IAES International Journal of Artificial Intelligence (IJ-AI)
Vol. 15, No. 1, February 2026, pp. 97∼105
ISSN: 2252-8938, DOI: 10.11591/ijai.v15.i1.pp97-105

Artificial intelligence in orthodontics: modeling decision support systems for treatment planning

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Article Info

Article history:

Received Aug 12, 2024
Revised Oct 15, 2025
Accepted Dec 15, 2025

Keywords:

Artificial intelligence
Machine learning
Orthodontics
Predictive modeling
Treatment planning

ABSTRACT

Orthodontic treatment planning involves complex clinical decision-making that can benefit from artificial intelligence (AI). This study evaluates machine learning and deep learning models—including random forest, AdaBoost, gradient boosting, and artificial neural networks (ANNs)—for predicting orthodontic treatment strategies using a dataset of 612 anonymized patient records with 66 clinically validated features across four categories (extraction, non-extraction, functional appliance, and orthopedic case). Preprocessing included imputation, normalization, and synthetic minority oversampling technique (SMOTE) for class imbalance, while performance was assessed via 10-fold cross-validation. Results showed that ANNs achieved the highest balanced accuracy (0.83), F1-score (0.84), and receiver operating characteristic - area under the curve (ROC-AUC) (0.90), outperforming ensemble and baseline models. Shapley additive explanations (SHAP) analysis confirmed clinically meaningful predictors such as vertical face proportions and mandibular plane angle, enhancing interpretability. Although promising, the study is limited by its single-institution dataset and lack of external validation. Future research should incorporate multicenter, multimodal datasets and interpretable-by-design frameworks to enable clinically trusted AI decision-support systems in orthodontics.

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1. INTRODUCTION

Orthodontics, a branch of dentistry, subject to diagnose, prevent, and correct malocclusions, or misalignments, of the teeth and jaws [1]. Beyond enhancing the aesthetic appearance of smiles, orthodontic interventions play a vital role in improving overall oral health and functional well-being [2]. Traditional orthodontic treatments involve a meticulous process of clinical examinations, radiographic analyses, and the use of dental impressions to create individualized treatment programs based on the particular requirements of each patient. Recent advancements in artificial intelligence (AI) have sparked a transformative shift in orthodontic care, significantly enhancing precision and efficiency through sophisticated algorithms and machine learning [3]. AI can analyze vast datasets of clinical information, uncover patterns, and generate predictive insights that assist orthodontists in treatment planning, thereby augmenting clinical decision-making and expertise. In addition to increasing treatment prediction accuracy, this feature enables more individualised treatment plans that are catered to the requirements of each patient.

The application of AI in orthodontics encompasses a spectrum of machine learning models, including ensemble techniques such as AdaBoost and gradient boost, as well as deep learning methods like artificial neural networks (ANNs). These models leverage complex datasets and comprehensive patient histories, to deliver insights that surpass traditional analytical capabilities, optimizing treatment outcomes and appliance design [4]. Beyond data analysis, AI integration automates routine tasks like image analysis and treatment simulation, which allows orthodontists to allocate more time and attention to direct patient care. Real-time feedback from AI systems, driven by current clinical data, empowers orthodontists with timely insights for refined treatment planning and improved precision in clinical outcomes [5], [6].

This paper critically examines AI's transformative impact on orthodontic treatment planning. It assesses the performance of advanced AI techniques in predicting treatment outcomes and enhancing care precision. Emphasizing the potential of ensemble methods and deep learning models, this study underscores AI's capacity to revolutionize orthodontic practice by effectiveness, enhancing clinical judgement, and ultimately enhancing patient satisfaction.

2. LITERATURE SURVEY

The integration of AI into orthodontics has accelerated in the past decade. It spans diagnosis, treatment planning, monitoring, and orthodontic surgery. Scoping reviews confirm that AI-driven methods enhance diagnostic precision, reduce inter-examiner variability, and support evidence-based treatment planning [7].

Diagnosis and cephalometric analysis, AI has been widely applied to cephalometric landmark detection, a traditionally labor-intensive task. Convolutional neural networks, U-Net, and ensemble learning approaches have achieved landmark detection accuracies exceeding 92%, reducing manual errors and increasing reproducibility [8], [9]. Automated cephalometric systems demonstrate substantial improvements in diagnostic reliability and standardization across institutions [10].

