Original Article

Comparison of individualized facial growth prediction models based on the partial least squares and artificial intelligence

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ABSTRACT

Objectives: To compare facial growth prediction models based on the partial least squares and artificial intelligence (AI).

Materials and Methods: Serial longitudinal lateral cephalograms from 410 patients who had not undergone orthodontic treatment but had taken serial cephalograms were collected from January 2002 to December 2022. On every image, 46 skeletal and 32 soft-tissue landmarks were identified manually. Growth prediction models were constructed using multivariate partial least squares regression (PLS) and a deep learning method based on the TabNet deep neural network incorporating 161 predictor, and 156 response, variables. The prediction accuracy between the two methods was compared.

Results: On average, AI showed less prediction error by 2.11 mm than PLS. Among the 78 landmarks, AI was more accurate in 63 landmarks, whereas PLS was more accurate in nine landmarks, including cranial base landmarks. The remaining six landmarks showed no statistical difference between the two methods. Overall, soft-tissue landmarks, landmarks in the mandible, and growth in the vertical direction showed greater prediction errors than hard-tissue landmarks, landmarks in the maxilla, and growth changes in the horizontal direction, respectively.

Conclusions: PLS and AI methods seemed to be valuable tools for predicting growth. PLS accurately predicted landmarks with low variability in the cranial base. In general, however, AI outperformed, particularly for those landmarks in the maxilla and mandible. Applying AI for growth prediction might be more advantageous when uncertainty is considerable. (*Angle Orthod*. 2024;94:207–215.)

KEY WORDS: Growth prediction; Serial growth data; Partial least squares; Artificial intelligence

INTRODUCTION

The importance of craniofacial development in orthodontics cannot be overstated. Although growth prediction has been one of the classic subject matters in the orthodontic specialty, until fairly recently, over almost the last 20 years, only a few investigations regarding craniofacial growth prediction have been published.[1] The capability to predict growth patterns of growing patients is crucial since the craniofacial structures, which are likely directly related to clinical orthodontic practice, continue to change during growth. Various attempts have been made to achieve more accurate growth forecasts.[2–16] However, due to the complex nature of growth, which is influenced by diverse factors including genetic and environmental factors[3–5,16] leading to significant individual variation, predicting growth remains a challenging task.

Initial growth prediction methods tried to apply average annual growth to every patient. Those methods included

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Table 1. Subject Characteristics (n = 410)

Variable	N (%)	Mean	SD	Min	Max
Age at initial examination (y)					
All subjects		11.5	3.7	3.4	31.3
Female	236 (57.6%)	11.7	3.7	4.0	31.3
Male	174 (42.4%)	11.3	3.7	3.4	27.5
Age after growth observation (y)		15.3	4.8	5.4	32.6
Growth observation period (y)		3.8	3.3	0.3	17.4
Number of serial cephalograms taken					
Two	320 (78.0%)				
Three	66 (16.1%)				
Four or more times	24 (5.9%)				
Angle classification at the initial examination					
Class I	93 (22.7%)				
Class II	177 (43.2%)				
Class III	140 (34.1%)				

Max indicates maximum; Min, minimum; SD, standard deviation.

mesh diagrams,[10,17] forecast grids,[6,18] craniofacial templates,[11] and Ricketts' visual treatment objective.[12,13,19] Although these methods are relatively simple and easy to understand, they cannot effectively control for individual variation, which might lead to inaccurate prediction results. Subsequently, more statistical approaches were developed to control for individual characteristics such as age and gender. These methods applied discriminant function analysis,[20] multiple linear regression analysis,[15] Bayes' theorem,[14] nonlinear growth models,[7,8] and the multivariate partial least squares regression method (PLS).[1]

The PLS method, a statistical technique used in a recent growth prediction study, has proven more accurate than the conventional ordinary least squares method in predicting postoperative soft tissue response in several studies.[21–25] This method might have begun to be adopted in growth prediction studies since it can effectively handle intercorrelated variables and reflect individual skeletal and soft tissue attributes.

