치의학석사학위논문

A better statistical method of predicting post-surgery soft tissue response in Class II patients

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-ABSTRACT-

A better statistical method of predicting post-surgery soft tissue response in Class II patients

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Introduction: To propose a better statistical method of predicting post-surgery soft tissue response in Class II patients.

Methods: The subjects are comprised of 80 patients who had undergone the surgical correction of severe Class II malocclusions. Using 228 predictor and 64 soft tissue response variables, two multivariate methods of forming prediction equations, the conventional ordinary least squares (OLS) method and the partial least squares (PLS) method, were applied. After fitting the equation, the bias and a mean absolute prediction error were calculated. To evaluate the predictive performance of the prediction equations, a leave-one-out cross-validation method was used.

Results: The multivariate PLS method provided a significantly more accurate prediction than the conventional OLS method.

Conclusions: The multivariate PLS method was more satisfactory than the OLS method in accurately predicting the soft tissue profile change after surgical correction of severe Class II malocclusions.

국문초록

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본 연구의 목적은 II 급 부정교합 환자에서 턱교정 수술 후 연조직을 예측하는 더 나은 통계학적 방법을 제안하고자 하는 것이다. 서울대학교 치과병원 교정과에서 치료받은 환자 중 턱교정 수술을 받은 II 급 부정교합 환자 80 명 (남자 59 명, 여자 21 명)을 대상자로 선정하였다. 228 개의 예측 변수와 64 개의 연조직 반응 변수를 사용하여, 예측식을 구성하는 두 가지 다변량 기법인, 전통적인 최소자승법 (conventional ordinary least squares method, OLS)과 부분최소자승법 (partial least squares method, PLS)을 적용하였다. 식을 적합한 뒤, 편향과 예측 오차의 절대값의 평균을 계산하였다. 예측식의 예측 능력을 평가하기 위해, leave-one-out 교차 검정법을 사용하였다. 다변량 PLS 방법은 전통적 OLS 방법보다 의미 있게 더 정확하게 예측 결과를 도출하였다. 다변량 PLS 방법은 OLS 방법보다 심한 II 급 부정교합 환자에서 턱교정 수술 후 연조직 변화를 정확하게 예측하는데 있어 더 만족스러운 결과를 보여주었다.

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INTRODUCTION

Orthodontic literature is replete with studies regarding the association between surgical skeletal repositioning and the consequential soft tissue response. Accurate prediction of the postoperative facial profile is an essential step in the treatment planning of combined surgical-orthodontic treatment.[1-2] Defining a patient's projected post-surgery soft tissue profile used to be the starting point of planning the surgical-orthodontic treatment. This step also increases a patient's understanding and acceptance of the recommended treatment.[3] However, during surgical-orthodontic treatment in severe Class II malocclusion patients, the soft tissue profile does not directly follow the surgical changes in the underlying bony structures.

At present, several software systems allow clinicians to manually manipulate digital representations of soft tissue projections. However, manual predictions have a limited application due to the relative complexity of the soft and hard tissue relationships. Therefore, it is upon precise mathematical definitions of hard- and soft-tissue relationships that the development of computer-aided forecasting must depend.[4] Computer programs attempting to predict the soft tissue changes after surgery have been greatly improved by graphics and user interfaces.[5] The algorithms for the software programs should be based upon and derived from previous studies. Although the programs have been updated, the prediction results are still far from being accurate. In addition, the underlying algorithms for currently available commercial programs are all unknown. Furthermore, there have been several common problems in previous publications, such as small sample sizes and incorporating a limited number of both predictor and response variables.[2,6-9] Additionally, the prediction methods have been too simple. A frequently used guide for soft tissue simulation is still based simply on the 1-to-1

correspondence ratio for a specific bone to soft tissue change.[6-13] However, the ratio between bone and soft tissue changes varies extremely, lacks consistency across studies, and is inaccurate from patient to patient. For example, in relation to the forward positioning of the mandible, considerable variation in results has been reported for the proportional advancement of the lower lip.[6] After mandibular advancement surgery, even without genioplasty, the ratios for the lower lip to the incisor ranged from 13% to 108%, and from 71% to 127% for soft tissue pogonion to hard tissue Pogonion.[1,14-15]