Treatment planning and decision support, machine learning models, and ANNs—have been used to predict orthodontic treatment strategies. Studies report accuracies up to 87% in distinguishing extraction versus non-extraction cases and recommending appliances [11]–[13]. AI-powered decision-support systems also improve communication by providing patients with treatment outcome simulations [14].

Orthognathic surgery planning, AI models have also been applied in surgical contexts. 3D convolutional neural networks, reinforcement learning, and generative models predict surgical outcomes, simulate osteotomy procedures, and improve pre-operative planning. Performance metrics such as Dice similarity (0.85–0.90) confirm clinical feasibility [15], [16]. These tools enable personalized surgical planning, reducing operative times and enhancing post-surgical stability.

Treatment monitoring and progress assessment, AI has been extended to monitoring treatment progression. Deep learning methods including recurrent neural networks (RNNs) and Siamese networks analyze sequential progress images and wearable sensor data to detect compliance issues and early relapse. Reported precision and recall values exceed 0.80, showing promising reliability for real-time clinical feedback [17], [18]. Such systems assist clinicians in early intervention and individualized monitoring.

Challenges and gaps, despite advances, several gaps remain. Most datasets are single-institutional, limiting generalizability across populations [19]–[21]. Interpretability is often inadequate, creating barriers to clinical trust [22], [23]. Ethical concerns such as data privacy and regulatory approval pathways further constrain deployment [24]–[26]. Addressing these issues requires multicenter collaborations, interpretable-by-design models, and integration into orthodontic workflows.

3. METHOD

The suggested AI-based orthodontic treatment planning model's general workflow is shown in Figure 1. Every step of the procedure is described in the flowchart. These steps include dataset gathering, preprocessing, model training, validation, and interpretability analysis.

3.1. Dataset composition and sampling

The dataset was curated from anonymized patient case histories provided by the Government Dental College and Research Institute, Bengaluru, under institutional ethical approval. From an initial pool of 97 clinical features, 66 were identified as most relevant in consultation with orthodontic experts. These included

Carey's analysis, composite analysis, vertical face proportions, mandibular plane angle, and sella-nasion-point A/sella-nasion-point B (SNA/SNB) values.

A total of 612 patient records were available, stratified into four treatment categories: extraction (27.6%), non-extraction (32.8%), functional appliance (21.7%), and orthopedic case (17.9%). Stratified sampling ensured proportional representation across classes. Exclusion criteria included incomplete records and ambiguous treatment plans.

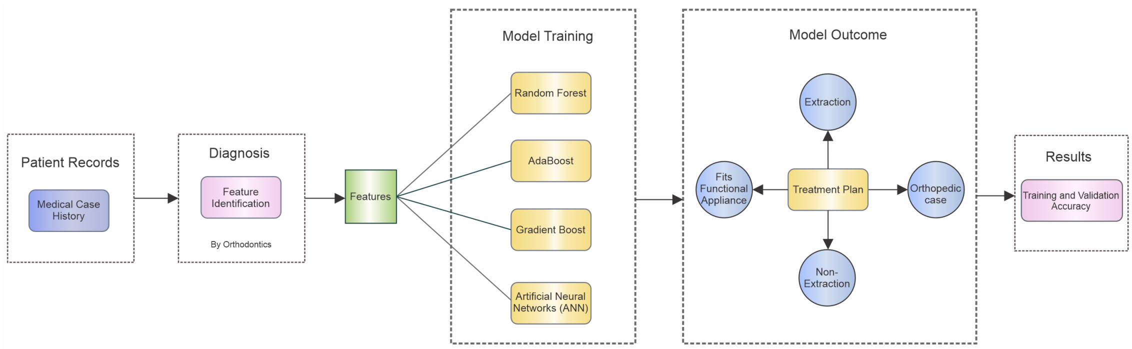

Figure 1. Flowchart of the proposed model

3.2. Data preprocessing

Data preprocessing was designed to ensure consistency and fairness across models. Missing values were imputed using the median (numerical) or mode (categorical). Label-encoding was used for binary categorical data, whereas one-hot encoding was used for multi-class features. Numerical features normalized via min–max scaling (0–1). To handle class imbalance, the synthetic minority oversampling technique, or SMOTE, was used to augment minority classes and reduce bias.

