Original Article

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pISSN 2234-7518 • eISSN 2005-372X
https://doi.org/10.4041/kjod25.214

THE KOREAN JOURNAL of ORTHODONTICS
KJO

# Development of Leading Enhancement Assistive Planning: A three-dimensional tooth classification system for orthodontic treatment with clear aligners

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**Objective:** To develop and validate the Leading Enhancement Assistive Planning (LEAP) system, a deep learning–based tool for automated malocclusion classification from three-dimensional (3D) intraoral scans, integrated into orthodontic computer-aided design (CAD) workflows to support clinical diagnosis and treatment planning. **Methods:** This retrospective study utilized 841 anonymized 3D intraoral scans in the standard tessellation language (STL) format, representing 8 malocclusion categories, labeled and validated by expert orthodontists. Preprocessing converted the STL meshes into standardized voxel grids, which served as inputs to a modified EfficientNet-based 3D convolutional neural network. The hierarchical classification logic distinguished primary and secondary malocclusions. Model performance was assessed using accuracy, precision, recall, and F1-score metrics on a held-out test set. Integration into orthodontic CAD software was demonstrated to provide real-time diagnostic feedback. **Results:** The LEAP system achieved robust classification performance, with 90.8% accuracy, 87.5% precision, 91.3% recall, and an F1 score of 89.2% across the eight malocclusion classes. Hierarchical logic enabled a clinically interpretable output for complex cases with overlapping conditions. The voxel-based pipeline supported resolutions of up to 256 × 256 × 256 with graphics processing unit acceleration for efficient inference. Readiness for integration into CAD platforms was demonstrated, providing automated malocclusion classification at the point of care. **Conclusions:** LEAP is an accurate, efficient, and scalable artificial intelligence–assisted system for classifying malocclusions using 3D dental scans. Its integration into orthodontic CAD software offers standardized, real-time diagnostic support, potentially improving workflow efficiency and consistency. The LEAP system may enhance diagnostic accuracy, reduce variability, and serve as a valuable decision-support tool in orthodontic practice.

**Keywords:** Classification, Orthodontic indices, Three-dimensional diagnosis and treatment planning, Computer algorithms

Received July 30, 2025; Revised December 22, 2025; Accepted December 28, 2025.

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**How to cite this article:** Lee HJ, Wee Ming How RA, Gan KB, Ashari A, Fadzlin Syed Mohamed AM, Abdul Wahab RM. Development of Leading Enhancement Assistive Planning: A three-dimensional tooth classification system for orthodontic treatment with clear aligners. Korean J Orthod. https://doi.org/10.4041/kjod25.214 Published online M D, 2026.

## INTRODUCTION

In orthodontics, dental occlusion refers to a state in which the maxillary and mandibular teeth touch when the mouth is closed. Malocclusion is defined as the misalignment of teeth or an abnormal relationship between the maxillary and mandibular dental arches, which can lead to functional and aesthetic problems. The concept of malocclusion was first introduced by Edward Angle, the "father of modern orthodontics."[1] Based on the anteroposterior relationship of the first molars, malocclusion can be classified into Class I, Class II (increased overjet, deep overbite), and Class III (negative overjet, underbite). Figure 1 illustrates a clinical example of Class II Division 1, characterized by increased overjet with a deep overbite, and serves as a contextual reference for one of the malocclusion types incorporated into the Leading Enhancement Assistive Planning (LEAP) classification system.

The evaluation of malocclusion requires the analysis of tooth alignment, position, and maxillary–mandibular interrelationships according to the defined classification criteria. Diagnostic records may include clinical examinations, dental model analyses, photographs, and radiographs.[2] However, no universally accepted minimum record set exists, and diagnosis depends heavily on the orthodontist's expertise and experience, making it a time-consuming process.

Advancements in artificial intelligence (AI) have demonstrated the potential to automate malocclusion classification, thereby improving diagnostic consistency and reducing the workload of clinicians. Deep convolutional neural networks (CNNs), such as Xception and DenseNet, have achieved reliable detection of crossbites from two-dimensional (2D) intraoral images.[3] A You Only Look Once–based CNN accurately identified crowding, spacing, overjet, crossbite, open bite, and deep bite from five standard views: left, right, and front occlusion, as well as maxillary and mandibular occlusal images.[4] Maxillary and mandibular occlusal views have been used exclusively to assess crowding, employing the Little Irregularity Index and arch length discrepancy, respectively.[5,6] AI using frontal and lateral occlusion images has been shown to outperform orthodontists in predicting Angle's classification, whereas inconsistent performance was observed when the SmileMate tool was applied to all five standard intraoral views.[7,8]

The introduction of three-dimensional (3D) digital dental models has advanced AI-assisted diagnostics. These models improve accuracy, eliminate physical storage, enhance patient comfort, and facilitate treatment planning.[9,10] Studies combining 3D models with CNNs and sparse voxel octrees have achieved tooth type classification accuracies of up to 95.96%, although without validation in more complex dental conditions such as caries, crowding, or missing teeth.[11] In another study, 3D intraoral scan data were converted into 2D images to test deep learning models, achieving the highest accuracy of 84.39%.[12] Additionally, 3D occlusal contact data have been employed to classify Angle's malocclusion, demonstrating a strong diagnostic accuracy.[13]

Accuracy alone can be misleading in imbalanced datasets; therefore, precision, recall, and F1 score are increasingly emphasized.[14,15] Annotated intraoral image datasets have supported strong AI performance across these metrics, although broader validation across devices is needed.[16] In oral cancer screening, smartphone-based AI achieved balanced accuracy, precision, recall, and F1 values of 94–95%.[17] Similarly, applications in detecting caries have reported excellent results, with a sensitivity of up to 99.4% and precision nearing 99.9%.[18] These findings show a trend toward nuanced metric reporting, which reflects clinical diagnostic requirements.