Recently, artificial intelligence (AI) in dentistry has gradually attracted attention. In orthodontics, there have been attempts to apply AI in cephalometric landmark detection, automatic image superimposition, and orthodontic diagnosis.[26–31] In 2021, Arik and Pfister (Stanford, California, USA) published the TabNet deep neural network (DNN) that can be applied to tabular data consisting of input and output matrices.[32] Evaluating and comparing the accuracy of the most recent growth prediction methods, including a new approach that employs the latest AI algorithm, may be of clinical interest to orthodontists.

This study aimed to compare growth prediction models by PLS and AI based on the TabNet DNN algorithm.

MATERIALS AND METHODS

Subjects

The institutional review board for the protection of human subjects of the Seoul National University School of Dentistry reviewed and approved the research protocol (S-D20200037). The subjects of this study were chosen from the digital patient files at the Department of Orthodontics, Seoul National University Dental Hospital, Seoul, Korea, from January 2002 to December 2022. Among 25,810 patients who had not undergone orthodontic treatment but had taken serial cephalograms, 410 growing patients (236 girls and 174 boys) were collated and selected.

Patients who had received space maintenance treatment were accepted as subjects. Patients with cleft lip and palate, craniofacial syndromes, or injuries, were excluded from the present study.

The growth observation period was variable among subjects because the intervals were not predetermined. Some of the reasons for the second visit without undergoing orthodontic treatment were monetary problems and poor personal timing.

Cephalometrics

A total of 935 cephalometric images of 410 subjects, taken before (T1) and after (T2) the growth observation period, were used. On these images, manual identification of 78 anatomic landmarks, consisting of 46 skeletal and 32 soft-tissue landmarks, was performed by a single examiner (SJL) with 32 years of clinical orthodontic practice experience. When the 78 landmarks were manually identified twice on 283 images by the same examiner and another examiner who was a third-year resident, the intra- and inter-examiner reliability measures were 0.97 ± 1.03 mm and 1.50 ± 1.48 mm, respectively.[27]

The Cartesian coordinate system was constructed on each image with its origin located at Sella, where the horizontal reference plane was established by drawing a line 7° downward from the Sella-Nasion plane.

Table 2. Comparison of Growth Prediction Models Based on the Partial Least Squares Regression (PLS) and the TabNet Artificial Intelligence (AI) Algorithm. Values are the Euclidean Distance between Prediction Results and Actual Growth in Millimeter Units. For a Given Landmark, the Model That Showed More Accurate Prediction Results is Indicated by the Symbol √