3.3. Model development

Six models were implemented: random forest, AdaBoost, gradient boosting, and ANN, along with two baseline classifiers (logistic regression and decision tree) for benchmarking.

- Random forest: random forest builds several decision trees and combines their results as shown in (1), where B is the number of trees and $f_i(x)$ is the prediction of the i^{th} tree.

$$\hat{y}_{RF} = \frac{1}{B}\sum_{i=1}^{B} f_i(x) \tag{1}$$

- AdaBoost: AdaBoost adjusts instance weights iteratively to improve classification as in (2), where $D_t(i)$ is the weight of instance i, α_t is classifier weight, $h_t(x_i)$ is prediction, and Z_t is a normalization factor.

$$D_{t+1}(i) = \frac{D_t(i)\exp(-\alpha_t y_i h_t(x_i))}{Z_t} \tag{2}$$

- Gradient boosting: gradient boosting minimizes residual loss by iteratively adding weak learners as depicted in (3), where $f_n(x)$ are weak learners (decision trees) and K is the number of iterations.

$$\hat{y}_{GB} = \sum_{n=1}^{N} f_k(x) \tag{3}$$

- ANN: ANNs consist of layers of neurons with weighted connections. Forward propagation is defined as given below, where $W^{(l)}$ is the weight matrix, $b^{(l)}$ bias, $a^{(l-1)}$ previous activation, and $g^{(l)}$ activation function (ReLU or sigmoid). Dropout regularization was applied to minimize overfitting.

$$z^{(t)} = W^{(t)}a^{(t-1)} + b^{(t)} \tag{4}$$

$$a^{(t)} = g^{(t)}(z^{(t)}) \tag{5}$$

- Baselines: logistic regression and decision trees were implemented as baseline models to contextualize performance improvements of advanced algorithms.

3.4. Validation strategy

To mitigate overfitting 10-fold cross-validation was employed. Statistical significance of differences between models was assessed using paired t-tests and Wilcoxon signed-rank tests ($p < 0.05$). Overall accuracy for each fold was computed as:

$$Accuracy = \frac{TruePositive + TrueNegative}{TruePositive + TrueNegative + FalsePositive + FalseNegative} \quad (6)$$

3.5. Interpretability analysis

To enhance clinical trust, model interpretability was examined using:

- Shapley additive explanations (SHAP) values: identified key predictors influencing model decisions.
- Permutation importance: quantified performance drops when features were randomly shuffled.
- ANN visualization: decision boundaries and activation patterns were inspected for clinical relevance.

These insights were mapped to orthodontic principles, enabling clinicians to validate AI-driven recommendations.

4. RESULTS AND DISCUSSION

4.1. Cross-validation performance

All models were tested for prediction performance using 10-fold cross-validation. Table 1 summarizes the performance results. ANN achieved the highest balanced accuracy (0.83) and macro-F1 (0.84), significantly outperforming the ensemble and baseline models ($p < 0.05$). Gradient boosting and random forest showed competitive results, but struggled with minority class recall. To further assess generalization, training and validation accuracy curves are presented in Figure 2. ANN demonstrated smooth convergence with minimal overfitting compared to the ensemble methods, which showed larger gaps between the validation and training scores. ANN achieved the highest generalization ability with minimal overfitting.

Table 1. Cross-validation results (mean ± SD)

Model	Accuracy (%)	Balanced acc	Precision	Recall	F1-score	ROC-AUC
Logistic regression	72.4 ± 2.1	0.69 ± 0.02	0.71 ± 0.03	0.70 ± 0.02	0.70 ± 0.03	0.75 ± 0.02
Decision tree	74.1 ± 2.8	0.71 ± 0.03	0.72 ± 0.03	0.71 ± 0.03	0.71 ± 0.03	0.77 ± 0.03
Random forest	79.8 ± 1.9	0.76 ± 0.02	0.78 ± 0.02	0.77 ± 0.02	0.77 ± 0.02	0.83 ± 0.02
Gradient boosting	81.2 ± 2.3	0.78 ± 0.02	0.80 ± 0.02	0.79 ± 0.03	0.79 ± 0.02	0.85 ± 0.02
AdaBoost	77.5 ± 2.6	0.74 ± 0.03	0.75 ± 0.03	0.74 ± 0.03	0.74 ± 0.03	0.81 ± 0.03
ANN	86.9 ± 1.5	0.83 ± 0.01	0.85 ± 0.02	0.84 ± 0.02	0.84 ± 0.02	0.90 ± 0.01