The lack of large, structured, and standardized datasets hampers model development and validation, raising concerns regarding generalizability. Effective clinical integration requires AI systems to demonstrate reliability, interpretability, and adherence to dental standards to foster professional trust.[19] Therefore, continued advances in AI technology are expected to further transform orthodontics, improving diagnostic accuracy and treatment planning efficiency.[20,21]

Despite advancements, a research gap remains in the development of AI systems based on 3D dental models that can accurately classify malocclusions and address specific conditions such as overbites, open bites, and

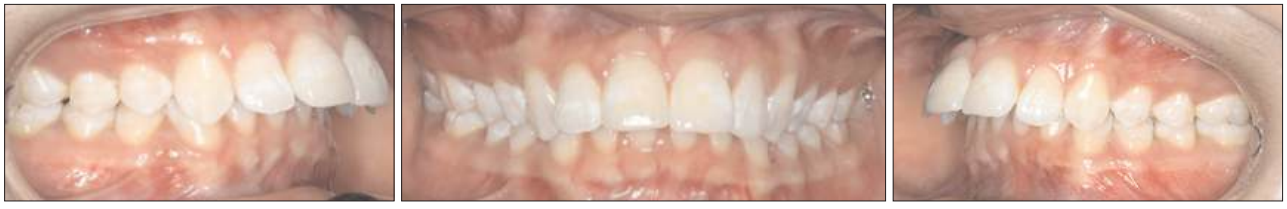

**Figure 1.** Clinical example of Class II Division 1 (deep bite), provided as a contextual reference to illustrate one of the malocclusion types included in the Leading Enhancement Assistive Planningclassification system.


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crossbites. This gap highlights the need to design AI solutions for practical clinical applications. For such systems to be successful, they must be user-friendly, efficient, highly accurate, and aligned with the expectations of clinicians. In this study, we present the development and validation of the LEAP system, a machine learning–based protocol designed to classify malocclusions using scanned study models within orthodontic computer-aided design (CAD) software (3Shape Holding A/S, Copenhagen, Denmark).

## MATERIALS AND METHODS

### Leading Enhancement Assistive Planning workflow and pipeline

Figure 2 summarizes the LEAP workflow and illustrates how 3D dental data are transformed into malocclusion classifications using deep learning. The process begins with data acquisition, during which intraoral scans are converted into voxel grids, followed by model training with 3D CNNs on labeled malocclusion data. In the classification logic stage, hierarchical rules interpret predictions to identify primary and secondary malocclusion classes. Finally, the deployment phase integrates the results into orthodontic CAD software to deliver automated classifications, with the potential for future extensions for diagnosis and treatment recommendations.

Figure 3 illustrates the LEAP system pipeline for orthodontic treatment, showing the end-to-end workflow from acquiring 3D dental scans to delivering treatment recommendations. It includes four main stages: Data Acquisition (standard tessellation language [STL] scan collection and voxelization), Model Training (using 3D CNNs), Classification Logic (hierarchical malocclusion prediction), and Deployment (integration into orthodontic CAD software). Each step demonstrates the transformation and interpretation of clinical data through deep learning to support precise, data-driven treatment planning.

### Data collection

The study models contain no identifiable participant information; therefore, individual participant consent was not required. This methodology was reviewed and approved by the Ethics Committee (Reference Code: JEP-2021-260). In this retrospective study, we utilized anonymized digital dental models obtained from patients who had previously undergone orthodontic evaluation at the university dental clinic. A total of 841 3D

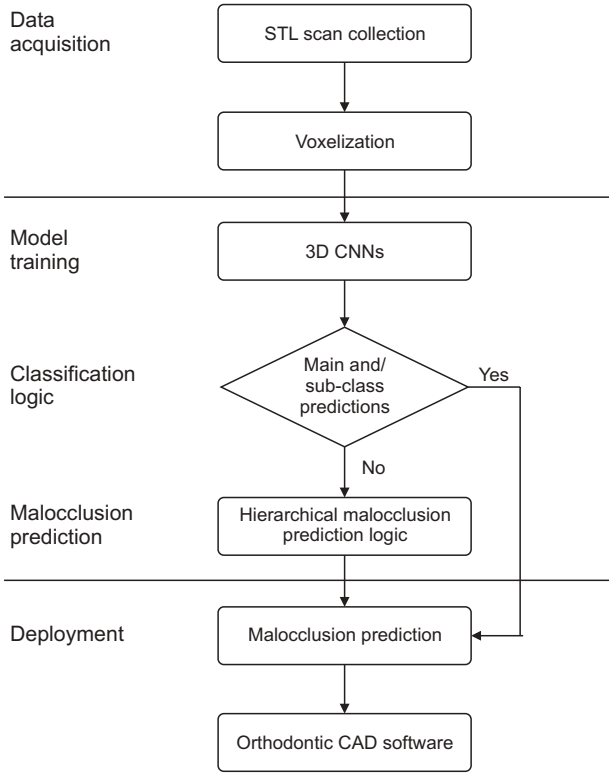


**Figure 2.** Leading Enhancement Assistive Planning research project workflow for deep learning–based orthodontic treatment.
STL, standard tessellation language; 3D, three-dimensional; CNN, convolutional neural network; CAD, computer-aided design.

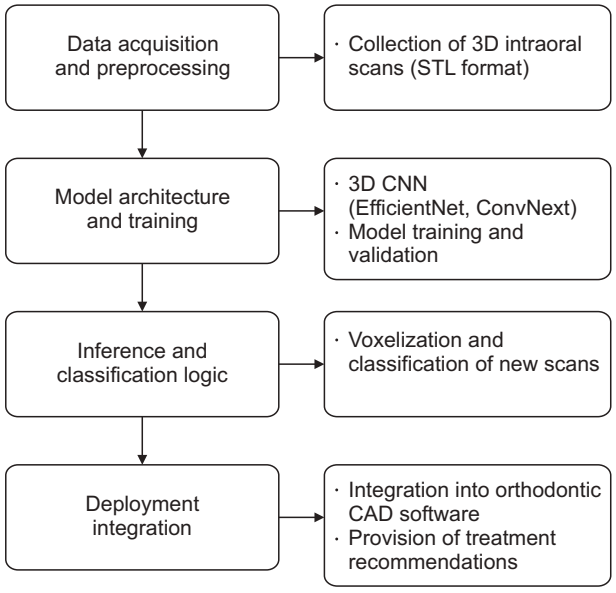


**Figure 3.** The Leading Enhancement Assistive Planning system pipeline for orthodontic treatment.
3D, three-dimensional; STL, standard tessellation language; CNN, convolutional neural network; CAD, computer-aided design.