When predicting soft tissue changes after surgery, by including as many predictors (independent variables) as possible, the multiple regression method has been found to be significantly more accurate than a simple proportional analysis or a simple regression equation.[4,8,16] However, regardless of the number of independent variables incorporated, this typical mode of analysis is unidirectional and univariate, including only a single response (dependent) variable.[2,4,7-9,12-13,17-19] This technique has been referred to as the conventional ordinary least squares (OLS) method. However, the conventional OLS has a significant drawback in predicting soft tissue response since soft tissue response is not simple. For example, a certain degree of vertical skeletal repositioning induces anteroposterior relocation also and vice versa. In addition, the soft tissue response at a specific point is highly dependent on its adjacent soft tissue response, and its neighboring points are also dependent on each other.[20] Therefore, the location of adjacent response points should also be taken into account when applying a prediction method. A multivariate method is an equation which calculates multiple responses and considers the mutual relationship that may exist among the multiple response variables. In this respect, the multivariate approach which involves multiple predictors and multiple response variables simultaneously is more appropriate when predicting a soft tissue response.[20-21]

The partial least squares (PLS) method developed in chemometrics is a comparatively new way of constructing prediction equations. When the number of predictor variables (p) far exceeds the number of observations (n), the conventional OLS method is not suitable for developing meaningful and robust results.[21-25] Predicting soft tissue responses after surgery requires a number of variables to consider, including the patient's age, sex, time after surgery, preoperative skeletal characteristics, pre-existing soft tissue thickness and position, amount of surgical replacement at various skeletal landmarks, direction of surgical replacement, and so forth. As the PLS method becomes more established, its application to various biologic disciplines is becoming increasingly widespread from bioinformatics and image analysis to dentistry.[20,26-28]

The aim of the present study is to propose a better statistical method of predicting post-surgery soft tissue response in Class II patients. The null hypothesis is that there is no difference in the soft tissue prediction accuracy and validity produced between the PLS and the conventional OLS methods.

REVIEW OF LITERATURE

Standardization of the reference system

When using cephalometric analysis, it is important to have appropriately constructed horizontal and vertical reference lines that increase the accuracy of interpretation of cephalometric analysis.[29]

Any x-y Cartesian coordinate system can be constructed. Traditionally in orthodontics, the Frankfort horizontal (FH) plane was used as the horizontal reference plane (HRP) and a line perpendicular to HRP through sella represented the vertical reference plane (VRP) (**Figure 1**, **A**).[15]

There have been a number of variations in establishing a reference system. A line parallel to the FH through sella was used as the HRP and a line perpendicular to HRP through sella represented the vertical reference plane (VRP) (**Figure 1**, **B**).[30] FH plane as the HRP, while a line perpendicular to the FH plane passing Nasion (N) was used as the VRP(**Figure 1**, **C**).[31] Pektas et al[32] used simply Sella-Nasion plane registered at Sella (**Figure 1**, **D**).

However, most researchers set Sella-Nasion plus 6˚ or 7˚ as a HRP. In these cases, a horizontal reference line with 6˚ or 7˚ of angular divergence from the line Sella-Nasion was constructed with the origin at Sella or Nasion. A vertical reference plane was then constructed perpendicular to the horizontal reference plane with its origin at Sella or Nasion. The reference system of which the vertical reference is perpendicular to Sella-Naion +7 ˚ , with the origin at Nasion was used by several studies (Chew et al[12]; Mankad et al 1999[33]; Naoumova et al 2008[9]; Jacobson and Sarver 2002[34]) (**Figure 1**, **E**). The vertical reference perpendicular to Sella-Naion +6 ˚ , with its origin at Sella was also used by several authors (**Figure 1**, **F**) (Burden et al 2007[35], Johnston et al 2006[36], Ksiezycki-Ostoya et al 2009[7], McCollum et al 2009[4,8]).