	PLS Method				TabNet AI Algorithm				More Accurate		
Landmark[a]	Mean	SD	Min	Max	Mean	SD	Min	Max	PLS	AI	*P* value[b]
Nasion	1.0	0.9	0.0	5.7	1.7	1.4	0.0	11.8	√		<.0001
Nasal tip	2.9	2.0	0.1	13.4	2.9	1.6	0.2	14.9			1.0000
Porion	2.1	1.4	0.1	14.7	3.2	1.8	0.1	13.2	√		<.0001
Orbitale	2.4	1.7	0.1	14.9	2.4	1.5	0.1	16.1			1.0000
Anterior nasal spine	3.8	3.3	0.1	29.8	2.4	1.6	0.1	23.2		√	<.0001
Posterior nasal spine	3.3	2.9	0.0	29.4	2.4	1.7	0.1	24.9		√	<.0001
Point A	4.0	3.7	0.2	31.6	2.3	1.8	0.2	25.0		√	<.0001
U1 root tip	4.3	4.0	0.0	35.0	2.4	1.9	0.1	26.5		√	<.0001
U1 incisal edge	5.6	5.1	0.2	47.2	3.0	2.4	0.2	37.4		√	<.0001
L1 incisal edge	5.6	5.1	0.1	48.2	2.7	2.2	0.1	33.0		√	<.0001
L1 root tip	6.3	5.8	0.4	52.5	2.5	2.3	0.1	42.0		√	<.0001
Point B	6.7	6.3	0.3	55.6	2.5	2.4	0.1	43.6		√	<.0001
Protuberance menti	7.0	6.5	0.4	60.7	2.6	2.7	0.1	47.2		√	<.0001
Pogonion	7.5	6.9	0.2	70.4	2.9	3.0	0.1	48.4		√	<.0001
Gnathion	7.7	7.1	0.4	71.2	2.9	3.1	0.0	50.5		√	<.0001
Menton	7.7	7.1	0.1	71.1	2.8	3.2	0.1	56.5		√	<.0001
Gonion, constructed	5.5	4.8	0.2	51.3	3.7	2.9	0.2	42.0		√	<.0001
Gonion, anatomic	5.3	4.6	0.2	50.3	3.5	2.7	0.1	35.9		√	<.0001
Articulare	2.5	2.1	0.1	22.6	2.9	1.8	0.1	23.7	√		.0003
Condylion	2.2	3.6	0.0	87.3	2.9	3.7	0.2	88.2	√		<.0001
Pterygoid	2.0	1.5	0.1	15.7	2.6	1.6	0.1	17.5	√		<.0001
Basion	2.9	2.5	0.1	27.3	3.4	2.2	0.1	26.1	√		.0005
glabella	3.6	2.4	0.1	14.7	4.3	2.9	0.3	20.9	√		<.0001
nasion	2.3	1.4	0.1	8.4	2.7	1.5	0.1	8.4	√		<.0001
supranasal tip	3.9	2.9	0.2	22.4	2.8	1.7	0.1	19.6		√	<.0001
pronasale	4.1	3.2	0.1	26.5	2.5	1.7	0.0	24.2		√	<.0001
columella	4.3	3.5	0.1	29.6	2.5	1.7	0.2	25.7		√	<.0001
subnasale	4.1	3.6	0.2	30.9	2.2	1.8	0.0	26.0		√	<.0001
point A	4.1	3.7	0.1	31.4	2.1	1.6	0.1	27.0		√	<.0001
superior labial sulcus	4.6	4.2	0.0	37.4	2.3	1.9	0.1	28.8		√	<.0001
labiale superius	4.9	4.4	0.1	41.0	2.5	2.0	0.0	30.7		√	<.0001
upper lip	5.1	4.7	0.2	42.9	2.5	2.0	0.0	32.9		√	<.0001
stomion superius	5.4	5.1	0.1	45.6	2.5	2.0	0.1	33.7		√	<.0001
stomion inferius	5.7	5.1	0.2	44.4	2.8	2.2	0.2	31.2		√	<.0001
lower lip	6.2	5.7	0.1	51.3	2.9	2.3	0.1	33.8		√	<.0001
labiale inferius	6.5	6.0	0.2	52.5	3.1	2.6	0.1	35.7		√	<.0001
point B	6.9	6.1	0.2	51.0	3.1	2.6	0.1	43.4		√	<.0001
protuberance menti	7.2	6.3	0.4	54.4	3.0	2.8	0.1	44.1		√	<.0001
pogonion	7.7	6.8	0.2	61.6	3.5	3.2	0.1	49.7		√	<.0001
gnathion	8.2	7.4	0.4	68.8	3.3	3.5	0.1	62.0		√	<.0001
menton	8.2	7.6	0.3	73.5	2.9	3.5	0.1	62.9		√	<.0001

[a] Soft tissue landmarks were indicated by small case letters and hard tissue landmarks by capital letters. Among the 78 landmarks, to succinctly provide the results, the prediction results of only 41 landmarks are listed in this table. The omitted 37 landmarks were complementary to draw and connect smooth curves between anatomically meaningful landmarks or arbitrary landmarks to support the extension of soft-tissue lines.

[b] Results from *t*-tests with Bonferroni correction. Max indicates maximum; Min, minimum; SD, standard deviation.

