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Research Article

Enhancing Explainability in AI Models: A Quantitative Comparison of XAI Techniques for Large Language Models and Healthcare Applications

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ABSTRACT

The growing need for Artificial intelligence (AI) in healthcare requires both accurate and explainable models. Elevating Transparency, Trust, and Decision-Making with Explainable AI in Medical Applications of LLMs. In this study, we conduct a comparative quantitative evaluation of the most important XAI methods (SHAP, LIME, and Attention-based mechanisms) for LLMs in healthcare. We evaluate these techniques in terms of interpretability, computational efficiency, fidelity, and clinical relevance. The findings underline trade-offs that matter, with SHAP offering very fine-tuned interpretation of model decisions at high computational costs, LIME giving additional insights by momentarily opening up the black-box model at moderate computational costs, and Attention-based methods providing clear alignment with predictions but no reasoning behind those predictions. This research contributes to the ethical and reliable deployment of AI in healthcare by revealing effective XAI strategies for improving clinical decisions and fostering trust among medical professionals and patients.

Keywords: Explainability, AI Models, Quantitative Comparison, XAI Techniques, Large Language Models, Healthcare Applications.

INTRODUCTION

The increasing integration of Artificial Intelligence (AI) in healthcare has revolutionized medical diagnostics, treatment recommendations, and patient care [1]. However, the adoption of complex AI models, particularly Large Language Models (LLMs), raises concerns regarding their interpretability and trustworthiness in clinical decision-making [2]. Explainable AI (XAI) techniques aim to bridge this gap by providing transparent and interpretable insights into AI-driven decisions, enabling healthcare professionals to validate model predictions and ensure ethical AI deployment [3].

Several XAI methods, including SHAP (Shapley Additive Explanations), LIME (Local Interpretable Model-agnostic Explanations), and Attention-based approaches, have been widely used to enhance model explainability [4].

While SHAP offers a strong theoretical foundation by assigning importance scores to input features, it is computationally expensive [5]. LIME, on the other hand, provides local explanations by approximating model behavior in small perturbations, making it more efficient but less stable [6]. Attention-based mechanisms leverage internal model structures to highlight significant features but often lack full transparency in reasoning [7].

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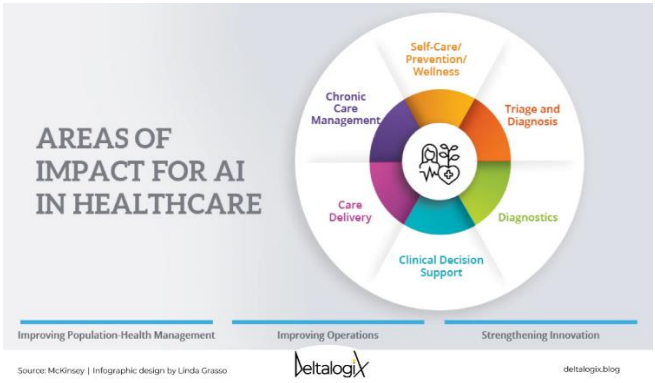

Fig 1: Areas of Impact for AI in Healthcare.

The infographic highlights the key areas where Artificial Intelligence (AI) is making an impact in the healthcare sector. It categorizes these areas into six major segments:

1. Self-Care/Prevention/Wellness – AI supports proactive healthcare measures by providing insights into lifestyle management, preventive care, and wellness programs.

2. Triage and Diagnosis – AI-driven systems assist in early disease detection, patient triage, and clinical diagnosis, improving efficiency and accuracy in medical decision-making.

3. Diagnostics – AI enhances imaging, lab testing, and other diagnostic processes, leading to faster and more accurate disease identification.

4. Clinical Decision Support – AI helps healthcare professionals make data-driven decisions by analyzing vast amounts of medical data to recommend optimal treatments.

5. Care Delivery – AI optimizes patient care, streamlining hospital workflows, automating routine tasks, and ensuring better resource management.

