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Research on Incisor Target Position Design Based on Orthodontic Profile Changes
Assisted by Artificial Intelligence

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ABSTRACT

Background: Improving the soft tissue profile is an important goal in orthodontics, and incisor positioning plays a critical role in determining facial aesthetics. Artificial intelligence (AI) has shown potential in orthodontic treatment planning; however, limited research has been conducted on predicting incisor target positions based on soft tissue changes. We aimed to develop and validate an AI model based on a diffusion framework for predicting target incisor positions by integrating cephalometric and soft tissue parameters.

Methodology: A total of 300 patients who met the inclusion criteria were enrolled in the study. Pre- and posttreatment lateral cephalograms were preprocessed and used to train the Ceph-DDPM, a latent-space diffusion model. The model, comprising of a variational autoencoder and a condition-guided diffusion denoising network, generated predicted posttreatment images from pretreatment scans and soft tissue change vectors. An efficient 10-step sampling strategy was used. Model accuracy was quantitatively evaluated by comparing landmark errors and cephalometric measurements between the predicted and actual outcomes. Statistical analyses were performed using the SPSS software.

Results: The errors across the nine cephalometric parameters were not statistically significant. Predictions of the sagittal positions of the incisors fell within clinically acceptable ranges, although inaccuracies persisted in other parameters, indicating the need for further refinement. Visualization of the generated incisor positions demonstrated the model's ability to simulate clinically relevant outcomes.

Conclusions: The Ceph-DDPM model is a promising decision-support tool for orthodontic treatment planning that links soft tissue changes with incisor movement. Although predictions of sagittal incisor positions are clinically useful, additional optimization and integration of anatomical constraints will improve overall accuracy and physiological plausibility. Future studies should focus on incorporating interactive manipulation and expert-driven rules to enhance the clinical applicability of the model.

KEYWORDS: Artificial Intelligence, Orthodontic Treatment Planning, Incisor Position Prediction, Cephalometric Analysis, Diffusion Model

BACKGROUND

Improving the soft tissue profile has become a major demand for many orthodontic patients^[1]. Lip protrusion is common in East Asian populations. Orthodontic treatment not only aligns teeth and improves occlusion but also affects facial soft tissues. Therefore, orthodontists should develop targeted treatment goals and plans based on patients' individual needs and preferences to achieve optimal therapeutic outcomes^[2].

The incisor position objective (IPO) is typically set on the pre-treatment cephalogram and comprises three elements: the sagittal location, vertical location, and labiolingual angulation of the central incisors.^[3] Given that the incisor retraction results in retrusion of the lips, the sagittal location within IPO is crucial for the post-treatment facial profile^[4-6]. Incisor aesthetic positioning is a central issue in precision orthodontics^[7]. It is widely recognized that the

inclination and sagittal position of incisors are closely related to the profile contour and smile aesthetics^[8, 9]. Andrews demonstrated that the sagittal position of incisors plays a significant role in establishing lip aesthetics^[10]. In *The Six Elements of Orofacial Harmony*^[11], he elaborated on the theory of sagittal positioning of the anterior teeth, emphasizing the aesthetic positioning of the maxillary central incisors and the importance of tailoring treatment to the patient's individual facial profile characteristics^[12]. The Forehead's Anterior Limit Line and Goal Anterior Limit Line, as relatively stable, quantifiable, and reproducible facial reference lines, help determine the target position of maxillary incisors in orthodontic treatment and establish an evaluation benchmark^[13-16]. According to studies, the "Diagnostic Facial Triangle" suggests that the upright positioning of the mandibular incisors over the basal bone i.e., when the posterosuperior angle between the axis of the lower central incisor and the mandibular plane ($\angle L1-MP$) is $90\pm 5^\circ$ contributes to both profile aesthetics^[17] and dental stability^[18].

Precision medicine is becoming a cutting-edge focus in the international medical field owing to rapid advancements in artificial intelligence (AI) technology^[19]. In AI-enabled healthcare, image-based applications, such as the evaluation of radiological, dermatological, pathological, and retinal images, are among the most extensively researched and widely implemented applications^[20]. AI-based models outperform those developed using conventional epidemiological methods and can be applied to predict diseases^[21], estimate prognosis^[22], and forecast all-cause mortality^[23]. Diffusion models are a unique type of generative model that focuses on simulating the gradual evolution of data distribution from a simple starting point to

increasingly complex distributions^[24]. Furthermore, diffusion models have surpassed traditional generative adversarial networks in the field of image synthesis^[25].

Traditionally, determining the ideal target position for teeth in orthodontics has relied on manual measurements and clinical observations, a process that is relatively cumbersome and susceptible to human error. The introduction of digital technologies has made clinical orthodontic examinations and measurements more precise, efficient, and convenient. With the advancement of AI, the development of orthodontic treatment plans has become a prominent research focus^[26]. Numerous studies have confirmed the advantages of AI models in predicting changes in soft tissue profiles during orthodontic treatment. However, research on inferring incisor positions based on soft tissue changes remains limited. A deep learning model capable of accurately predicting incisor positions from morphological changes in soft tissues could assist clinicians in formulating more rational treatment plans, reduce the risks associated with planning errors, and improve communication among doctors, patients, and clinical teams, thereby minimizing conflicts arising from mismatched aesthetic expectations.