Variables

The prediction equation included 161 predictor variables (input **X** matrix) and 156 response variables (output **Y** matrix). The predictor variables comprised five variables representing individual characteristics: age, gender, Angle classification, growth observation interval, and 156 variables of the x and y coordinates of 78 anatomic landmarks at T1. The positions of these 78 landmarks, in the x and y axes at T2, were set as the 156 response variables.

Validation

When developing a prediction model, a validation process is essential to evaluate the accuracy of predicting new subjects (also called *test/validation data*) that are not included in the model construction process. For this purpose, the leave-one-out cross-validation technique (LOOCV) was applied after establishing prediction equations including all subjects (also called *training data*). In other words, a prediction model was constructed by excluding one subject at a time and

Table 3. Multiple Linear Regression Analysis of Variables Affecting the Accuracy of Growth Predictions

Variables		β	SE (β)	*P* Value
Prediction method	Partial least squares	*Reference*		
	Artificial intelligence (TabNet DNN)	−2.11	0.028	<.0001
Subject characteristics	Gender			
	Female	*Reference*		
	Male	0.40	0.029	<.0001
	Angle classification			
	Class I	*Reference*		
	Class II	0.35	0.038	<.0001
	Class III	0.17	0.040	<.0001
Landmark characteristics	Direction of growth			
	Horizontal direction (*x* axis)	*Reference*		
	Vertical direction (*y* axis)	0.57	0.028	<.0001
	Type of landmark			
	Hard tissue	*Reference*		
	Soft tissue	0.16	0.028	<.0001
	Position of landmark			
	Maxilla	*Reference*		
	Mandible	0.97	0.029	<.0001

β indicates regression coefficients; DNN, deep neural network; SE, standard error.

using the remaining subjects. After building the model, a prediction was made for the excluded subject, yielding a test error for that individual. This process was repeated N times to collect the test errors, where N was the total number of subjects.[33]

PLS and AI Prediction Models

The PLS prediction model was coded in the open-source program language R and included 30 PLS components, which was also determined through the leave-one-out cross-validation technique.[1]

The original TabNet DNN architecture by Arik and Pfister (2021, Stanford, California, USA)[32] was modified using Python programming (Python Software Foundation, Wilmington, Delaware, USA).

Statistics

The Euclidean distance between real growth and the prediction result of a given landmark was calculated. The *t*-tests with Bonferroni correction were used to compare the prediction accuracy between PLS and AI.

Scatterplots with 95% confidence ellipses were drawn to visualize the pattern of prediction errors.

Multiple linear regression analysis was conducted to examine the effect of subject and landmark characteristics on the accuracy of prediction models. This analysis used the absolute value of the prediction error as a dependent variable.

RESULTS

Table 1 presents the ages and characteristics of the subjects at the time of growth observation. The average observation period was 3.8 years, with a mean starting age of 11.5. Most subjects had radiographs taken twice, while about 22% had radiographs taken more than three times. When the proportion of malocclusion was considered, nearly 80% of the subjects had Class II or III malocclusions.

Among the 78 anatomical landmarks, the AI-based prediction model showed better prediction accuracy in 63 landmarks. The PLS-based prediction model was more accurate in nine landmarks. There was no statistical difference in the remaining six landmarks (Table 2).

On average, the AI prediction error was 2.11 mm smaller than that of PLS. The prediction accuracy was higher for girls with Class II malocclusion than for boys with Class I or III malocclusion. The soft-tissue landmarks demonstrated 0.16 mm greater prediction error than hard-tissue landmarks. Mandibular landmarks in vertical directions resulted in greater prediction errors than maxillary landmarks in horizontal directions (Table 3).

The pattern of growth prediction errors for representative landmarks are shown in Figure 1. Orbitale showed no statistical difference between the two prediction methods. The PLS method showed better prediction accuracy in Porion and Basion. However, in general, AI showed significantly more accurate results than PLS. In addition, AI showed more accurate prediction results in landmarks with more variability during growth (Figure 2).