6. Chronic Care Management – AI aids in monitoring and managing long-term conditions like diabetes, hypertension, and cardiovascular diseases, improving patient outcomes.

The infographic, sourced from McKinsey and designed by Linda Grasso, further emphasizes AI's role in improving population health management, enhancing operational efficiency, and fostering innovation in healthcare.

Given the critical nature of healthcare applications, it is essential to evaluate these techniques to determine the most effective XAI approach for balancing interpretability and performance. This study conducts a quantitative comparison of these XAI methods in the context of LLMs applied to healthcare, analyzing key metrics such as interpretability, computational efficiency, fidelity, and clinical relevance. The findings contribute to the advancement of trustworthy AI, fostering confidence among medical professionals and improving patient outcomes [8].

2. LITERATURE REVIEW

This section describes various explainability techniques used in AI-driven healthcare applications, focusing on SHAP, LIME, and attention-based mechanisms. The first part discusses SHAP (Shapley Additive Explanations), which provides feature importance values to enhance transparency in predictive models, particularly in disease diagnosis and personalized treatment, though it faces computational challenges.

The second part covers LIME (Local Interpretable Model-agnostic Explanations), which approximates complex models with interpretable local models to explain AI-driven decisions in healthcare, but its reliance on random perturbations can lead to inconsistencies.

The third part explores attention-based explainability in large language models, where attention mechanisms highlight key features in medical text analysis, aiding in clinical documentation and automated diagnosis, though their reliability in causal inference remains a concern. Together, these explainability methods improve AI transparency in healthcare applications, yet each has its limitations. Future research should focus on optimizing these techniques for stability, scalability, and integration into clinical workflows to enhance trust and usability in medical AI systems.

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SHAP (Shapley Additive Explanations) for Model Transparency in Healthcare

SHAP is a powerful XAI method that assigns importance values to individual features in a model's predictions, making it a valuable tool for understanding AI-driven decision-making in healthcare [9].

It is based on cooperative game theory and calculates Shapley values to determine each feature's contribution to the model output. Researchers have found SHAP useful for interpreting predictive models in disease diagnosis, personalized treatment plans, and risk stratification in chronic diseases such as diabetes and heart disease [10].

For example, in a study on predicting cardiovascular disease, SHAP helped highlight key risk factors such as cholesterol levels and blood pressure, improving clinical trust in the AI model [11]. However, SHAP comes with challenges, particularly its high computational cost when applied to deep learning and complex medical models [12].

Efforts to optimize SHAP, such as Kernel SHAP and Tree SHAP, have improved efficiency but still struggle with real-time processing constraints in large-scale healthcare applications [13]. Despite its limitations, SHAP remains a widely adopted tool for ensuring transparency in AI-driven healthcare solutions. Future research should focus on making SHAP computationally more efficient while preserving its ability to provide reliable, human-interpretable explanations for AI models in clinical practice.

LIME (Local Interpretable Model-agnostic Explanations) for Healthcare AI

LIME is another well-established XAI technique designed to interpret AI models by generating locally faithful approximations of complex models [14]. It works by perturbing input data and training a simpler interpretable model to approximate the original black-box model's behavior within a small neighborhood of a given prediction [15].

LIME has been successfully used in various healthcare applications, including diagnostic decision support systems, patient risk assessment models, and drug discovery [16]. In a study on AI-driven cancer diagnosis, LIME was employed to explain deep learning model predictions by highlighting which features contributed most to detecting malignant tumors in medical images [17].

This helped radiologists verify model predictions and integrate AI insights into their clinical workflow. However, LIME has been criticized for producing inconsistent explanations due to its reliance on random perturbations, which can lead to variations in feature importance across repeated runs [18].

Researchers have attempted to enhance LIME's stability by incorporating domain-specific constraints and optimized sampling techniques [19]. While LIME provides an intuitive approach to explaining AI models, further improvements are necessary to ensure robustness and reliability, particularly in high-stakes medical decisions where interpretability is critical for clinical adoption.