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dental models were collected, representing a balanced distribution of Class I, Class II Division 1, Class II Division 2, Class III, crossbite, deep bite, open bite, and scissor bite malocclusions, as clinically diagnosed by 4 certified orthodontists, each with over 10 years of clinical experience. Figure 4 shows an example of multiview images of an intraoral scan file. The multiview images of the STL files provide a more complete representation, which helps in understanding the 3D structures of the teeth and their supporting structures for machine learning tasks.

Using a dataset of 841 STL files, each representing a 3D intraoral model labeled and cross-validated by experts, the system classified cases of deep bite based on learned patterns of malocclusion. Instead of manually defining anatomical landmarks (the lowest point on the mandibular midline), the model used deep learning to automatically extract features and classify malocclusion types. Figure 5 shows a sample visualization of dental arch mesh editing using Meshmixer software (version 3.5.474; Autodesk, Inc., San Francisco, CA, USA). Autodesk Meshmixer is a free 3D modeling and editing software designed primarily for working with triangular meshes (STL and OBJ files).

Table 1 shows the malocclusion types and numbers of samples. The dataset used for model training and evaluation consisted of 841 3D intraoral scan files in STL format. Each scan was labeled by expert orthodontists and cross-validated to ensure annotation reliability. The dataset was balanced across eight clinically relevant malocclusion categories.

- Classes I to III: anteroposterior relationships based on Angle's classification
- Vertical discrepancies: deep bite, open bite, cross-

**Table 1.** Overview of datasets used to train the model

| Incisor relationship | Number of samples | Malocclusion | Number of samples |
|---|---|---|---|
| Class I | 110 | Cross bite | 104 |
| Class II Division 1 | 102 | Deep bite | 101 |
| Class II Division 2 | 106 | Open bite | 106 |
| Class III | 104 | Scissor bite | 108 |
| Total | | 841 | |

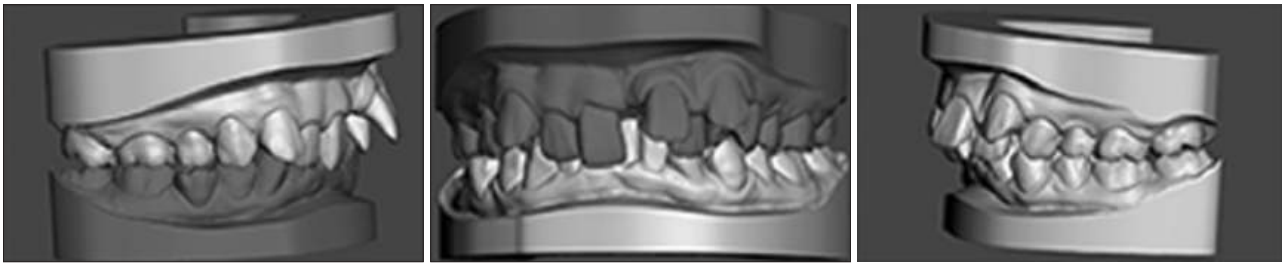

**Figure 4.** Multi-view intraoral scan file showing left-side, frontal, and right-side views from left to right.

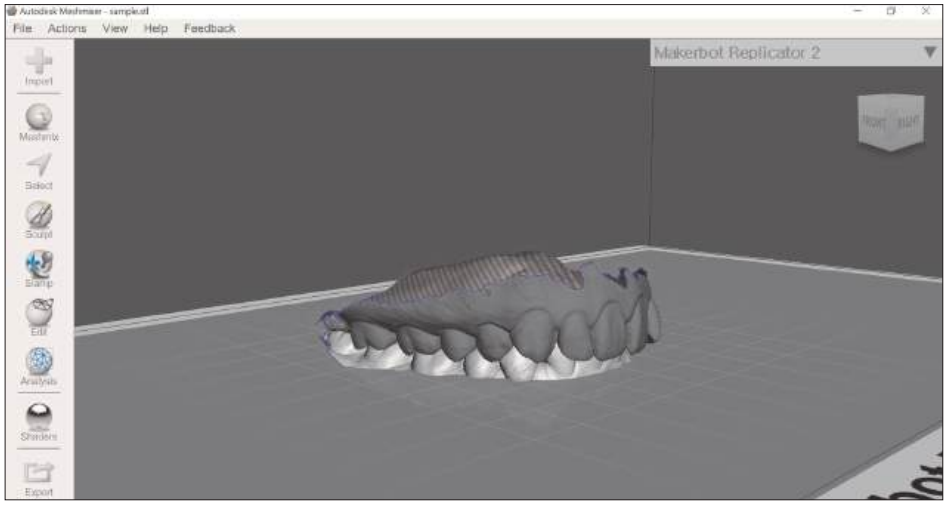


**Figure 5.** Standard tessellation language dental arch model processed in Autodesk Meshmixer.


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bite, and scissor bite

### Data preprocessing and preparation

In the data preparation module, raw 3D dental scans were converted into inputs for deep learning classification. A custom PyTorch dataset class was implemented to process STL files parsed with the NumPy-STL library to extract triangular mesh vertices. The meshes were voxelized into fixed-resolution grids (128 × 128 × 128 or 256 × 256 × 256). The voxelization function computed each model's bounding box, scaled the mesh points to the voxel resolution, and translated them into a centered grid. The coordinates were normalized using the maximum bounding box dimensions and discretized into integer voxel indices with clipping to prevent out-of-bounds errors. The resulting binary voxel arrays preserved geometric accuracy and provided 3D occupancy data for CNNs to learn spatial features.

The dataset was organized into folders according to the malocclusion classes (Class I, Class II Division 2). The STL3D class indexed STL files, mapped class names to numeric labels, and returned each sample as a labeled 3D tensor. Data augmentation and normalization were performed using PyTorch DataLoader (version 2.6.0; PyTorch Foundation, San Francisco, CA, USA) and TQDM (version 4.67.1; tqdm developers, London, United Kingdom), respectively, for efficient batching and monitoring. The STL files were converted into a standardized format for 3D CNN input. This module supported preprocessing and dataset handling for training and evaluation, integrating seamlessly with PyTorch pipelines. Table 2 presents the pseudocode for the pipeline, covering mesh normalization, voxelization, class labeling, and dataset integration.