Comparisons of real growth and the prediction outcomes based on the PLS method and AI for real-case examples are shown in Figure 3. Although the prediction results were distant from real growth changes, AI-based predictions generally appeared to be a little closer to actual growth changes.

DISCUSSION

The results of the present study showed that the growth prediction was imperfect and inaccurate. However,

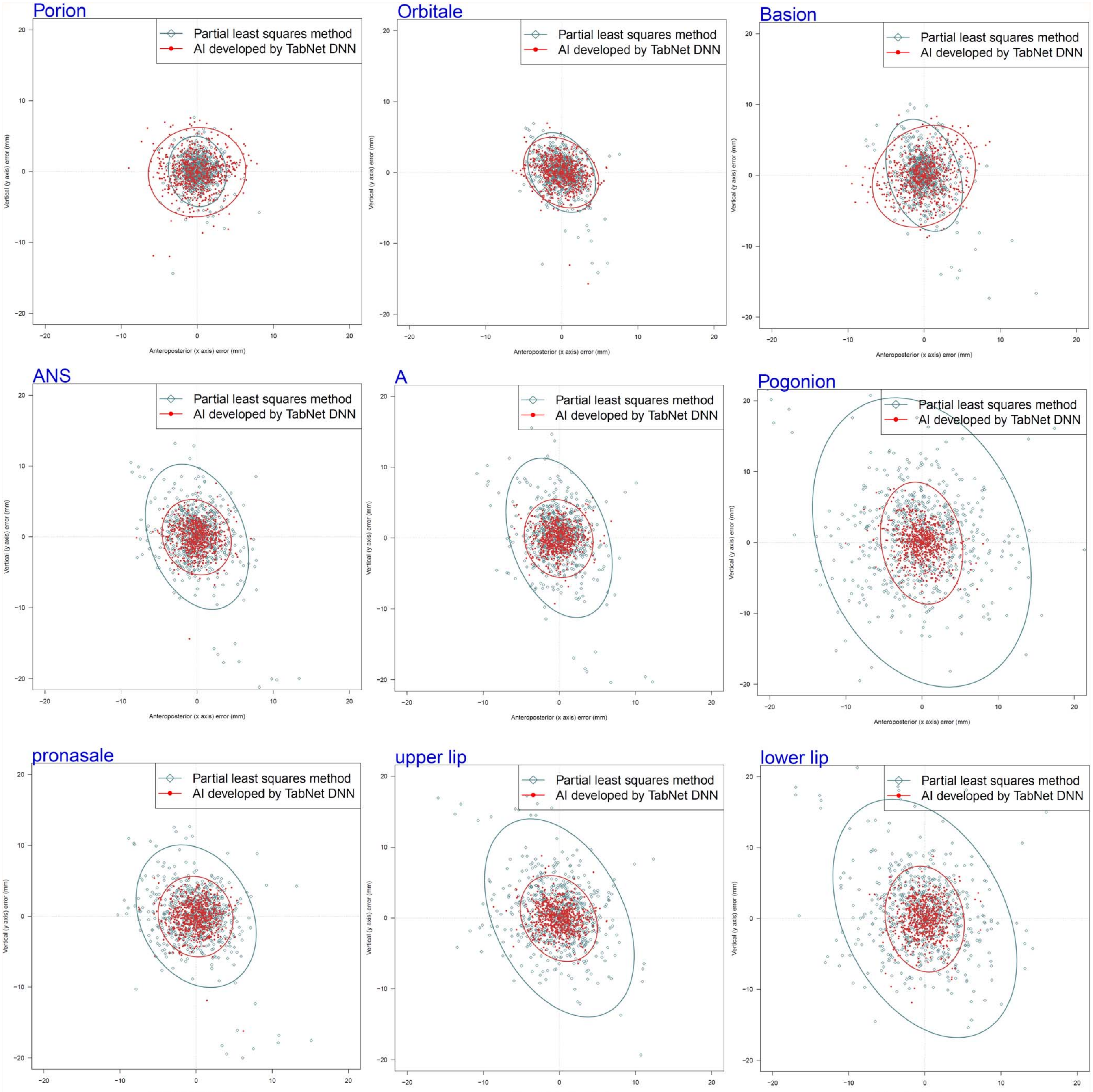

Figure 1. Scatterplots and 95% confidence ellipses illustrate the pattern of growth prediction errors (mm): in the cranial base (*top*); in the maxilla and mandible (*middle*); in soft-tissue landmarks (*bottom*). AI generally showed more accurate prediction results than the PLS method, except for those landmarks in the cranial base.