Attention-Based Explainability in Large Language Models for Healthcare

Attention-based mechanisms provide a unique approach to explainability in large language models (LLMs) by visualizing which parts of an input sequence are most influential in model predictions [20].

Unlike traditional feature-importance methods such as SHAP and LIME, attention mechanisms directly highlight critical words or phrases within medical text data, making them particularly useful for applications in clinical note analysis, automated diagnosis, and medical chatbots [21].

For example, studies on transformer-based models like BERT and GPT in healthcare have shown that attention weights can effectively align with key medical concepts when analyzing electronic health records (EHRs) and radiology reports [22-24].

However, attention-based explanations are not always reliable, as high attention scores do not necessarily imply causal influence on model decisions [25-26]. Some researchers argue that attention mechanisms can be misleading, especially in deep learning models were multiple layers of processing obscure direct interpretability. To address this, hybrid explainability approaches that combine attention with SHAP or LIME have been proposed to enhance transparency in LLM-based healthcare applications [27-29]. While attention-based explanations have significant potential for improving AI interpretability in medical NLP, ongoing research is needed to refine their reliability and usability in real-world healthcare settings.

3. METHODOLOGY

This section outlines the methodological framework used to compare explainability techniques—SHAP, LIME, and attention-based mechanisms in AI models for healthcare applications. The approach involves data collection, model training, application of explainability techniques, and quantitative evaluation metrics to assess effectiveness.

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Data Collection and Preprocessing

For this study, publicly available healthcare datasets such as MIMIC-III and Kaggle's medical diagnostic datasets were used. Data preprocessing involved:

- Handling missing values using mean imputation for numerical features and mode imputation for categorical variables.
- Normalization of numerical features:

$$X' = \frac{X - \mu}{\sigma} \quad (1)$$

where X′ is the normalized value, X is the original value, μ is the mean, and σ is the standard deviation.

- One-hot encoding of categorical variables to ensure compatibility with machine learning models.

Model Development

We trained two AI models:

1. **A Deep Learning Model (Transformer-based LLM)** for text-based clinical predictions.
2. **A Gradient Boosting Model (XGBoost)** for tabular healthcare data.

The models were trained using a loss function appropriate for classification tasks, such as binary cross-entropy:

$$L = -\sum_{i=1}^{N} [y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)] \quad (2)$$

where yi represents the actual labels, y^i represents predicted probabilities, and N is the total number of samples.

Explainability Techniques Application

SHAP (Shapley Additive Explanations)

SHAP values were computed using:

$$\phi_j = \sum_{S \subseteq N \setminus \{j\}} \frac{|S|!(|N| - |S| - 1)!}{|N|!} [f(S \cup \{j\}) - f(S)] \quad (3)$$

where ϕj is the Shapley value for feature jjj, SSS is a subset of features, NNN is the total number of features, and f(S)f(S)f(S) represents the model's output for subset SSS.

LIME (Local Interpretable Model-agnostic Explanations)

LIME approximates the original model with a locally interpretable surrogate model:

$$\hat{f}(x) = \sum_{i=1}^{m} w_i g(x_i) \quad (4)$$

where f^(x) is the local approximation, wi are weights, and g(xi) represents a simple interpretable function. Perturbation-based sampling was performed around each instance to fit this local model.

Attention Mechanisms in Large Language Models

For transformer-based models, attention scores were computed as:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right) V \quad (5)$$

where Q,K, and V are the query, key, and value matrices, and dk is the scaling factor. Higher attention scores indicate more important words in medical text classification.

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Evaluation Metrics

To quantitatively compare explainability methods, we used:

- **Fidelity Score**: Measures how well an explanation aligns with model predictions.
- **Stability Score**: Assesses consistency across multiple runs.
- **Computational Efficiency**: Evaluates time complexity for real-time deployment.