### AI model architecture

This study used a 3D CNN based on EfficientNet to classify voxelized STL data from 3D dental models. EfficientNet-3D is designed to efficiently process volumetric data, such as medical scans and voxel grids, and performs well with a small number of parameters and low computational cost. The single-channel input structure is listed in Table 3. In the implementation, the first convolutional layer ("conv_stem") is modified to accept a single-channel 3D input, accommodating the grayscale voxel representation of STL files.

### Training and inference

The voxel resolution was set to 128 × 128 × 128 for model performance and efficiency, and Weights & Biases (W&B) made it easy to adjust and track hyperparameters. The inference pipeline was designed to process STL files to classify malocclusions and integrate the results into CAD software. The entire process, from preprocessing to prediction, was integrated into inference.py to support real-time classification. The input data were normalized and voxelized in the same manner as that during training, and the model output major and minor classes along with confidence scores to aid clinical decision-making. The step-by-step inference process is illustrated in Figure 6.

### Classification logic and prediction flow

In this study, malocclusions were organized hierarchically to align with standard clinical orthodontic diagnostic reasoning. During routine orthodontic assessments, the primary sagittal relationship is first established and documented. This is followed by a description

**Table 2.** STL-to-voxel preprocessing and dataset initialization

| Algorithm |
|---|
| Input: Root directory R containing STL files organized in subfolders by class Target voxel grid resolution V_dim<br>Output: Dataset D containing voxelized 3D models with labels |
| 1: procedure STL3DDataset(R, V_dim)<br>2: Initialize empty list F ← [] ▷ File paths<br>3: Initialize empty list L ← [] ▷ Corresponding labels<br>4: ClassNames ← sorted list of subdirectories in R<br>5: for each class index c, class_name in ClassNames do<br>6: Path_c ← R / class_name<br>7: for each file f in Path_c do<br>8: if f ends with ".stl" then<br>9: Append full path (Path_c / f) to F<br>10: Append label c to L<br>11: return Dataset(F, L, ClassNames, V_dim) |
| 12: procedure STLToVoxel(FilePath, V_dim)<br>13: Mesh ← LoadSTL(FilePath)<br>14: Vertices ← Extract all triangle vertices from Mesh<br>15: MinBound ← min(Vertices), MaxBound ← max(Vertices)<br>16: Scale ← V_dim / max(MaxBound - MinBound)<br>17: Scaled ← (Vertices - MinBound) × Scale<br>18: Clipped ← Clip(Scaled, 0, V_dim - 1)<br>19: Voxels ← Zero matrix of shape (V_dim, V_dim, V_dim)<br>20: for each point p in Clipped do<br>21: i, j, k ← round(p_x), round(p_y), round(p_z)<br>22: Voxels[i, j, k] ← 1<br>23: return Voxels<br>24: procedure GetItem(i)<br>25: FilePath ← F[i], Label ← L[i]<br>26: Voxel ← STLToVoxel(FilePath, V_dim)<br>27: return Tensor(Voxel), Label |
| 28: procedure LoadData(Dataset, BatchSize)<br>29: return DataLoader with batches of size BatchSize and shuffling |

STL, standard tessellation language; 3D, three-dimensional.

 https://doi.org/10.4041/kjod25.214 

**Table 3.** EfficientNet-3D architecture (modified for single-channel input)

| Algorithm |
|---|
| Input: [1 × D × H × W] voxel grid (1 × 128 × 128 × 128) |
| 1. Stem:<br>Conv3d(1, 32, kernel_size=3, stride=2, padding=1)<br>BatchNorm3d<br>Swish (SiLU) |
| 2. MBConv Blocks:<br>Stage 1: MBConv1 (expand=1, out_channels=16, num_blocks=1)<br>Stage 2: MBConv6 (expand=6, out_channels=24, num_blocks=2, stride=2)<br>Stage 3: MBConv6 (expand=6, out_channels=40, num_blocks=2, stride=2)<br>Stage 4: MBConv6 (expand=6, out_channels=80, num_blocks=3, stride=2)<br>Stage 5: MBConv6 (expand=6, out_channels=112, num_blocks=3, stride=1)<br>Stage 6: MBConv6 (expand=6, out_channels=192, num_blocks=4, stride=2)<br>Stage 7: MBConv6 (expand=6, out_channels=320, num_blocks=1, stride=1) |
| 3. Head:<br>Conv3d(320, 1280, kernel_size=1)<br>BatchNorm3d<br>Swish (SiLU) |
| 4. Global Average Pooling:<br>AdaptiveAvgPool3d(1) |
| 5. Classifier:<br>Dropout<br>Linear(1280, num_classes) |

3D, three-dimensional.