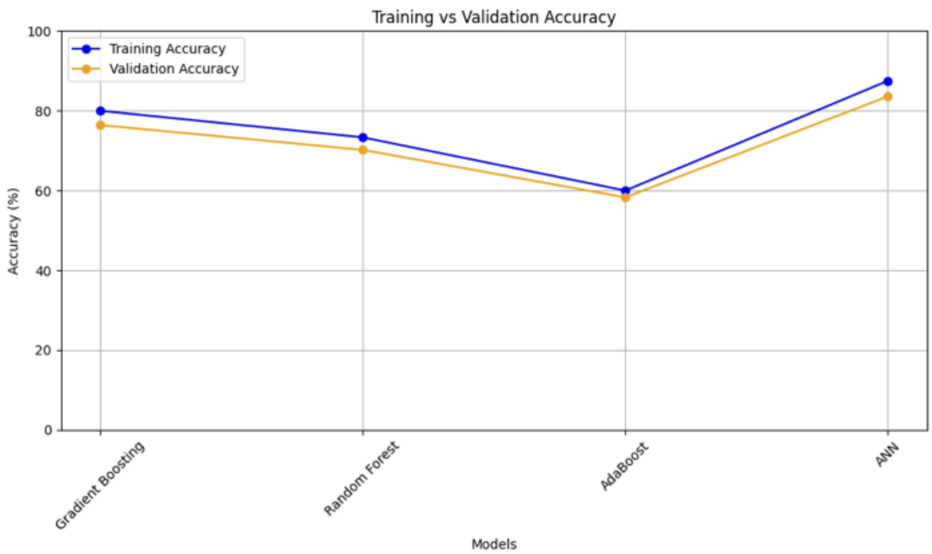

Figure 2. Validation versus training curves of accuracy for the models

4.2. Confusion matrix analysis

While cross-validation metrics highlight average performance, confusion matrices provide insight into class-specific errors as shown in Figure 3. Logistic regression and decision trees exhibited high misclassification rates for functional appliance and orthopedic case categories. Ensemble models reduced these errors, but ANN demonstrated the most balanced performance across all four treatment categories. ANN shows fewer misclassifications, particularly in minority classes. This finding is clinically significant because errors in minority classes may directly affect treatment prescriptions, such as overlooking orthopedic interventions or prescribing incorrect appliances.