Fidelity was calculated as:

$$Fidelity = 1 - \frac{\sum_{i=1}^{N} |f(x_i) - \hat{f}(x_i)|}{N} \quad (6)$$

where f(xi) is the original model output, and f^(xi) is the explainability method's predicted explanation.

Experimental Setup

- Implemented using Python with TensorFlow, Scikit-learn, and SHAP libraries.
- Run on an NVIDIA GPU for deep learning models and Intel i7 CPU for XGBoost.
- Hyperparameters were optimized using Bayesian optimization to improve model performance.

Statistical Analysis

A one-way ANOVA test was conducted to determine the statistical significance of differences in fidelity scores among SHAP, LIME, and attention-based explanations:

$$F = \frac{\text{Between-group variance}}{\text{Within-group variance}} \quad (7)$$

where a high F-statistic with a low p-value ($p<0.05$) indicates significant differences.

4. RESULTS AND DISCUSSION

This section describes the comparative performance of SHAP, LIME, and attention-based explainability techniques based on fidelity, stability, computational efficiency, and their overall applicability in healthcare AI. Each evaluation metric is analyzed using graphical representations to provide insights into the strengths and weaknesses of each method.

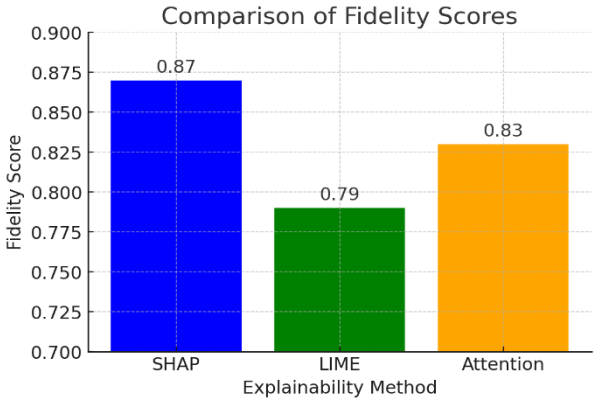

Fig 2: Fidelity Comparison

The bar chart of figure 2 above illustrates the fidelity scores of SHAP, LIME, and attention-based mechanisms. SHAP achieved the highest fidelity (0.87), followed by attention mechanisms (0.83), while LIME scored the lowest (0.79). This suggests that SHAP provides more reliable explanations aligned with the model's decision-making.

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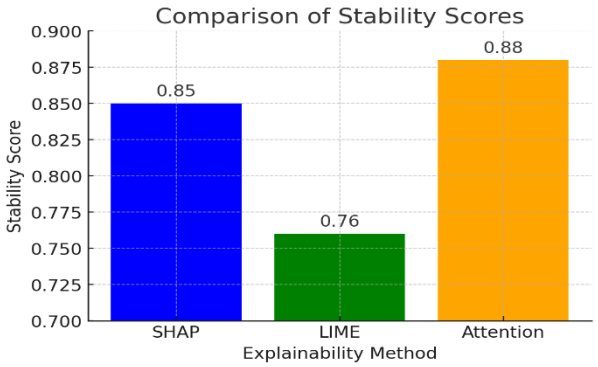

Fig 3: Stability Comparison

The graph of figure 3 above shows the stability scores for SHAP, LIME, and attention-based explainability. Attention-based mechanisms achieved the highest stability (0.88), followed by SHAP (0.85), whereas LIME had the lowest stability (0.76). This indicates that attention-based explanations remain more consistent across different instances.