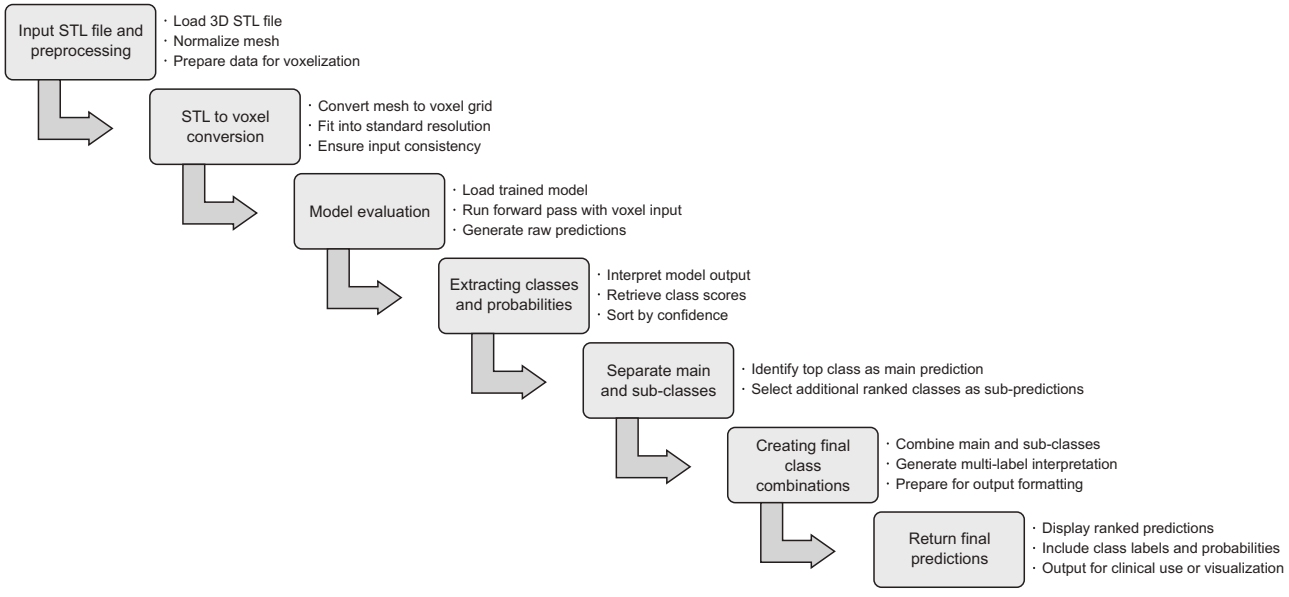


**Figure 6.** Inference process.
STL, standard tessellation language; 3D, three-dimensional.


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of other coexisting occlusal traits, including vertical and transverse discrepancies. The main classes representing primary sagittal malocclusions according to Angle's classification are as follows:

- Class I
- Class II Division 1
- Class II Division 2
- Class III

These main classes correspond to the dominant anteroposterior relationship of the dental arches and serve as primary orthodontic diagnoses. Subclasses represent secondary occlusal characteristics that may coexist with any main class and further characterize malocclusion. These are the following:

- Deep Bite
- Open Bite
- Anterior Crossbite
- Posterior Crossbite
- Crowding (mild/moderate/severe, where applicable)

Subclasses do not replace sagittal diagnosis but provide complementary information that reflects the multidimensional nature of malocclusion.

In LEAP, the STL file was voxelized and processed by a 3D CNN, which output the top five predicted classes with confidence scores categorized into main classes and subclasses. Subsequently, a rule-based combination logic was applied. The system first examined whether an incisor relationship was present among the top predictions. If an incisor relationship was detected, the system evaluated whether valid labelling combinations could be formed. When no valid combinations were possible, only the detected incisor relationship was provided (e.g., Class II). Otherwise, the system output the individual classes together with all valid pairwise combinations, including clinically relevant conditions, such as Class II Division 1, open bite, and crossbite. All decision paths converged at a unified output stage, ensuring a consistent and deterministic classification outcome.

Figure 7 shows the rule-based logic, where the LEAP system predicts the final malocclusion based on the major-minor classification, as defined. The outputs were the top five diagnostic-ranking classes. The logic in the make_possible_combinations() function was designed to filter low-probability predictions and generate a clinically meaningful class. Through this structured prediction approach, LEAP improved the accuracy for effective treatment planning support.

## RESULTS

### Model training hyperparameters

A customized version of the EfficientNet architecture, optimized for 3D volumetric data, was used to train the 3D malocclusion classification model. The model was trained using the Adam optimizer, which has the advantages of handling sparse gradients and adaptively adjusting the learning rate, with a batch size of 10 and total of 100 epochs. The classification target consisted of eight orthodontic categories, and the cross-entropy loss function was used as the loss criterion, which is well-suited for multiclass classification problems. These hyperparameters were selected based on empirical tuning for optimal convergence and generalization, as summarized in Table 4.

### Classification performance

The orthodontists and dentists used the testing datasets to confirm the model's accuracy. The experimental outcomes confirmed the system's technical reliability and clinical applicability. The trained model achieved an accuracy of 90.8%, precision of 87.5%, recall of 91.3%, and F1 score of 89.2%. Furthermore, the classification performance of the LEAP was analyzed for each malocclusion type. Table 5 presents the performance metrics

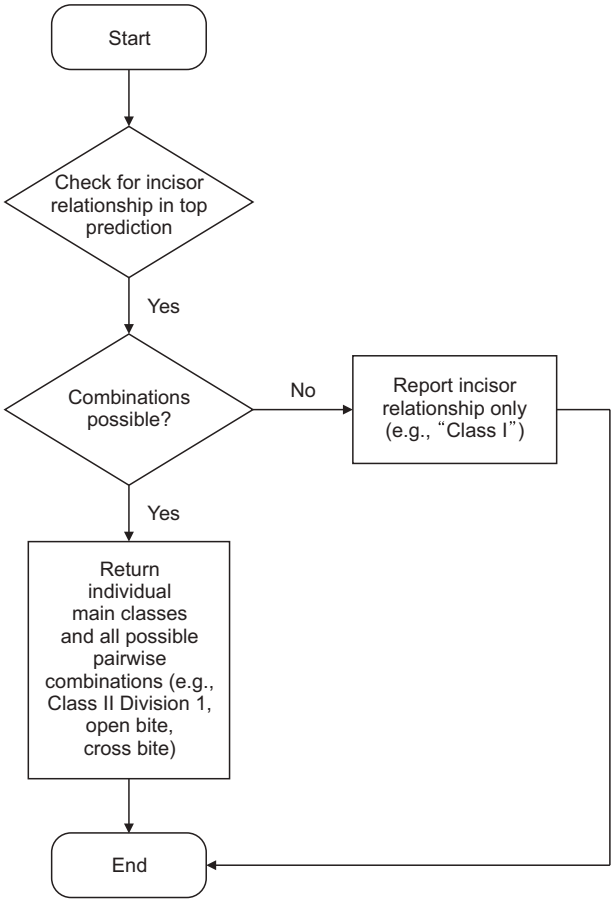


**Figure 7.** Rule-based logic flowchart for generating a final malocclusion prediction in Leading Enhancement Assistive Planning inference.

for each class. The model maintained balanced performance across most categories, consistent with the overall metrics. Class I achieved an accuracy of 90.0%, precision of 91.0%, recall of 89.0%, and F1 score of 90.0%. The highest performance was observed for the anterior open bite (accuracy: 94.7%, F1 score: 94.7%), indicating that the model could distinguish this condition with the greatest confidence. In contrast, lower results were observed for Class II Division 2 (accuracy: 83.0%, F1 score: 83.0%) and severe crowding (accuracy: 83.2%, F1 score: 83.2%), suggesting that these categories exhibit greater morphological variability (i.e., larger differences in tooth shapes and arrangements), making automatic classification by LEAP more challenging.