Based on this, the study proposes a diffusion model-based method for predicting orthodontic soft tissue-guided treatment outcomes and evaluates the accuracy of the algorithm in orthodontic hard and soft tissue correlation analysis by comparing the predicted incisor positions generated by the model with actual treatment results.

METHODS

Sample selection

This study was approved by the Research Ethics Committee of Beijing Stomatological Hospital, Capital Medical University (CMUSH-IRB-KJ-PJ-2022–25). A total of 300 adult patients who completed orthodontic treatment at the Department of Orthodontics, Beijing Stomatological Hospital, Capital Medical University, between 2013 and 2023 were screened for inclusion. The inclusion criteria were as follows: (1) age 18–45 years; (2) orthodontic treatment with tooth extractions; (3) no history of craniomaxillofacial trauma, previous orthodontic treatment, or orthognathic surgery; (4) complete pretreatment (T1) and posttreatment (T2) medical records; and (5) diagnosis of skeletal Class I malocclusion. The exclusion criteria were as follows: (1) requirement for correction of dental midline deviation; (2) history of cosmetic surgery during the treatment period; (3) presence of facial features such as birthmarks or scars that could interfere with landmark identification; and (4) occurrence of soft or hard tissue facial trauma during the treatment period.

Based on previous research^[27], the sample size required for this study was estimated based on hypothesis testing. The significance level (α) was set at 0.05 (two-tailed), statistical power (1- β) at 95%, and the standard deviation at 1.50 mm. This study was designed to detect a 2.0 mm difference between the predicted treatment outcomes and actual measurements. Using PASS software, the minimum sample size was calculated as 10 participants. In line with prior studies^[28], the sample size was appropriately increased in this study.

Image processing

Two operators used the LabelMe® software to annotate landmarks on all T1 images to determine the region of interest for cropping and to obtain the condition vectors. A total of 13 cephalometric landmarks were plotted: Nasion, Orbitale, Porion, Pronasale, Columella point, Subnasale, Soft tissue A point, Upper lip, Lower lip, Soft tissue B point, Soft tissue Pogonion, and Cervical point. In addition, five soft tissue measurements were obtained. The landmarks and parameters used in this study are shown in Figure 1 and Table 1.

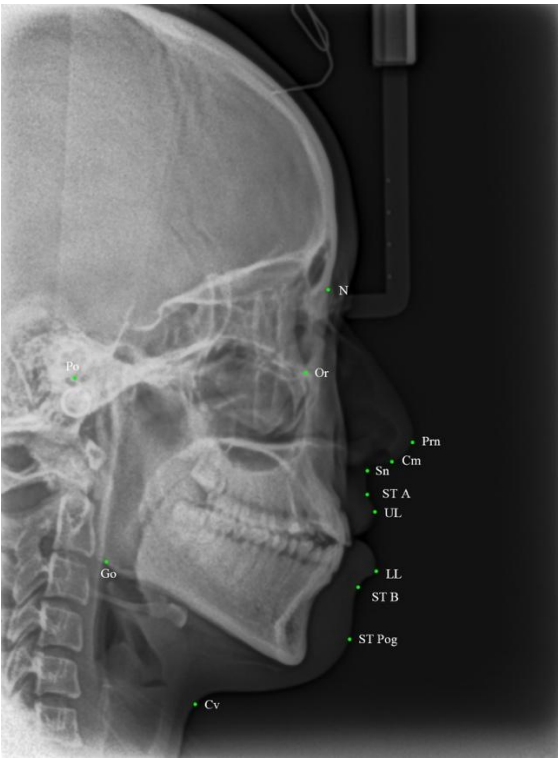


Figure 1. Landmarks (A) and soft tissue analysis parameters (B, C) used in this study.

Table 1. The parameters used in this study

Variable	Description
Upper lip to E line (mm)	The distance from point UL to the E line
Lower lip to E line (mm)	The distance from point LL to the E line

Upper lip sulcus depth (mm)	The distance from point ST A to the perpendicular line of the Frankfort plane through point upper lip
Lower lip sulcus depth (mm)	The distance from point ST B to the H line
Nasolabial angle ($^{\circ}$)	The intersection angle of the line of point columella and Sn with the line of point Sn and point upper lip
H line	Holdaway line. The tangent line drawn from point ST Pog to the upper lip

132 UL: Upper lip

133 LL: Lower lip

134 ST A: Soft tissue A point

135 ST B: Soft tissue B point

136 ST Pog: Soft tissue Pogonion

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138 The same operators used Dolphin Imaging 18.0 software to annotate landmarks on both
139 T1 and T2 images, further characterizing changes in the five soft tissue measurements and
140 converting these data into vectorized form. All X-ray images were resized to a uniform
141 dimension of 256×256 pixels while maintaining the original aspect ratio, with any insufficient
142 areas padded with zeros. The image intensity was linearly normalized by mapping the pixel
143 values to the range of $[-1, 1]$.

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Model construction and training

We propose the use of Ceph-DDPM, an orthodontic target position prediction model based on latent-space diffusion, which consists of two modules: a variational autoencoder (VAE) and a condition-guided latent diffusion denoising network (Figure 2). The preoperative cephalometric radiograph X_{pre} and target soft tissue deformation vector S are fed as joint inputs, and the predicted post-treatment cephalometric image PT2 (denoted as X_{post}) is generated as the output.