In this study, an x axis was created at a 7˚angle to Sella-Nasion and the y axis was constructed as a perpendicular to Sella-Nasion at Sella turcica. The researchers who adopted this reference system are as follows. In other words, the coordinate system had its origin at Sella, and its x-axis formed an angle of 7° with the reference line Sella-Nasion (**Figure 1**, **G**) (Jones et al 2007[37], Joss et al 2008[2], Shaughnessy et al 2006[10]).

Any of the above reference system can be used and each reference system would have

had an advantage and disadvantage of its own. If the landmark of interest is located far from the reference line or plane, it is difficult to manually measure the exact coordinate and/or distance from the reference. Today, the distance from the reference does not mean much for clinicians because of the development in the digitizing interfaces. In this study, the coordinate system had its origin at Sella, and its x-axis formed an angle of 7° with the reference line Sella-Nasion.[2,10,37] This reference coordinate system has a several advantages. First, Sella-Nasion is easier to locate and more reproducible than FH plane, which produces more reliable comparison during superimposition. Second, Sella-Nasion is considered to relatively stable beyond 7 years of age.[36] Third, the origin at Sella is better than the origin at Nasion in that a modification of maxillary surgery, high Le Fort I or Le Fort II osteotomy often changes the Orbitale area locating the same FH plane difficult. Fourth, when using the origin at Nasion, the vertical reference line drawings have a possibility to obscure the surgical and/or orthodontic changes in anterior region of face. Selecting a cranial deflection angle between 6° and 7°, there was no preference to choose one of the two. For the subjects in this study, it has been an arbitrary decision to adopt 7° defining the amount of the cranial deflection between Sella-Nasion and FH plane.

According to the reference system negative values imply a backward movement and positive values imply a forward movement of the point in the horizontal plane. Negative values imply an upward movement and positive values imply a downward movement of the point in the vertical plane.

In case of investigating the accuracy of prediction, for horizontal measurements, a negative value indicates that the actual result was posterior to predicted position; a positive value indicates that the actual result was anterior to the predicted position. For vertical measurements, a negative value indicates that the actual result was superior to the predicted position, whereas a positive value indicates that the actual result was

inferior to the prediction.

Superimposition methods

During superimposition, particular attention should be given to fit the consecutive tracings. The references axes should not be simply determined on the second tracings but should be transferred from the first tracing to the second tracing after the tracing were accurately overlaid by superimposing the 2 locating crosses which had been copied onto each tracing directly from the radiograph. This standardized reference system for each set of tracings for each patient was suggested by McCollum et al.[4], which was applied in this study also.

Then, in each set of tracings the reference axes were transferred from the pre-surgical tracings to the post surgical tracings. This can be achieved by finding the closest orientation between the two tracings by closely superimposing the outlines of sella turcica, de Coster's lines, superior orbital rim, orbit and the fronto-nasal area structures.[4] The tracings of the cribriform plate and the anterior wall of the Sella turcica are also important since these are areas that undergo minimal remodelling.[2]

When comparing the two tracings from the same subject, it has been usual to assess the differences as the followings. Difference in x-axis = $x_{after} - x_{before}$; difference in y-axis = $y_{after} - y_{before}$ result, where a negative value indicates the second cephalogram was more posterior in the x-axis or more superior in the y-axis compared to the first cephalogram.