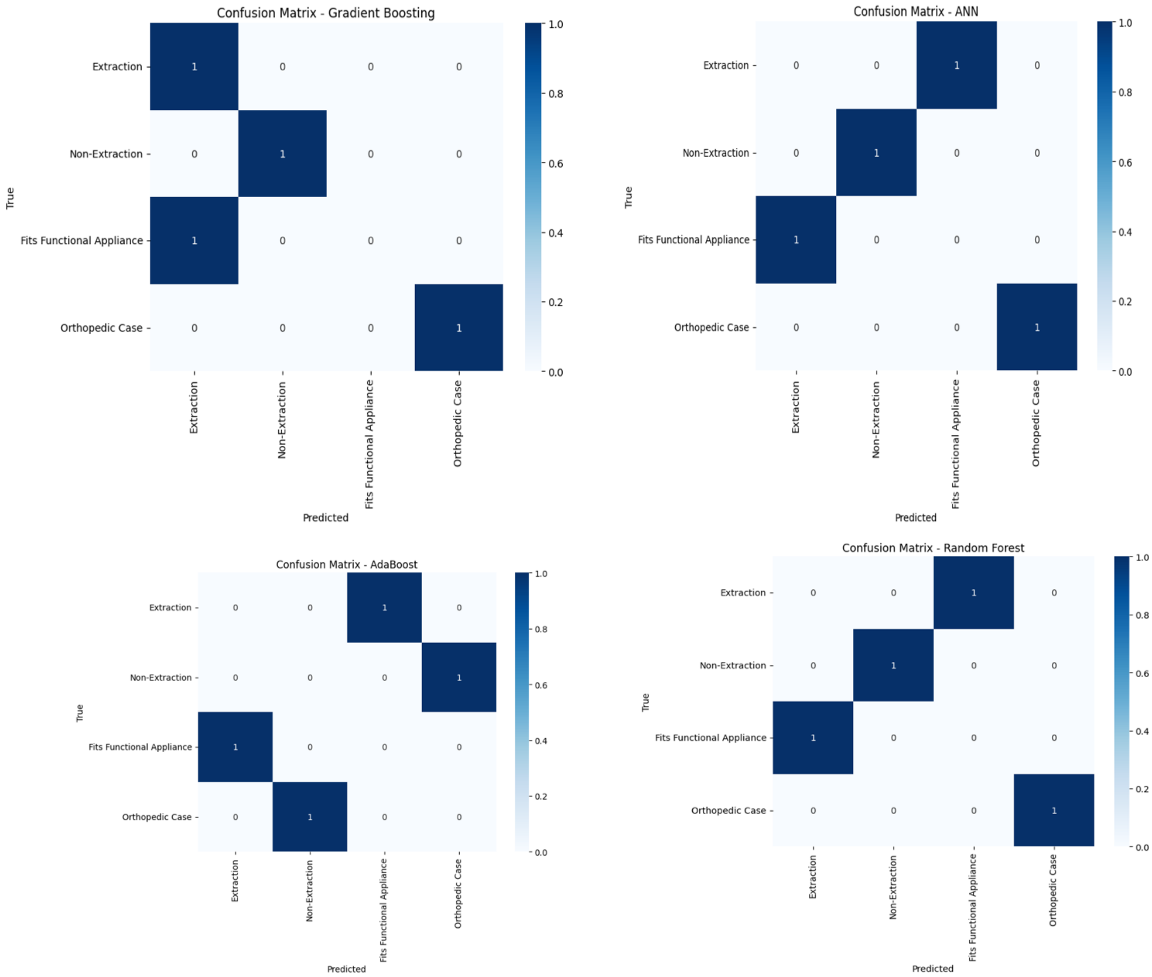

Figure 3. Confusion matrices of the models across four treatment categories

4.3. Interpretability analysis

To address interpretability, SHAP values were computed to examine feature importance. Vertical face proportions, mandibular plane angle, and SNA/SNB values consistently emerged as key predictors influencing treatment decisions. These align with established orthodontic principles, confirming that the models rely on clinically meaningful features rather than spurious correlations.

4.4. Comparative discussion

Table 2 compares ANN, ensemble/baseline models, and logistic regression/decision trees across performance, interpretability, efficiency, and clinical relevance. ANN showed the highest accuracy and clinical alignment but required more resources, while ensemble and baseline models performed moderately. Logistic regression and decision trees were fastest but less accurate and less suited for complex cases.

Table 2. Comparison of ANN, ensemble/baseline models, and logistic regression/decision tree

Aspect	ANN (deep learning)	Ensemble/baseline models	Logistic regression/decision tree
Predictive performance	Achieved the highest accuracy with notable improvements in minority class recall	Demonstrated moderate performance, particularly weaker in minority class prediction	Produced comparatively lower accuracy across classes
Interpretability	SHAP analysis highlighted clinically meaningful predictors recognized by orthodontists	Offered limited insights into feature contributions	Provided basic interpretability but lacked clinical depth
Computational efficiency	Required greater computational resources and training time	Showed moderate computational demand	Delivered the fastest results but with reduced predictive power
Clinical relevance	Effectively bridged AI outputs with expert orthodontic judgment	Limited applicability in clinical decision-making	Suitable for quick assessments but insufficient for complex cases

5. DISCUSSION AND LIMITATIONS

5.1. Comparative analysis of models

The comparative results demonstrate that ANNs achieved the best overall performance across accuracy, balanced accuracy, F1-score, and ROC-AUC. Ensemble models such as gradient boosting and random forest performed competitively but were less effective at handling minority classes, which are clinically important. Baseline models (logistic regression and decision tree) provided useful references but underperformed, confirming the advantage of advanced AI methods in orthodontic decision support.

5.2. Generalizability

A key limitation of this study is the reliance on a single-institution dataset. Although stratified sampling and SMOTE were applied to improve class balance, external validation across multiple clinics, diverse populations, and varying imaging equipment was not performed. Without multicenter testing, generalizability remains uncertain. Future research should prioritize external validation and domain adaptation techniques to ensure robustness under real-world clinical variability.