it might be said that there would be a better method than others in predicting something. Research on growth prediction has not been actively conducted for about two decades. The difficulty and complexity of predicting craniofacial development, which is influenced by multiple factors leading to significant individual variation, might have been a reason for the lack of active research in this area. However, the recent development of high-performance computers that can handle the enormous computational burden required by sophisticated algorithms, has enabled the development of growth prediction methods that can take a vast number of variables into account. This study attempted to overcome challenges in predicting growth by applying TabNet, one of the state-of-the-art DNN algorithms.[32] Although AI has been an area of interest in the field of orthodontics, the

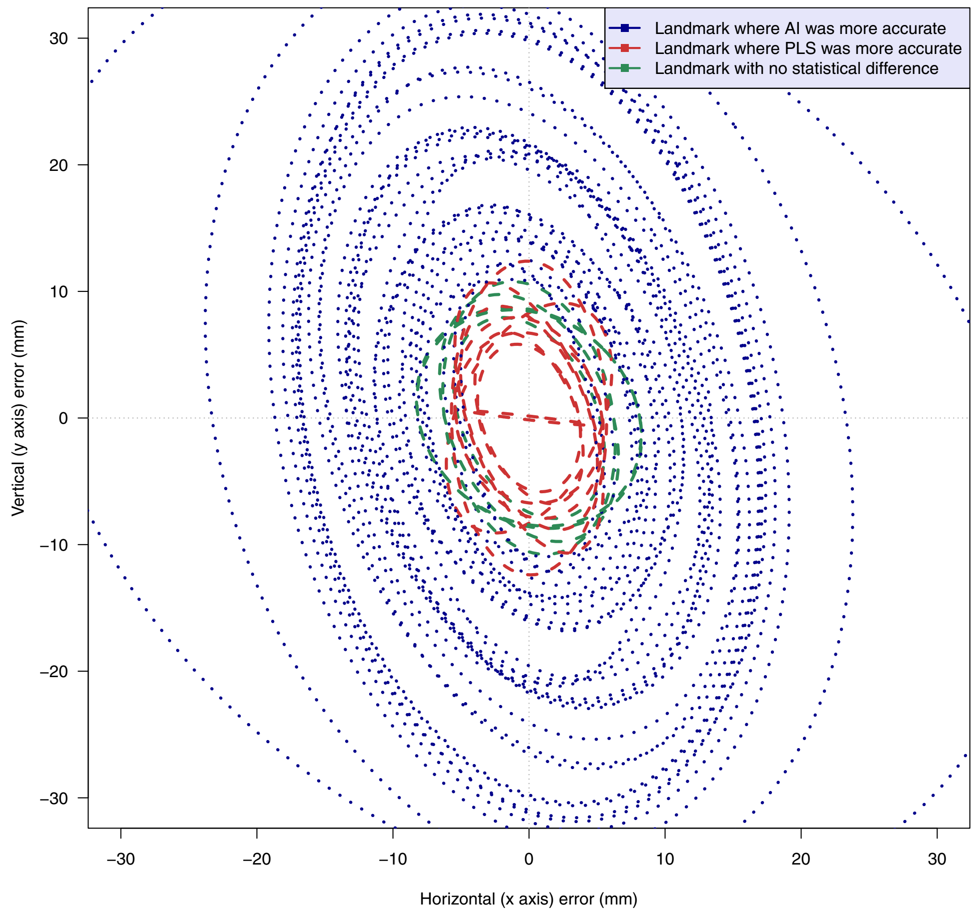

Figure 2. Growth pattern and variability of each landmark according to the model that showed more accurate predictions. Landmarks for which PLS was superior tended to have less variability in growth than landmarks with excellent AI prediction results.

focus has been on improving the precision of automatic landmark identification. There are areas beyond landmark identification in orthodontics that can benefit from using AI. The present study seems to be the first to use AI technology for craniofacial growth prediction.