However, classification accuracy dropped below 87.0% for certain malocclusion types. Specifically, classification accuracies were 84.0% for Class II Division 1, 83.0% for Class II Division 2, 85.6% for edge-to-edge, and 85.4%, 84.7%, and 83.2% for mild, moderate, and severe crowding, respectively. These findings indicate that some malocclusion types are more challenging to classify, likely because of morphological similarities between adjacent classes, limited variability in the sample, or overlapping diagnostic features.

Class II Division 2 malocclusion is difficult to diagnose because of its variable presentation and dentoalveolar compensation, which often mask underlying skeletal discrepancies. Features such as retroclined upper incisors, deep overbite, and inconsistent molar/canine relationships can resemble those of Class I or Class II Division 1, thus creating ambiguity. Severe crowding adds complexity because it exists on a continuum and is influenced by multiple factors beyond the arch length discrepancy, such as tooth size and rotations. Both conditions are prone to interclinician variability, which introduces label noise into datasets and reduces model reliability. Despite these challenges, the LEAP model maintained clinically acceptable F1 scores; however, future improvements should incorporate additional diagnostic data, such as cephalometric analysis and quantitative arch length measurements, to better distinguish overlapping and morphologically complex cases.

**Table 4.** Model training hyperparameters

| Hyperparameter | Value |
|---|---|
| Deep learning model | EfficientNet (3D architecture) |
| Number of epochs | 100 |
| Batch size | 10 |
| Optimizer | Adam |
| Number of classes | 8 |
| Loss function | Cross entropy loss |

3D, three-dimensional.

### Model and system performance

The model architecture was designed for batch inference and production deployment. The system supports scalability and fast inference for integration into clinical settings and large-scale studies, and the efficiency of the 3D-CNN is crucial to its application in clinical workflows where speed and reliability are critical.

**Table 5.** Performance metrics of Leading Enhancement Assistive Planning for each malocclusion class

| Class | Accuracy (%) | Precision (%) | Recall (%) | F1-score (%) |
|---|---|---|---|---|
| Class I | 90.0 | 91.0 | 89.0 | 90.0 |
| Class II Division 1 | 84.0 | 85.0 | 83.0 | 84.0 |
| Class II Division 2 | 83.0 | 82.0 | 84.0 | 83.0 |
| Class III | 87.0 | 88.0 | 86.0 | 87.0 |
| Deep bite | 87.4 | 83.2 | 88.2 | 85.6 |
| Cross bite | 86.3 | 86.5 | 86.0 | 86.3 |
| Scissor bite | 89.4 | 84.2 | 87.9 | 87.5 |
| Open bite | 88.7 | 84.5 | 90.0 | 87.1 |
| Anterior open bite | 94.7 | 95.1 | 94.5 | 94.7 |
| Posterior open bite | 93.6 | 93.5 | 93.8 | 93.6 |
| Edge-to-edge | 85.6 | 83.2 | 87.8 | 85.4 |
| Spacing | 91.2 | 88.5 | 89.1 | 88.8 |
| Mild crowding | 85.4 | 86.1 | 85.2 | 85.5 |
| Moderate crowding | 84.7 | 85.2 | 84.3 | 84.5 |
| Severe crowding | 83.2 | 83.0 | 83.5 | 83.2 |


https://doi.org/10.4041/kjod25.214

The LEAP inference pipeline processed newly acquired STL files in real-time. The scans were normalized and voxelized before being passed to a CNN that output the top five malocclusion classes and their confidence scores. Hierarchical logic was developed to display the major and minor classes, improving the diagnostic clarity for overlapping conditions. Single-class predictions were displayed when only the dominant patterns were detected. LEAP voxelization supported 128 × 128 × 128 and 256 × 256 × 256 resolutions and worked reliably in both cases. The 256 × 256 × 256 resolution had a slightly higher precision but increased memory usage, requiring approximately 67 MB per sample. Deployment on a graphics processing unit resulted in a 5- to 10-fold improvement in the inference speed, thereby enhancing the feasibility of the proposed system for both clinical and research applications. Batch inference also handled multiple STL files reliably, and the pipeline performed well in error situations.

The LEAP workflow for automated malocclusion classification from oral scans is illustrated in Figure 8. It begins with an oral scan that generates an STL file that is preprocessed and converted into a normalized 3D grid. The data are then analyzed, and hierarchical rule-based logic determines the main and subclasses while addressing overlaps (e.g., Class II Division 2 with deep bite). The outputs include a final classification with confidence, spacing, and crowding assessment and clinically interpretable results. Once integrated into orthodontic CAD, the packaged LEAP model will enable automated classification directly from STL input, supporting clinicians with faster, more consistent, and standardized diagnostic feedback.

## DISCUSSION

LEAP demonstrates the integration of deep learning into orthodontic workflows, and in doing so, it shows the high clinical potential of using AI in digital dentistry. The results showed that automated classification based on 3D oral scans can reduce delays caused by errors and the lack of standardization of traditional diagnostics.

### Clinical implications

LEAP's high accuracy of 90.8% and recall rate of 91.3% indicate that even complex classes with overlapping patterns can be reliably identified. Owing to the hierarchical prediction algorithms developed to reflect the multifactorial nature of malocclusions, the system provides more accurate and practical diagnoses. For example, the ability to identify combinations such as "Class II Division 2 with deep bite" reflects a nuanced understanding of tooth morphology that correlates well with clinical reasoning.