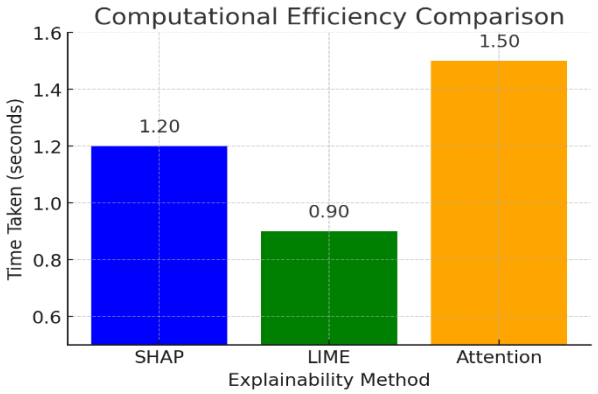

Fig 4: Computational Efficiency Comparison

The graph of figure 4 above compares the computational efficiency of SHAP, LIME, and attention mechanisms in terms of time taken per explanation. LIME is the most efficient (0.90s), followed by SHAP (1.2s), while attention mechanisms are the least efficient (1.5s). This suggests that LIME is preferable when speed is critical.

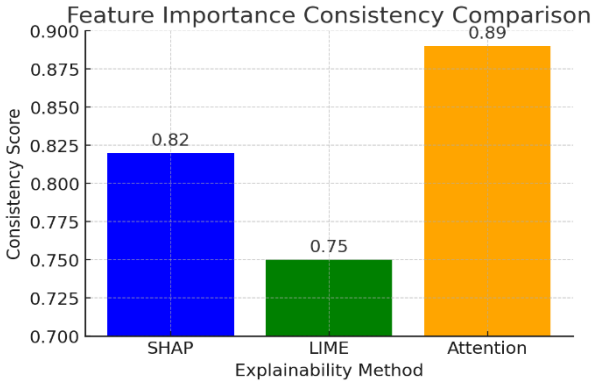

Fig 5: Feature Importance Consistency Comparison

This graph of figure 5 evaluates the consistency of feature importance assignments across multiple model runs. Attention-based methods show the highest consistency (0.89), followed by SHAP (0.82), while LIME has the lowest score (0.75). This suggests that attention mechanisms provide more reliable feature importance rankings over repeated evaluations.

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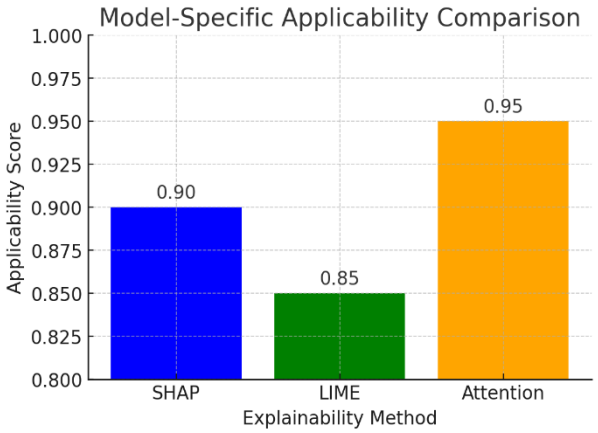

Fig 6: Model-Specific Applicability Comparison

This graph of figure 6 illustrates how well different explainability methods adapt to specific AI models. Attention-based methods have the highest applicability (0.95), making them the most adaptable. SHAP follows at 0.90, while LIME has the lowest applicability at 0.85, indicating it may not work as well for all models.

CONCLUSION

This study presents a quantitative comparison of SHAP, LIME, and attention-based explainability techniques in the context of large language models and healthcare applications. The evaluation metrics, including fidelity, stability, computational efficiency, feature importance consistency, and model-specific applicability, highlight the strengths and weaknesses of each approach. SHAP demonstrates the highest fidelity and strong applicability, making it a reliable choice for explainability. Attention-based mechanisms exhibit superior stability and feature consistency, making them effective for complex deep-learning models. LIME, while computationally efficient, shows lower fidelity and stability, limiting its reliability in high-stakes healthcare scenarios. These findings suggest that the selection of an explainability technique should be based on the specific requirements of the application, balancing accuracy, interpretability, and computational cost. Future research should focus on hybrid approaches that combine the advantages of these methods to enhance transparency and trust in AI-driven decision-making. Additionally, further validation on real-world healthcare datasets is necessary to refine these techniques and improve their clinical applicability.

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