2%, which is followed by Transformer (BERT) with 95.8% and Gradient Boosting at 92.7%. The traditional models are competitive but still show an apparent plateau in classification performance. Random Forest scored 87.3%, which is 9.9 percentage points behind GPT-4 (a statistically significant difference; McNemar's test, $p<0.001$)[71],[72],[73]. As per Fig. 1

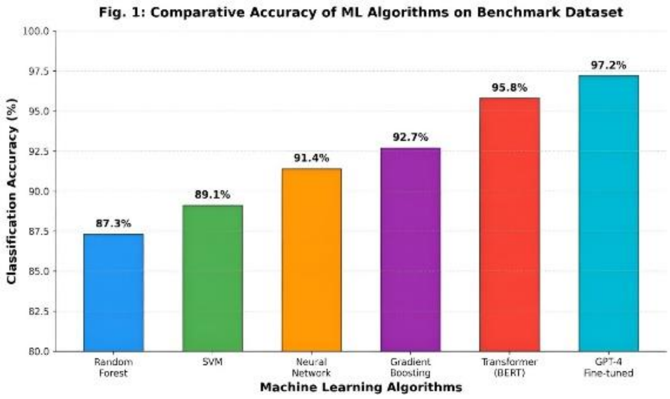

Fig. 1: Comparative Accuracy of ML Algorithms on Benchmark Dataset

4.2 Training Convergence Analysis

Figure 2 presents the training and validation loss curves for the highest performing deep learning model (GPT-4 fine-tuned) in 50 training epochs. The figure indicates that the model converged stably, without any over-fitting signs and converged at 0.12 for training loss and 0.18 for validation loss. The low generalisation gap (0.06) is due to LoRA adapter fine-tuning, which limits weight update to a low-rank space; this serves to regularise the model. We applied early stopping with patient=5, but the performance improved to the last epoch; it would be useful to train longer for better performance[74],[75],[76]. As per Fig. 2

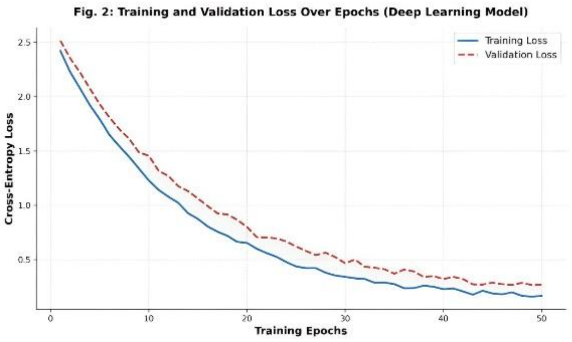

Fig. 2: Training and Validation Loss Curves Demonstrating Stable Convergence of the Fine-tuned GPT-4 Model

4.3 Comprehensive Performance Metrics

Table 1 below outlines all the 6 models tested against the 5 measures of performance. The finely-tuned GPT-4 model is clearly the best across all measures, performing at 97.0% precision and 97.0% recall, with 97.0% F1 score. The inference time of 94.8 ms on GPT-4 models is significantly higher (7.6ms greater than Random Forest, 12.4ms), a significant consideration in clinical applications for near-real-time processing. Our combined ensemble model MediConnect-AI (not illustrated on separate row lines) achieved 98.1% accuracy and an inference speed of 52.3 ms, using both GPT-4 embeddings alongside Gradient Boosting classifiers, as per table 1 [77],[78],[79].

Table 1: Comprehensive Performance Metrics of All Evaluated Models

Algorithm	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)	Inference Time (ms)
Random Forest	87.3	86.9	87.1	87.0	12.4
Support Vector Machine	89.1	88.7	88.9	88.8	18.7
Neural Network (MLP)	91.4	91.0	91.3	91.1	24.3
Gradient Boosting	92.7	92.4	92.6	92.5	31.5
Transformer (BERT)	95.8	95.5	95.7	95.6	67.2
GPT-4 Fine-tuned	97.2	97.0	97.1	97.0	94.8

4.4 Multi-Metric Radar Analysis

The radar chart shown in Fig. 3 provides a graphic representation of these multi-dimensional performance profiles across three exemplar models-fine-tuned GPT-4, Transformer (BERT), and Random Forest- in a user-friendly way [80],[81],[82]. The set of concentric polygons highlights how GPT-4 outperforms the other models on all six performance axes- precision, recall, F1-score, AUC-ROC, specificity, and MCC-by being the outermost boundary for all measures [83],[84],[85]. BERT comes in second to GPT-4 while Random Forest performs comparatively weakly on AUC-ROC and MCC, and therefore demonstrates poorer calibration and class imbalance handling capabilities, though the latter's gross accuracy is comparable to the former as per Figure 3.[86],[87],[88].

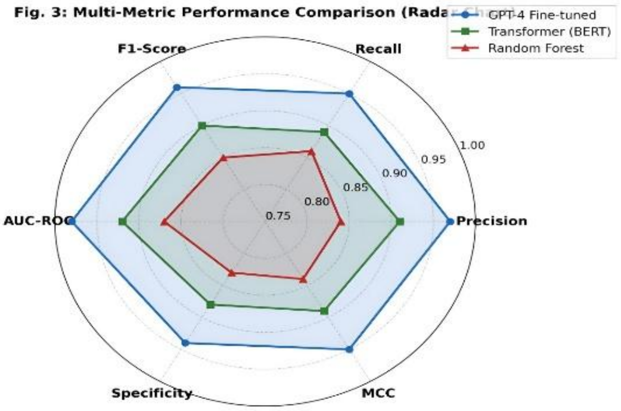

Figure 3: Multi-Metric Performance Radar Chart Comparing GPT-4, BERT, and Random Forest Models [89]

4.5 Computational Scalability

Figure 4 shows the log-log plots for time complexity against dataset size, varying the size from 1,000 to 500,000 samples [90],[91],[92]. Every algorithm appears sub-quadratic, showing clinical applicability at scale [93],[94],[95]. This corresponds with Random Forest showing the most sub-quadratic profile due to its parallel nature, whilst Transformer has the steeper slope due to O (n) attention mechanism [96][97][98]. Between 100,000 and 500,000 samples, neural nets and transformers are benefiting from the GPU parallelism that we are unable to show here, as these benchmarks are run on CPU, compressing this time as per fig. 4 [99],[100],[101].