Embedding automatic inference pipelines into CAD software can accelerate the treatment-planning process by providing clinicians with real-time diagnostic feedback. This is especially useful in high-volume clinical settings or in areas with limited access to orthodontic specialists. In addition, by providing consistent classifi-

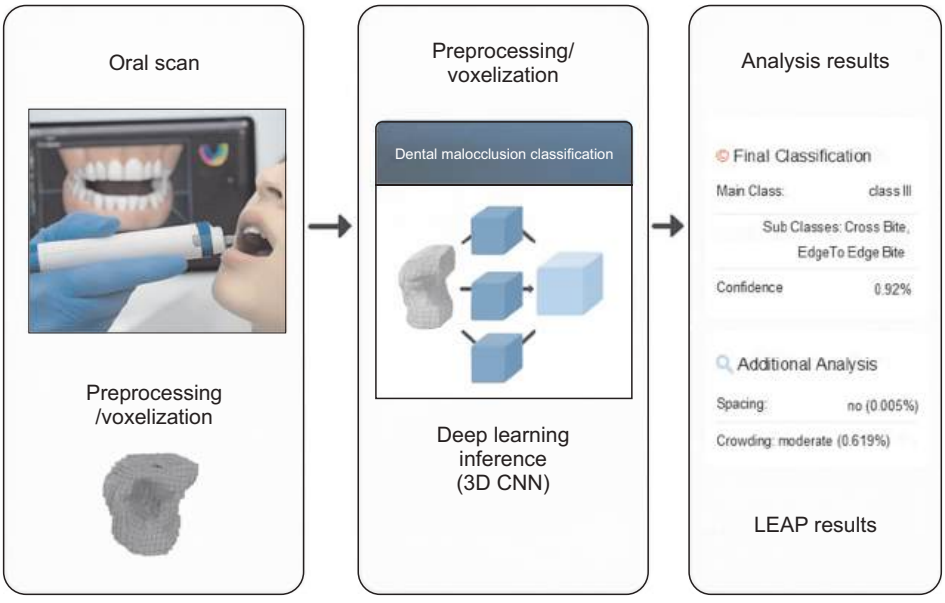


**Figure 8.** Leading Enhancement Assistive Planning (LEAP) workflow for automated malocclusion classification from oral scans.
3D, three-dimensional; CNN, convolutional neural network.

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cations based on patterns learned from expert-labeled data, LEAP can be used as a training tool by less-experienced practitioners.

### Technical contributions

From a technical perspective, applying image-based CNN architectures such as EfficientNet and ConvNeXt[22] worked well for 3D dental data. Voxel grids (3D equivalents of pixels, consisting of many small cubes used to represent a tooth) allow spatial relationships (the relative positions of teeth, roots, or jaws) to be maintained and provide uniform inputs (the same grid size and structure). Hierarchical logic is a decision-making framework that organizes malocclusion classifications into layers, allowing for realistic representation and flexible interpretation of complex malocclusions.

The learning and inference pipeline modules integrate STL preprocessing, model optimization, batch processing, and error handling. These successful integrations make LEAP suitable for clinical applications. In addition, we developed performance-monitoring modules using W&B, which allowed us to systematically track the behavior and reproducibility of the model.

### Limitations

While the LEAP system has demonstrated accurate classification of malocclusions that can support treatment planning, it has a few limitations.[23] Current models depend on expert-annotated dataset labels, which, although reviewed and validated by human experts such as dentists and dental technicians, are still likely to contain some subjective bias due to human judgment.[24] Additionally, voxel representations effectively preserve spatial information, which is valuable for AI models to understand the relationships between teeth; however, they can be computationally expensive at high resolution.

To address this trade-off (high spatial accuracy vs. high computational load), future versions of LEAP may need to explore point clouds (sets of points in space) or mesh-based (surfaces composed of triangles) models to improve performance and efficiency. Furthermore, the system has only been tested on controlled datasets, and its generalizability to different scanners has not yet been validated.

### Future directions

LEAP was designed to evolve toward seamless integration into clinical CAD workflows, ultimately serving as a key component of AI-assisted orthodontics. To accommodate diverse clinical environments, we envision multiple deployment strategies, including embedding LEAP as an on-premises module within CAD software, deploying it as a secure cloud-based Application Programming Interface, or connecting through workflow automation tools. These approaches would enable automated classification and treatment planning directly within existing digital systems. However, a critical limitation is that LEAP's generalizability across different intraoral scanners has not yet been validated, posing a major barrier to clinical applicability. To address this, we plan to conduct a multicenter validation study across diverse clinical settings and scanning devices to enhance system robustness and reliability prior to commercial integration. Integrating LEAP with treatment simulation tools, including predictive models of tooth movements under different aligner protocols, could convert it into a comprehensive treatment planning assistant. Embedding LEAP directly into intraoral scanning devices would enable real-time diagnostic feedback during patient examinations, streamlining workflows and improving chairside efficiency. Ultimately, these advancements position LEAP to improve diagnostic accuracy, reduce clinical workload, and enable more personalized patient care.

## CONCLUSIONS

This study presents LEAP, an AI protocol that automatically classifies malocclusions and integrates them into treatment planning. LEAP uses 3D CNNs and hierarchical classification to identify major and minor malocclusions with high accuracy and provides an automated workflow from STL preprocessing to real-time prediction. The LEAP system demonstrated high classification performance across multiple malocclusion types, with accuracy, precision, recall, and F1 scores all exceeding 87%. Notably, the system generated classification results in real time, immediately after the STL file was uploaded from a 3D scan, underscoring its potential for seamless integration into routine clinical practice.

Although it is limited to treatment planning, as it does not provide specific guidance on how to move teeth, LEAP lays the groundwork for AI-assisted orthodontics and is expected to advance further. Future plans include expanding the dataset, such as larger or more diverse cases, including multilabeled instances (e.g., Class II Division 1 and deep bite), and integrating treatment outcomes (e.g., did this patient's bite improve as expected?) to enhance treatment support and real-time diagnostic feedback.

## AUTHOR CONTRIBUTIONS

Conceptualization: RAWMH. Data curation: RAWMH, AA, AMFSM, RMAW. Formal analysis: HJL. Funding acquisition: HJL. Methodology: KBG. Validation: KBG. Visualization: HJL, Writing–original draft: HJL. Writing–review & editing: AA, AMFSM, RMAW.


https://doi.org/10.4041/kjod25.214

## CONFLICTS OF INTEREST

No conflicts of interest relevant to this article were reported.

## FUNDING

This work was supported in part by the National Research Foundation of Korea (NRF), funded by the Korean Government (MSIT) under Grant RS-2023-00250496, and by the Institute of Information & Communications Technology Planning & Evaluation (IITP), funded by the Korean Government (MSIT) under Grant RS-2019-II190421 (AI Graduate School Support Program, Sungkyunkwan University).