Overall, AI predicted growth more accurately than PLS. However, the growth prediction accuracy was different according to the landmarks that were predicted. Among the 78 cephalometric landmarks, AI was more accurate in 81%. The PLS-based prediction showed higher accuracy in nine landmarks, mainly cranial base landmarks such as Nasion, Porion, and Basion.

Soft-tissue growth was more difficult to predict than changes in skeletal landmarks. This was likely due to the fact that soft-tissue landmarks can be influenced by unpredictable factors such as abnormal posture and muscle tonicity. Regarding the growth variability of each landmark, the PLS method showed better performance in landmarks with small growth variations. Conversely, landmarks where AI was more accurate generally showed great variability in growth. In other words, AI was powerful when uncertainty was high. This tendency might be helpful in choosing which method to use in building prediction models.

Prediction of growth may not be perfect and accurate. Nonetheless, the prediction method might be better than having nothing to estimate individualized growth changes.[1] One strength of this study was the largest sample size among all previous growth prediction studies. Including many subjects in the study improved statistical power and enabled more accurate predictions. However, one of the limitations of this study was that the study population may not be representative of the general population. Contrary to the prevalence of Class I malocclusion, the majority of subjects included in this study had Class II or Class III malocclusions. This might have been because Class II or III growing patients frequently require growth monitoring before starting comprehensive orthodontic treatment. Another limitation was that the growth observation periods were not prearranged, predetermined, or planned in advance. The subjects were actually patients who sought orthodontic treatment. They were collected retrospectively based on those who had not undergone treatment but had taken