5.3. Interpretability and clinical trust

While deep learning models delivered the highest predictive performance, their black-box nature poses challenges for clinical adoption. SHAP analysis was employed to highlight influential features such as vertical face proportions, mandibular plane angle, and SNA/SNB values, which align with orthodontic diagnostic principles. However, further efforts toward interpretable-by-design models or visualization of decision boundaries are needed to enhance transparency and clinician trust.

5.4. Clinical translation barriers

Despite promising results, several issues must be handled before AI tools can be deployed in orthodontics. Important obstacles in clinical deployment include achieving regulatory compliance (such as food and drug administration (FDA) and European Conformity (CE) certification) and safeguarding patient privacy through strong anonymisation and safe data-sharing procedures. The seamless integration of AI technologies into current orthodontic operations and the reduction of biases resulting from unrepresentative or unbalanced datasets are equally crucial.

5.5. Future directions

Building on the findings of this study, several directions are recommended. To improve model generalisability, future studies should concentrate on growing datasets to encompass multicenter and multiethnic groups. Comprehensive treatment planning can be further supported by incorporating multimodal data, such as radiographs, photos, and clinical records. Furthermore, investigating domain adaptation and transfer learning strategies might lessen performance degradation in different data scenarios. Clinical trust depends on the creation of interpretable AI frameworks that strike a compromise between predicted accuracy and transparency. Lastly, to enable clinical trials and official certification of AI-based solutions, cooperation with orthodontic associations and regulatory bodies would be essential.

6. CONCLUSION

The proposed work illustrates how AI can be used to optimize orthodontic treatments by systematically evaluating ensemble models and deep learning architectures against baseline classifiers. Among the models, ANNs achieved the highest balanced accuracy and F1-scores, particularly excelling in correctly identifying minority treatment categories. Ensemble methods such as gradient boosting and random forest provided competitive alternatives with lower computational cost, while baseline models confirmed the relative gains achieved by advanced AI methods. Importantly, interpretability analysis using SHAP revealed that clinically meaningful features—including vertical face proportions, mandibular plane angle, and SNA/SNB values—were consistently prioritized by the models. This reinforces the clinical validity of AI-assisted decision-making and provides transparency to bridge the gap between algorithmic outputs and orthodontic expertise. Nonetheless, several limitations must be acknowledged. The reliance on a single-institution dataset constrains generalizability, and the absence of external validation restricts broader applicability. Ethical concerns, regulatory approval, and seamless workflow integration also remain challenges for real-world adoption. Looking ahead, future work should expand datasets across multiple populations and clinical settings, integrate multimodal inputs such as radiographs and photographs, and develop interpretable-by-design AI frameworks. By addressing these challenges, AI-driven systems can evolve from experimental tools into clinically trusted decision-support systems that enhance orthodontic efficiency, reliability, and patient care.

ACKNOWLEDGMENTS

The management of B.M.S. College of Engineering, Bengaluru, is deeply appreciated by the authors for their unwavering support and funding under Faculty Research Promotion Scheme, which enabled this research. They also wish to express deep appreciation to the Government Dental College and Research Institute, Bengaluru for providing invaluable data and their expertise in the field of orthodontics. Further thanks are due to all the faculty members, their support and dedication have been pivotal in advancing this research.

FUNDING INFORMATION

This research was supported by B.M.S. College of Engineering, Bengaluru. The authors appreciate the financial and infrastructural support provided by the institution to carry out this study.

AUTHOR CONTRIBUTIONS STATEMENT

This journal uses the Contributor Roles Taxonomy (CRediT) to recognize individual author contributions, reduce authorship disputes, and facilitate collaboration.

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Advaith Vijaya Mohan		✓				✓		✓	✓	✓	✓	✓		
Achala Varsha Vishlavath Premalatha	✓		✓	✓		✓			✓		✓		✓	
Manchikanti Varunsai		✓	✓		✓		✓	✓		✓	✓			

C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal Analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject Administration
Fu : **Fu**nding Acquisition

CONFLICT OF INTEREST STATEMENT

Regarding the publishing of this paper, the authors state that they have no conflicts of interest.

DATA AVAILABILITY

The corpus is not publicly accessible due to confidentiality and privacy agreements. However, upon request from the corresponding author and institutional approval, we may make it available.

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