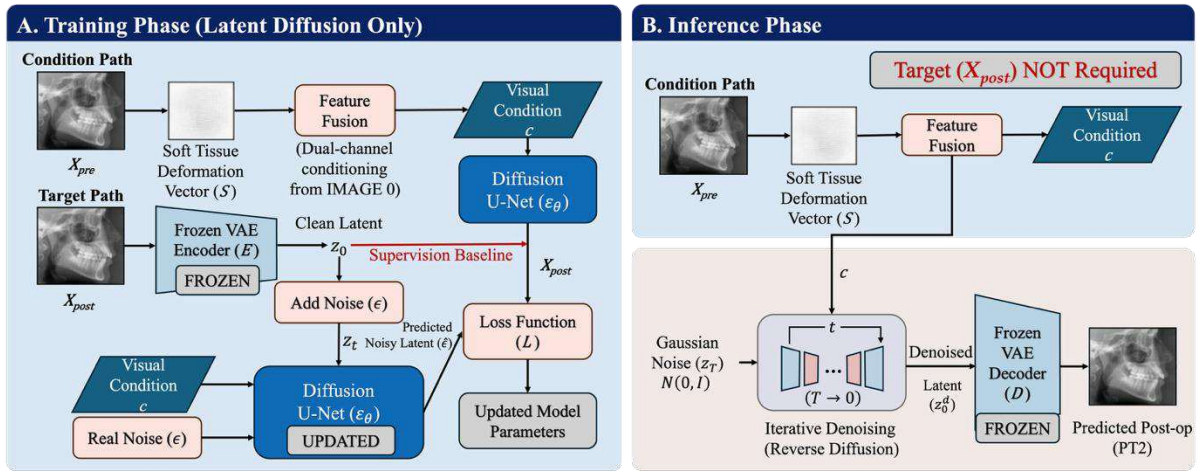


Figure 2. Workflow for Ceph-DDPM. Input thumbnails are illustrative examples and PT2 (X_{post}) is generated as output. The ‘Supervision Baseline’ connection is corrected only in the training panel.

A Kullback–Leibler (KL)–regularized VAE was adopted to compress high-resolution X-ray images into low-dimensional latent space, separating image reconstruction from latent diffusion denoising and drastically reducing computational overhead. The encoder E takes 256×256 single-channel grayscale cephalometric radiographs as input and outputs 8-channel

latent feature maps with a resolution of 32×32 (denoted as $z \in \mathbb{R}^{8 \times 32 \times 32}$). The decoder D reconstructs original 256×256 grayscale X-ray images from latent variables.

The VAE was pre-trained independently and was optimized by a composite loss function combining reconstruction loss, multi-scale perceptual loss, and KL regularization loss. After pre-training, the weights of both encoder and decoder were fully frozen throughout the subsequent training phase; only the parameters of the diffusion U-Net were updated.

During training, real post-treatment radiographs X_{post} were encoded into clean latent variables z_0 , serving as the supervision baseline for the diffusion model. In the inference stage, real post-treatment images were no longer required; the denoised latent representations were directly decoded by the decoder to generate predicted post-treatment radiographs.

A dual-channel conditional input mechanism was implemented to fuse visual features from preoperative radiographs and numerical soft tissue measurement conditions simultaneously. The visual preoperative condition c enforces pixel-wise spatial alignment between preoperative images and latent-space features. Five soft tissue metrics (nasolabial angle, upper/lower lip E-line distance, superior/inferior labial sulcus depth) were encoded into a one-dimensional feature vector S , which was mapped via fully connected layers into feature maps matching the resolution of latent variables. The noisy latent variable z_t , visual preoperative condition c , and soft tissue feature vector S were concatenated along the channel dimension and fed into the network.

The total diffusion timestep was set to $T = 1000$, with a linear noise schedule β_t ranging from 1.5×10^{-3} to 2.05×10^{-2} . In the forward diffusion process, noise is gradually injected into z_0 . The formula for noisy latent variables at arbitrary timestep t is as follows:

$$z_t = \sqrt{\bar{\alpha}_t} z_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, \quad \epsilon \sim \mathcal{N}(0, I), \quad \text{Eq. A1}$$

where $\bar{\alpha}_t = \prod_{i=1}^t \alpha_i$, $\alpha_i = 1 - \beta_i$, and ϵ denotes randomly sampled Gaussian noise.

For reverse denoising, a modified OpenAI-style U-Net (Figure 3) was utilized as the noise prediction network ϵ_θ . The base channel count was set to 160 with channel multipliers [1,2,4,4], and feature resolution transitions followed $32 \rightarrow 16 \rightarrow 8 \rightarrow 4$. Two residual blocks were deployed at each resolution level, and self-attention modules were integrated at the 32, 16, and 8 resolution layers to capture global anatomical correlations. Embedded timestep t was injected into all residual blocks via feature-wise linear modulation layers; no cross-attention layers were used, and all conditional information was incorporated solely through channel-wise concatenation. The iterative formula for reverse denoising is written as follows:

$$z_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left[z_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon_\theta(z_t, t, X_{pre}, S) \right] + \sigma_t z, \quad \text{Eq. A2}$$

where $\epsilon_\theta(z_t, t, X_{pre}, S)$ represents the noise predicted by the network, z is standard normal random noise, and σ_t is the noise coefficient corresponding to timestep t .