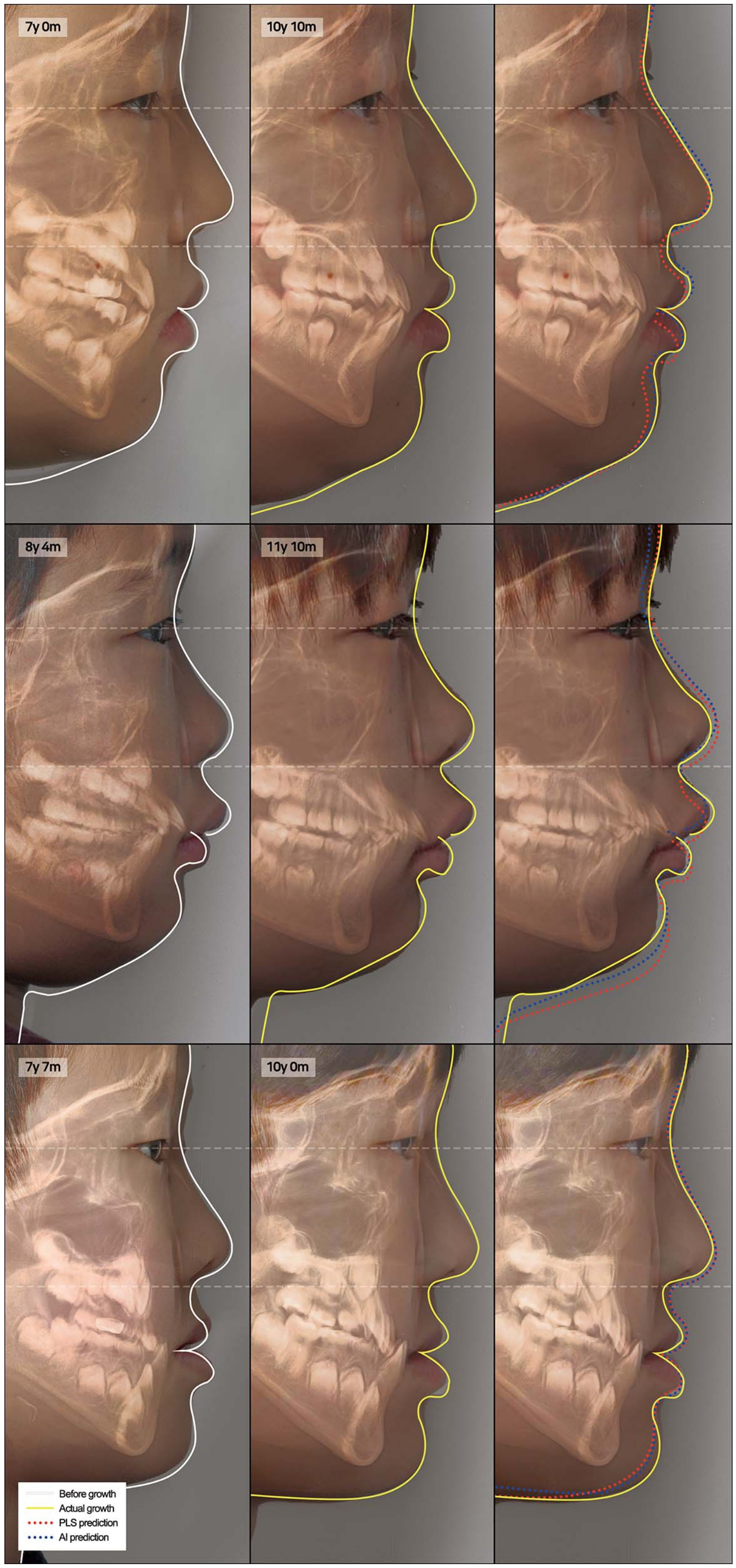

Figure 3. Comparisons between actual growth and prediction results for patients with Class I (*top*), Class II (*middle*), and Class III malocclusion (*bottom*). To concisely showcase the prediction result, only soft tissue outlines are shown.

serial cephalometric images. Therefore, the growth period varied considerably, ranging from 0.3 to 17.4 years. The result of growth observation could have been varied according to the growth observation interval.[7]

With the advent of computer technology, AI research has become familiar to clinicians. To develop an automated growth prediction method, identifying a number of landmarks and applying reliable superimposition methods were significant hurdles. Recently, AI began substituting human labor by automatically identifying 80 landmarks,[26,27,31] and superimposing serial images.[28,29] Irrespective of the growth prediction accuracy, it can be conjectured that a growth prediction study will not be a difficult task in the future. Currently, however, due to ethical issues, collecting longitudinal growth data has been becoming more difficult than it was in the past. For example, the longitudinal growth data for 410 patients in the present study were collected among 25,810 new patients seeking orthodontic treatment from January 2002 to December 2022. Collating and collecting patients who had longitudinal growth data was a challenging task that demanded considerable time and effort. In the meantime, the American Association of Orthodontists Foundation (AAOF) completed the AAOF Craniofacial Growth Legacy Collection project that collected the nine famous longitudinal collections scattered throughout the United States and Canada. Presently available on the AAOF website are about 20,000 digital images from 842 subjects gathered from nine different collections, including the Bolton-Brush, Burlington, Fels Longitudinal, Forsyth Twin, Iowa, Denver, Michigan, Oregon, and Mathews growth studies. By applying the aforementioned AI to the mass growth database that is open to the public and freely available on the AAOF website, it is envisioned that a more accurate growth prediction method can be developed in the near future.

CONCLUSIONS

- Since the PLS method and the TabNet AI algorithm are capable of building models that incorporate numerous variables, these algorithms seem suitable for use in predicting craniofacial growth.
- In general, the TabNet AI algorithm predicted growth more accurately than the PLS method. However, the PLS method was favorable in predicting landmarks with low variability.

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