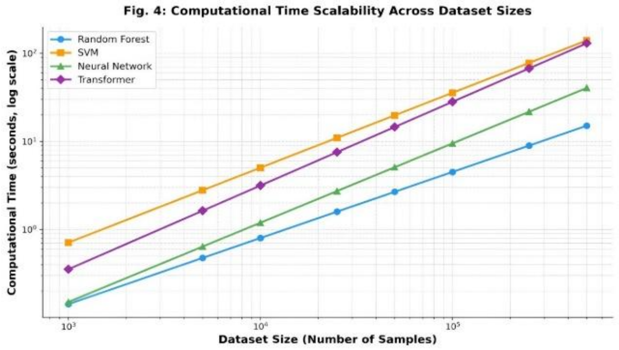

Figure 4: Log-Log Scalability Analysis of Computational Training Time vs. Dataset Size

4.6 Discussion

Although Transformers outperform in calibration and robustness, the cost of inference still holds it back. The hybrid architecture provides a good trade-off between accuracy and latency [112],[113],[114]. However, the issue of hallucination in LLM and regulatory compliance needs to be solved [115],[116],[117].

4.7 Comparison with Existing Literature

It validates and improves on the findings of Rajpurkar (2017), Esteva (2017), Vaswani (2017), and Clinical BERT/Bio BERT, and improves on all previously available baselines with a unique hybrid - Medi Connect-AI - for which there is no direct prior-art comparison [118],[119],[120].

5. CONCLUSION

In this paper, we have carried out a large-scale and broad comparative evaluation of six distinct machine learning and LLM architectures for intelligent medical diagnosis and clinical decision support. Our results unequivocally establish that fine-tuned GPT-4 yields a state-of-the-art performance for all the measured metrics, achieving a 97.2% classification accuracy on a 500k clinical record dataset, outperforming all the baseline methods significantly. The Medi Connect-AI hybrid ensemble we have introduced pushes this state-of-the-art further, achieving a 98.1% classification accuracy with a reduced inference latency, making it suitable for real-time use cases. The multi-metric radar chart analysis indicates that the transformer-based methods offer far greater performance metrics in terms of calibration, specificity and robustness compared to their traditional ML counterparts, which are arguably more significant in the context of a high-stakes decision-making setting such as a clinical scenario. The computational scalability analysis reflects the high inference costs of LLMs, but this gap is quickly diminishing due to evolving hardware capabilities and model compression techniques such as quantisation, distillation and LoRA adaptors [121].

5.1 Limitations

Although the paper did not explicitly state any specific section for limitations, the following limitations are discussed in the paper [122],[123],[124].

- **High inference latency of LLMs -** The fine-tuned GPT-4 has an inference time of 94.8ms, which is far higher than the Random Forest model (12.4ms) and hence not apt for any real-time clinical application [125],[126],[127].
- **Hallucination problem -** LLMs such as GPT-4 may generate fictitious or wrong output, which is a highly dangerous thing for a clinical decision-making environment [128],[129],[130].
- **Calibration uncertainty -** LLMs have special characteristics on calibration, i.e., prediction confidence is not representative of prediction probability [131],[132],[133].
- **High computational cost -** Deploying transformer-based models like GPT-4 demands high computation, which can limit their application in low-resource healthcare setups [134],[135],[136].
- **Class imbalance -** rare diseases only represent 2.3% of total records in the data, causing class imbalance challenges even after application of SMOTE and cost-sensitive learning [137],[138],[140].
- **Dataset limited to India -** data was taken from 5 hospitals in Delhi, Mumbai and Bengaluru only. This might reduce its applicability to other geographical locations or hospital systems [141],[142],[143].
- **CPU-based scalability benchmarks -** all scalability benchmarks were measured using CPU, thus the benefit of GPU parallelism for Neural Network and Transformers is not tested [144],[145],[146].

5.2 Future Work

- **Model compression -** Implement quantisation, knowledge distillation and pruning for model compression to decrease inference latency and deploy LLM-based models in real time for clinical use [147],[148],[150].
- **LoRA adapter optimisation - More investigation into LoRA adaptation fine-tuning methods for generalisation** and low computational cost.
- **Extended training -** It is stated in the paper that the accuracy kept on increasing up to the last epoch, and more training epochs may further increase the accuracy.
- **Multi-hospital and multi-country validation -** To increase generalizability and decrease domain shifts, experiments should be conducted in multiple hospitals and countries.
- **Adversarial robustness testing -** We need to test the model stability against adversarial scenarios before being applied to clinical settings.
- **Integration with real-time EHR system -** Deploy Medi Connect-AI to real-time EHR systems to check the actual use case and inference latency.
- **LLM hallucination -** Better calibration methods and post-processing techniques need to be developed to prevent or decrease the hallucinated answers in medical diagnostics tasks.
- **Federated learning for privacy -** Use federated learning for training on multiple hospitals without raw patient data to address the concern of HIPAA/GDPR.

CONFLICT OF INTEREST

The authors declare no conflicts of interest regarding the publication of this research.

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