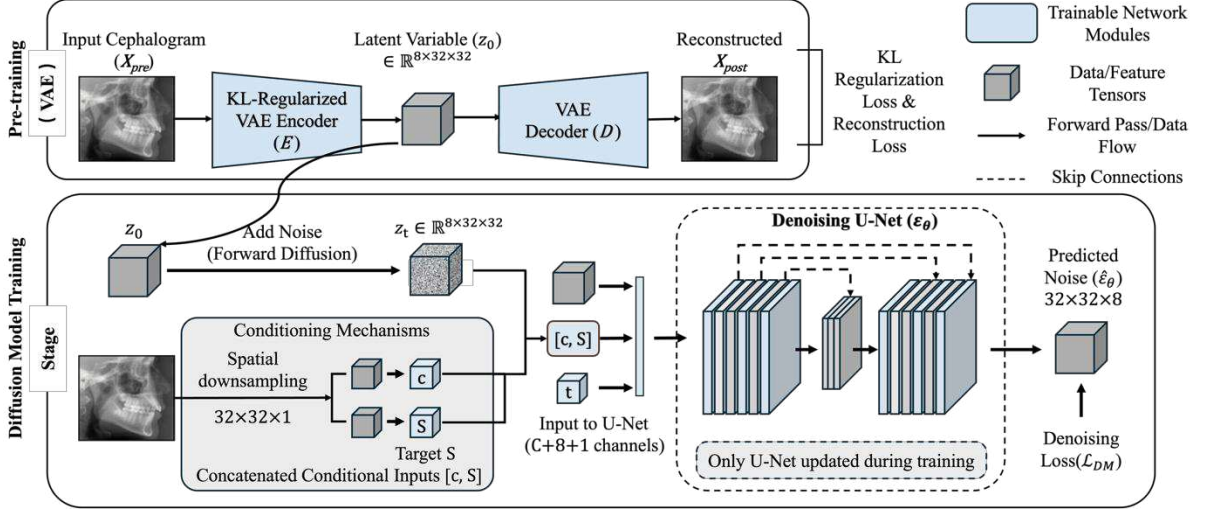


Figure 3. Overall architecture of Ceph-DDPM.

A weighted composite total loss function was designed to balance noise prediction precision, anatomical plausibility, and visual similarity of generated images:

1. Basic diffusion loss:

$$\mathcal{L}_{diff} = \mathbb{E}_{t, z_0, \epsilon} \left[\|\epsilon - \epsilon_{\theta}(z_t, t, X_{pre}, S)\|^2 \right] \quad \text{Eq. A3}$$

2. Anatomical consistency loss:

$$\mathcal{L}_{anatomy} = \sum_i \lambda_i \|A_i(X_{pred}) - A_i(X_{gt})\|_1 \quad \text{Eq. A4}$$

3. Multi-scale perceptual loss:

$$\mathcal{L}_{perceptual} = \sum_{l=1}^L \lambda_l \|\phi_l(X_{pred}) - \phi_l(X_{gt})\|_1 \quad \text{Eq. A5}$$

The final total loss function is defined as follows:

$$\mathcal{L}_{total} = \mathcal{L}_{diff} + \lambda_{anatomy} \mathcal{L}_{anatomy} + \lambda_{perceptual} \mathcal{L}_{perceptual}, \quad \text{Eq. A6}$$

where $\lambda_{anatomy}$ and $\lambda_{perceptual}$ are weighting coefficients to balance the magnitude of each loss component.

To reduce inference latency, a Fast-DDPM-accelerated sampling strategy was introduced to compress the original 1000-step diffusion cycle into 10 denoising iterations. Two sets of sampling timesteps were formulated:

Uniform sampling schedule:

$$T_{uniform} = \{0, 100, 200, 300, 400, 500, 600, 700, 800, 900, 999\}.$$

Non-uniform sampling schedule:

$$T_{non-uniform} = \{0, 199, 399, 599, 699, 799, 849, 949, 999\}.$$

During inference, T1 cephalometric radiographs were standardized to 256×256 pixels with intensity values normalized to $[-1, 1]$ and then downsampled to extract visual condition c . Clinically expected soft tissue improvement metrics were converted into the condition vector S . Initial latent variables $z_t \sim \mathcal{N}(0, I)$ were randomly sampled from the standard normal distribution. The 10-step Fast-DDPM reverse denoising iteration was executed to gradually eliminate latent-space noise and obtain clean latent representation z_0 . The decoder D reconstructed z_0 into a 256×256 grayscale predicted post-treatment radiograph PT2. Pixel intensity inverse normalization and anatomical consistency verification were performed to output the final predicted cephalogram.

Quantitative evaluation of model performance

Two investigators independently annotated the following landmarks on all T2 and PT2 images by using LabelMe[®] software: incisal edge of the upper central incisor (U1I), apex of the upper central incisor (U1A), incisal edge of the lower central incisor (L1I), and apex of the lower

central incisor (L1A). The final position of each landmark was determined by averaging the measurements of the two investigators after two rounds. The mean radial error (MRE) and successful detection rate (SDR) within thresholds of 2.0, 2.5, 3.0, and 4.0 mm were calculated to evaluate landmark identification accuracy.