## REFERENCES

1. Ghodasra R, Brizuela M. Orthodontics, malocclusion. In: StatPearls. Treasure Island: StatPearls Publishing; 2025. https://pubmed.ncbi.nlm.nih.gov/37276298/
2. Rischen RJ, Breuning KH, Bronkhorst EM, Kuijpers-Jagtman AM. Records needed for orthodontic diagnosis and treatment planning: a systematic review. PLoS One 2013;8:e74186. https://doi.org/10.1371/journal.pone.0074186
3. Noeldeke B, Vassis S, Sefidroodi M, Pauwels R, Stoustrup P. Comparison of deep learning models to detect crossbites on 2D intraoral photographs. Head Face Med 2024;20:45. https://doi.org/10.1186/s13005-024-00448-8
4. Talaat S, Kaboudan A, Talaat W, Kusnoto B, Sanchez F, Elnagar MH, et al. The validity of an artificial intelligence application for assessment of orthodontic treatment need from clinical images. Semin Orthod 2021;27:164-71. https://doi.org/10.1053/j.sodo.2021.05.012
5. Hertig G, van Nistelrooij N, Schols J, Xi T, Vinayahalingam S, Patcas R. Quantitative tooth crowding analysis in occlusal intra-oral photographs using a convolutional neural network. Eur J Orthod 2025;47:cjaf025. https://doi.org/10.1093/ejo/cjaf025
6. Ryu J, Kim YH, Kim TW, Jung SK. Evaluation of artificial intelligence model for crowding categorization and extraction diagnosis using intraoral photographs. Sci Rep 2023;13:5177. https://doi.org/10.1038/s41598-023-32514-7
7. Bardideh E, Lal Alizadeh F, Amiri M, Ghorbani M. Designing an artificial intelligence system for dental occlusion classification using intraoral photographs: a comparative analysis between artificial intelligence-based and clinical diagnoses. Am J Orthod Dentofacial Orthop 2024;166:125-37. https://doi.org/10.1016/j.ajodo.2024.03.012
8. Vaughan M, Mheissen S, Cobourne M, Ahmed F. Diagnostic accuracy of artificial intelligence for dental and occlusal parameters using standardized clinical photographs. Am J Orthod Dentofacial Orthop 2025;167:733-40. https://doi.org/10.1016/j.ajodo.2025.01.017
9. Nakajima A, Murata M, Tanaka E, Arai Y, Fukase Y, Nishi Y, et al. Development of three-dimensional FE modeling system from the limited cone beam CT images for orthodontic tipping tooth movement. Dent Mater J 2007;26:882-91. https://doi.org/10.4012/dmj.26.882
10. Semerci ZM, Yardımcı S. Empowering modern dentistry: the impact of artificial intelligence on patient care and clinical decision making. Diagnostics (Basel) 2024;14:1260. https://doi.org/10.3390/diagnostics14121260
11. Tian S, Dai N, Zhang B, Yuan F, Yu Q, Cheng X. Automatic classification and segmentation of teeth on 3D dental model using hierarchical deep learning networks. IEEE Access 2019;7:84817-28. https://doi.org/10.1109/ACCESS.2019.2924262
12. Juneja M, Saini SK, Kaur H, Jindal P. Application of convolutional neural networks for dentistry occlusion classification. Wirel Pers Commun 2024;136:1749-67. https://doi.org/10.1007/s11277-024-11358-y
13. Yao Z, Wang P, Li Y, Yang X, Zhou X, Wang Y, et al. Automatic Angle's classification based on the occlusal contact information. Paper presented at: 2022 IEEE International Conference on Systems, Man, and Cybernetics (SMC); 2022 Oct 9-12; Prague, Czech Republic. New York: IEEE, 2022. p. 761-7. https://doi.org/10.1109/SMC53654.2022.9945529
14. Khanagar SB, Alfouzan K, Awawdeh M, Alkadi L, Albalawi F, Alfadley A. Application and performance of artificial intelligence technology in detection, diagnosis and prediction of dental caries (DC)-a systematic review. Diagnostics (Basel) 2022;12:1083. https://doi.org/10.3390/diagnostics12051083
15. Luke AM, Rezallah NNF. Accuracy of artificial intelligence in caries detection: a systematic review and meta-analysis. Head Face Med 2025;21:24. https://doi.org/10.1186/s13005-025-00496-8
16. Faizan Ahmed SM, Ghori MH, Khalid A, Nooruddin A, Adnan N, Lal A, et al. Annotated intraoral image dataset for dental caries detection. Sci Data 2025;12:1297. https://doi.org/10.1038/s41597-025-05647-9
17. Chai Y, Chai X, Zhang L, Ye G, Sheykhahmad FR. Oral cancer detection via Vanilla CNN optimized by improved artificial protozoa optimizer. Sci Rep 2025;15:29218. https://doi.org/10.1038/s41598-025-11861-7

18. Mao YC, Lin YJ, Hu JP, Liu ZY, Chen SL, Chen CA, et al. Automated caries detection under dental restorations and braces using deep learning. Bioengineering (Basel) 2025;12:533. https://doi.org/10.3390/bioengineering12050533
19. Leonardi R, Vaiid N. Artificial intelligence in orthodontics: concerns, conjectures, and ethical dilemmas. Int Dent J 2025;75:20-2. https://doi.org/10.1016/j.identj.2024.11.002
20. Babu A, Andrew Onesimu J, Martin Sagayam K. Artificial intelligence in dentistry: concepts, applications and research challenges. E3S Web Conf 2021;297:01074. https://doi.org/10.1051/e3sconf/202129701074
21. Ding H, Wu J, Zhao W, Matinlinna JP, Burrow MF, Tsoi JKH. Artificial intelligence in dentistry-a review. Front Dent Med 2023;4:1085251. https://doi.org/10.3389/fdmed.2023.1085251
22. Tan M, Le QV. EfficientNet: rethinking model scaling for convolutional neural networks. arXiv 2019. https://doi.org/10.48550/arXiv.1905.11946
23. Auconi P, Gili T, Capuani S, Saccucci M, Caldarelli G, Polimeni A, et al. The validity of machine learning procedures in orthodontics: what is still missing? J Pers Med 2022;12:957. https://doi.org/10.3390/jpm12060957
24. Liu J, Chen Y, Li S, Zhao Z, Wu Z. Machine learning in orthodontics: challenges and perspectives. Adv Clin Exp Med 2021;30:1065-74. https://doi.org/10.17219/acem/138702