The same investigators performed cephalometric analyses of the PT2 and T2 images by using Dolphin Imaging software. The target angulation and positional measurements of the upper and lower incisors were calculated, with the error defined as the difference between the actual and predicted values of the measurements. The definitions of the measured variables are listed in Table 2.

Table 2. Measurement Items for Evaluating the Accuracy of Upper and Lower Incisor

Positioning	
Variable	Description
$\angle U1-SN (^{\circ})$	The angle between the axis of the upper central incisor and the sella-nasion plane.
$\angle U1-NA (^{\circ})$	The angle between the axis of the upper central incisor and the nasion-A point line.
$\angle U1-PP (^{\circ})$	The angle between the axis of the upper central incisor and the palatal plane.
$\angle L1-APog (^{\circ})$	The superior angle between the axis of the lower central incisor and A point-Pogonion line.

∠L1-MP (°)	The posterosuperior angle between the axis of the lower central incisor and the mandibular plane.
U1-TVL (mm)	Distance from the incisal edge of the upper central incisor to the true vertical line (TVL) passing through Subnasale and perpendicular to the Frankfort horizontal plane.
U1-PP (mm)	Distance from the incisal edge of the upper central incisor to the palatal plane.
L1-APog (mm)	The horizontal distance from the incisal edge of the lower central incisor to the A-Pogonion line.
L1-MP (mm)	Distance from the incisal edge of the lower central incisor to the mandibular plane.

Statistical analysis was performed using SPSS software (version 28.0.1). The normality of the cephalometric measurements from PT2 and T2 was first assessed using the Shapiro–Wilk test and quantile–quantile (Q–Q) plots. Paired t-tests were used to compare measurements that followed a normal distribution in both groups. For measurements in which either the PT2 or T2 group did not follow a normal distribution, the Wilcoxon signed-rank test was used. The significance level was set at $P < 0.05$.

RESULTS

Landmark prediction error

The prediction errors for the incisor landmarks are presented in Table 3. The MRE for all incisor landmarks was 0.91 ± 0.73 mm. The average SDRs within thresholds of 2.0, 2.5, 3.0, and 4.0 mm were 89.58%, 93.75%, 97.92%, and 100.00%, respectively.

Table 3. Error of the Predicted Incisor Landmarks

Landmarks	MRE (Mean ± SD)	SDR (%)			
		<2.0 mm	<2.5 mm	<3.0 mm	<4.0 mm
U1I	0.53±0.53	91.67	100.00	100.00	100.00
U1A	1.47±0.88	75.00	75.00	91.67	100.00
L1I	0.51±0.37	100.00	100.00	100.00	100.00
L1A	1.13±0.52	91.67	100.00	100.00	100.00
Mean	0.91±0.73	89.58	93.75	97.92	100.00

MRE: mean radial error

SD: standard deviation

SDR: successful detection rate

U1I: incisal edge of the upper central incisor

U1A: apex of the upper central incisor

L1I: incisal edge of the lower central incisor

L1A: apex of the lower central incisor

Prediction results and errors of incisor measurements

The angular measurements of the upper and lower incisors are listed in Table 4. A positive relative error (RE) indicates that the predicted value is smaller than the actual value, whereas a negative RE indicates that the predicted value is larger. The mean RE for all predicted incisor angles was $0.20^{\circ} \pm 3.70^{\circ}$, and the mean absolute error (AE) was $2.94^{\circ} \pm 2.27^{\circ}$.

Table 4. Predicted Errors of Upper and Lower Incisors

Variable	Predicted values (Mean $\pm$ SD)	Actual values (Mean $\pm$ SD)	RE (Mean $\pm$ SD)	AE (Mean $\pm$ SD)
$\angle$ U1-SN ($^{\circ}$)	97.58 $\pm$ 6.84	97.83 $\pm$ 7.63	0.25 $\pm$ 2.84	2.18 $\pm$ 1.83
$\angle$ U1-NA ($^{\circ}$)	16.84 $\pm$ 6.09	15.71 $\pm$ 7.07	-1.13 $\pm$ 2.89	2.38 $\pm$ 2.00
$\angle$ U1-PP ($^{\circ}$)	107.98 $\pm$ 6.67	107.72 $\pm$ 7.55	-0.27 $\pm$ 3.11	2.40 $\pm$ 2.00
$\angle$ L1-APog ($^{\circ}$)	23.68 $\pm$ 7.30	25.08 $\pm$ 5.94	1.39 $\pm$ 4.19	3.78 $\pm$ 2.29
$\angle$ L1-MP ($^{\circ}$)	96.96 $\pm$ 10.49	97.88 $\pm$ 9.54	0.92 $\pm$ 4.58	3.95 $\pm$ 2.49
Mean	-	-	0.20 $\pm$ 3.70	2.94 $\pm$ 2.27

SD: standard deviation

RE: relative error

AE: absolute error

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The predicted linear measurements and corresponding errors for the upper and lower incisors are listed in Table 5. The overall mean RE for all incisors was 0.97 ± 3.41 mm and the mean AE was 2.32 ± 2.69 mm. Further analysis revealed that the mean RE for sagittal linear measurements was 0.01 ± 0.59 mm, with a mean AE of 0.47 ± 0.36 mm, and the mean RE for vertical linear measurements was 1.93 ± 4.45 mm, with a mean AE of 4.17 ± 2.64 mm.

Table 5. Predicted Linear Measurements and Errors of Upper and Lower Incisors

Variable	Predicted values (Mean $\pm$ SD)	Actual values (Mean $\pm$ SD)	RE (Mean $\pm$ SD)	AE (Mean $\pm$ SD)
U1-TVL (mm)	9.85 $\pm$ 3.01	9.65 $\pm$ 3.19	-0.21 $\pm$ 0.42	0.39 $\pm$ 0.25
U1-PP (mm)	27.11 $\pm$ 4.99	29.33 $\pm$ 3.53	2.23 $\pm$ 4.10	4.08 $\pm$ 2.27
L1-APog (mm)	1.78 $\pm$ 1.13	2.01 $\pm$ 1.10	0.23 $\pm$ 0.65	0.54 $\pm$ 0.43
L1-MP (mm)	36.34 $\pm$ 4.53	37.97 $\pm$ 2.61	1.63 $\pm$ 5.02	4.26 $\pm$ 3.12
Mean	-	-	0.97 $\pm$ 3.41	2.32 $\pm$ 2.69

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SD: standard deviation

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RE: relative error

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AE: absolute error

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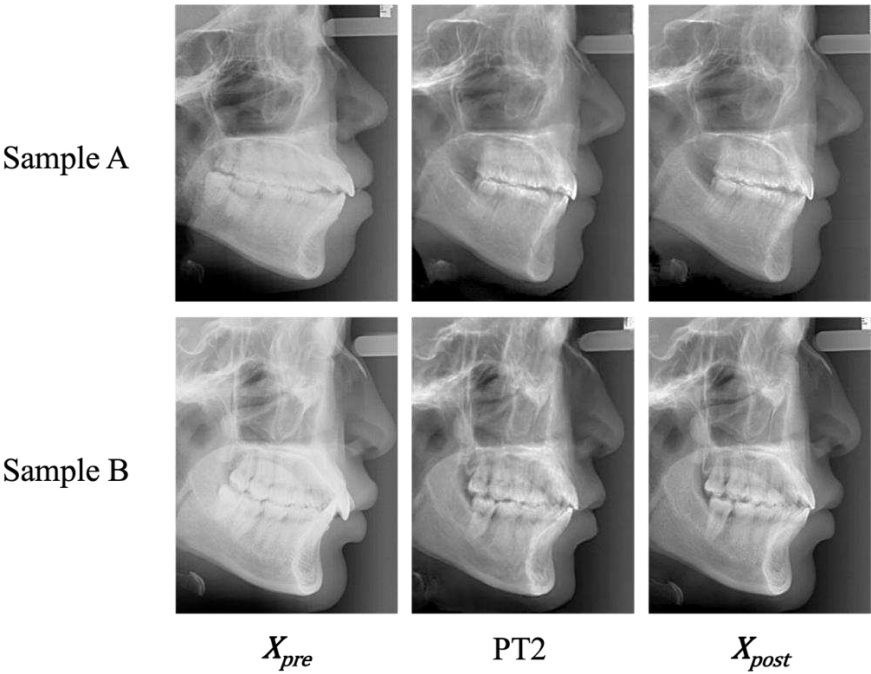
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The results of the Shapiro–Wilk test and Q–Q plots indicated that all measurements were normally distributed ($P > 0.05$). The paired t-test results between the cephalometric measurements of PT2 and T2 are presented in Table 6. No statistically significant differences were observed between the predicted and actual values for any of the measurements ($P > 0.05$). Figure 4 shows exemplary visualizations of the target tooth positions generated by the diffusion model.



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Figure 4. Visualization of the generated target tooth positions.

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Table 6. Results of Paired t-tests Between Predicted and Actual Posttreatment Cephalometric

Measurements			
Variable	t value	Significance of the paired t-test	
		One-tailed P -value	Two-tailed P -value

∠U1-SN (°)	0.29	0.39	0.78
∠U1-NA (°)	-1.30	0.11	0.22
∠U1-PP (°)	-0.28	0.39	0.78
∠L1-APog (°)	1.10	0.15	0.30
∠L1-MP (°)	0.66	0.26	0.52
U1-TVL (mm)	-1.66	0.06	0.13
U1-PP (mm)	1.80	0.05	0.09
L1-APog (mm)	1.14	0.14	0.28
L1-MP (mm)	1.07	0.15	0.31

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300 **DISCUSSION**

301 Orthodontic aesthetics significantly emphasizes the harmony of the nasolabial–mental
302 relationship^[29]. The evaluation of the facial profile is a critical component of orthodontic
303 diagnosis and treatment planning^[30]. Although incisor retraction can influence profile
304 convexity, clinical observations have revealed considerable individual variability in soft tissue
305 responses to tooth movement. These soft tissue changes are further modulated by factors such
306 as lip tension, length, morphology, and discrepancy^[4]. Individuals with different soft tissue
307 thicknesses exhibit markedly different responses to tooth movement. Thin soft tissue
308 phenotypes demonstrate better adaptability to dental repositioning, whereas thick soft tissue
309 phenotypes exhibit greater resistance and reduced displacement^[31]. Consequently, significant
310 dental retraction does not always translate into pronounced soft tissue changes in the profile.

To maintain an aesthetically pleasing facial profile, orthodontic practitioners must consider multiple factors, including the nasolabial angle, nasal prominence, convexity of the upper and lower lips, and depth of the mentolabial sulcus^[32]. Among the six commonly used clinical soft tissue analysis methods, most establish an aesthetic reference line based on two of the three key features (nose, lips, and chin) to evaluate their relative positions^[33-35]. Several scholars have identified analysis methods that are more sensitive, consistent, and clinically practical for assessing facial profiles^[36, 37]. According to Hsu ^[36], the B-line demonstrates superior consistency (with a smaller coefficient of variation indicating better reliability) and sensitivity (ability to distinguish between attractive and unattractive profiles) compared with other methods. Although the E-line is considered user-friendly for clinicians, the B-line provides the highest reference values. In contrast, reference lines that do not intersect the anatomical structures of the nose usually show poorer consistency and sensitivity. Hillesund et al. ^[37] reported that both the S-line and E-line exhibit good reproducibility. In clinical practice, reference lines that are closer to the facial contour are generally easier to apply and facilitate diagnosis. Because the E-line is closer to the facial profile than the B-line, it is more widely used in clinical settings for profile evaluation. However, the E-line has some limitations.

This study selected several commonly used cephalometric soft tissue parameters as conditional vectors and were chosen because their changes are associated with incisor movement and reflect alterations in the nasal, labial, and mental regions. The Parameters selected were: (1) Nasolabial angle: Defined as the position of the incisors after orthodontic treatment shows a significant correlation with the nasolabial angle^[32]. Lingual inclination and

retraction of the upper and lower incisors can increase the nasolabial angle value^[38], and under certain conditions, modifying the nasolabial angle may improve the facial profile^[4]. (2) Lower lip sulcus depth: Defined as the natural depression between the lower lip and chin that plays an irreplaceable role in harmonizing the lip-chin relationship^[39]. (3) Upper lip sulcus depth: This parameter reflects the curvature of the upper lip^[40], which crucially influences profile aesthetics^[41]. (4) Distance from the lips to the E-line: The E-line demonstrates good reproducibility^[36], and the distance from the lips to the E-line is widely used in the clinical assessment of lip prominence.

Current research at the intersection of AI and orthodontics primarily focuses on the development of intelligent decision-support systems, particularly algorithms for extraction decision-making^[26]. Neural networks can determine the necessity and specific plan for tooth extraction based on inputs such as lateral cephalometric radiographs, demographic characteristics, and other variables, achieving judgment accuracy rates exceeding 90%^[42, 43]. Scholars have also explored the automated formulation of complex orthodontic treatment plans from multiple perspectives, including the classification of sagittal skeletal patterns^[44], treatment planning for patients with deep overbites^[45], the necessity of orthognathic surgery^[46-48], and automatic segmentation of 3D jaw structures^[26, 49-51]. However, Leavitt et al.^[52] indicated that the prediction accuracy decreases for more complex extraction treatment plans. Shimizu et al.^[53] highlighted the limitations of current technology, noting that AI algorithms still perform significantly worse than experienced orthodontists in complex tasks such as prioritizing orthodontic issues and formulating treatment strategies. This performance gap may

stem from the multifactorial and nonlinear nature of clinical decision-making in treatment planning, suggesting that future research should prioritize the integration of structured orthodontic clinical knowledge graphs.

Although published studies have demonstrated promising outcomes of AI-assisted orthodontic decision-making^[26], most existing methods remain limited to feature selection and classification, nonlinear correlation analysis^[54], or prediction of numerical changes^[55]. Research on facial profile changes has largely focused on estimating soft tissue changes from tooth movement, rather than deducing the required tooth movement from the desired profile outcome. Rongo et al.^[56] attempted to develop a quantitative model linking facial profile changes to tooth movement, which inversely estimated the amount of incisor retraction required based on the desired profile outcomes such as the nasolabial angle and lip prominence. However, this method relies on finite element analysis to simulate biomechanical responses and has not yet been developed into a generalized tool for clinical use.

In interdisciplinary research combining AI and dental medicine, investigators are tasked with optimizing traditional algorithms for dental applications and translating clinicians' expertise into computable AI task frameworks. This study aimed to validate the ability of the Ceph-DDPM model to intuitively predict target incisor positions, thereby establishing, for the first time, an AI model that characterizes coupled hard and soft tissue changes in orthodontics. Our study addresses a gap in visualized orthodontic prediction research by integrating multiple parameters and offers a new reference for the clinical translation of medical AI systems.

The type of malocclusion is a significant factor influencing soft tissue response. For instance, differences have been observed in treatment changes between patients with Angle Class II Division 1 and those with Class I malocclusions^[57, 58]. Because no publicly available datasets of paired pre- and posttreatment lateral cephalograms currently exist, and to ensure a balanced distribution within the dataset, this study selected lateral cephalograms from skeletal Class I patients as the test set to minimize errors from training set bias^[54, 59].

This study has several limitations that may be attributed to the following factors. First, because the model input comprised changes in cephalometric parameters rather than complete lateral profile information, it could not fully or intuitively represent the overall soft tissue contour changes before and after the treatment. This limitation may have led to discrepancies between the generated cephalometric profile and actual posttreatment outcomes. Moreover, the input features were derived primarily from the displacements or angular changes of key soft tissue landmarks rather than from the comprehensive contour information of the nose, lips, and chin. Therefore, the model may have learned the local adjustment patterns of specific landmarks more effectively than the holistic harmonious changes in the entire profile.

It is well recognized that soft tissue profile alterations depend not just on isolated cephalometric metrics. Although these measurements provide discrete numerical features, the actual profile is a continuous curve. The prediction of incisor inclination in this study also requires further refinement. Inaccuracies may arise because different incisor inclinations can produce similar profile contours if the contact points with the lips remain unchanged. Therefore, the use of the inclination of the upper and lower incisors as an outcome variable

introduces additional uncertainty. Although the error in the “U1-TVL (mm)” reported in the results was not statistically significant, its clinical relevance should be interpreted with caution. The same profile convexity may correspond to different combinations of upper and lower incisor positions; thus, U1-TVL (mm) may not be uniquely determined for a given facial convexity.

Finally, the diffusion model proposed in this study was trained on only 270 cases of orthodontic cephalometric changes. Therefore, the predicted incisor target positions represent the most statistically suitable outcomes based on the training dataset, and their clinical applicability must be evaluated in conjunction with the individual patient characteristics.

Diffusion models also inherently carry the risk of generating unrealistic or anatomically implausible images^[60]. Factors such as alveolar bone thickness, root length, and crown length influence the safe range of incisor movement^[61-63]. Nakada^[64] recommended that, in addition to conventional model analysis and cephalometric evaluation, special attention should be paid to the relationship between the roots and cortical bone during orthodontic treatment planning. Because our model was not trained on such anatomical constraints, its predictions may occasionally suggest biologically unfeasible tooth displacements. Furthermore, the prediction of the incisor vertical position in this study was relatively suboptimal, likely because the model was not explicitly trained on prior knowledge, such as overbite relationships, but instead learned statistically probable incisor positions based solely on soft tissue change patterns. In summary, the incisor target positions generated by the Ceph-DDPM model require careful and expert supervision^[65]. Future research should incorporate these potential biomechanical risks

to ensure that the ideal incisor positions proposed by AI are clinically achievable and biologically safe.

Looking ahead, future research could explore synergistic frameworks that integrate point-driven image generation methods, such as Drag-GAN^[66], with the current model. Drag-GAN allows users to interactively adjust facial contours by dragging key points, enabling clinicians to manually modify landmarks in the nose, lips, or chin to simulate a more detailed and physiologically plausible posttreatment soft tissue profile. Incorporating orthodontic expert rules to constrain the dragging range could also help prevent the generation of non-physiological outcomes in the model. This approach may enhance the controllability of AI models, improve prediction accuracy, and provide a more effective tool for optimizing orthodontic and orthognathic treatment planning.

CONCLUSIONS

In this study, we constructed a Ceph-DDPM that could infer target incisor positions. The prediction errors for the sagittal positions of the upper and lower incisors were within clinically acceptable ranges, although inaccuracies remained in other measurements, highlighting the need for further optimizations. The Ceph-DDPM model may serve as a useful reference tool for clinicians to define orthodontic incisor-movement targets.

436 **List of Abbreviations**

437 IPO, incisor position objective; AI, Artificial Intelligence; MRE, Mean Radial Error; SDR,
438 Successful Detection Rate; RE, Relative Error; AE, Absolute Error

439

440 **DECLARATIONS**

441 **Ethics approval and consent to participate**

442 The study was approved by the Research Ethics Committee of Beijing Stomatological Hospital,
443 Capital Medical University (approval No. CMUSH-IRB-KJ-PJ-2024-72), and was registered
444 as a clinical trial at Beijing Stomatological Hospital, Capital Medical University (Registration
445 No. ChiCTR2400093660; registration date: 2024-11-29). All procedures involving human
446 participants were performed in accordance with the ethical standards of the Declaration of
447 Helsinki[BG2.1], as well as relevant national and institutional guidelines. Informed consent
448 was obtained from all participants. To ensure privacy, patient information was fully de-
449 identified, and written informed consent was obtained from all participants.

450

451 **Data availability statement**

452 The datasets generated and/or analysed during the current study are not publicly available due
453 [REASON WHY DATA ARE NOT PUBLIC] but are available from the corresponding author
454 on reasonable request.

455

456 **Competing interests**

The authors declare no conflicts of interest.

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Author contributions

Beiwen Gong: Formal analysis, Data curation, Interpretation of patient clinical data, Writing-original draft. Tianlei Shi: Methodology, Model development, Manuscript writing-original draft. Qiao Chang: Supervision, Writing – Reviewing and Editing; Yajie Wang: Supervision and Methodology; Feifei Zuo: Supervision and Methodology; Xianju Xie: Supervision, Writing – Reviewing and Editing; Yuxing Bai: Supervision, Writing – Reviewing and Editing. All authors have read and approved the final manuscript.

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