MATERIALS AND METHODS

The subjects consisted of 80 patients (59 women with an average age of 24 years, and 21 men with an average age of 24 years) who had undergone the surgical correction of a severe Class II malocclusion. From January 2001 through July 2012, the subjects were treated at the Department of Orthodontics, and surgery was performed at the Department of Oral and Maxillofacial Surgery, Seoul National University Dental Hospital in Seoul. All subjects are of Korean ethnicity. Subjects had a mandibular surgery and/or a maxillary surgery. An inclusion criterion was a non-syndromic skeletal Class II deformity. No patient included in this study had a cleft lip and palate, an injury, or a severe type of asymmetry. No medically compromised patients were included. All patients were treated with fixed orthodontic appliances before and after surgery. During the preoperative orthodontic treatment, the incisor teeth were appropriately decompensated, and the arches were coordinated and stabilized. Postoperative orthodontic treatment was limited to completing the adjustment of the occlusion, and minimal incisor movement was required. The institutional review board for the protection of human subjects reviewed and approved the research protocol (S-D20120019).

Lateral cephalograms were taken before and after orthognathic surgery for all patients. During imaging, the patient held their teeth in occlusion with lips relaxed. Preoperative lateral cephalograms were taken close to the time of surgical intervention. To ensure resolving of postoperative swelling, follow-up cephalograms were taken at least four months after surgery.[38] All cephalograms were traced by the same examiner (H-J L). With its origin at Sella, the vertical reference was established perpendicular to Sella-Nasion +7 °. The x coordinates were set to represent the horizontal distances from the vertical axis, and the y coordinates were set to represent the vertical distances from the horizontal axis

measured in millimeters. The cephalometric landmarks, soft tissue outline, and their abbreviations used in the study are illustrated in **Figure 2.** Upper-case letters were used to demarcate hard tissue landmarks. Lower-case letters were used to indicate the soft tissue landmarks.

A total of 228 predictor variables (**X** matrix) were entered into the prediction equation. The predictor variables included: patient's age, sex, time after surgery, the direction and amount of facial asymmetry, type of mandibular surgery, type of maxillary surgery, existence of genioplasty, 78 pre-surgical skeletal measurements, 64 pre-surgical soft tissue measurements; and 78 variables with regard to the surgical skeletal repositioning in both anteroposterior and vertical directions. Soft tissue changes in the 32 soft tissue landmarks both in x- and y-axes were comprised of the 64 response variables (**Y** matrix). This study denoted boldface capital letters for matrices, e.g., **X**, size $80(N)_{subjects} \times 228(K)_{variables}$ matrix of predictor variables and **Y**, size $80(N)_{subjects} \times 64(M)_{responses}$ matrix of response variables; superscripts for transposed matrices, e.g., $\mathbf{X}^{T}$; and boldface small characters for vectors, e.g., **x**, $\mathbf{x}_{i}$, and $\mathbf{y}_{m}$.

Two multivariate methods of forming prediction equations, the conventional ordinary least squares (OLS) method and the partial least squares (PLS) method, were calculated using 228 predictor variables and 64 response variables: The OLS method is the traditional and conventional multivariate linear regression method using forward variable selection. The prediction equation using the OLS solution can be written as $\mathbf{Y} = \mathbf{X}\mathbf{B}_{OLS} + \mathbf{E}$, where **E** is an $N \times M$ matrix of residual for **Y**, and $\mathbf{B}_{OLS}$ is a $K \times M$ matrix solution of least squares coefficients; $\mathbf{B}_{OLS} = (\mathbf{X}^{T}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{Y}$ by multivariate Gauss-Markov theorem.[39] The PLS prediction equation may be written as $\mathbf{Y} = \mathbf{X}\mathbf{B}_{PLS} + \mathbf{F}$, where **F** is an $N \times M$ matrix of residual for **Y**, and $\mathbf{B}_{PLS}$ is a $K \times M$ (size, 228×64) matrix of PLS prediction coefficients. In the equation itself, the PLS method resembles the stepwise OLS method, but, in

contrast to the latter, it is applicable even if the variables are strongly intercorrelated (multicollinear) and contain significant noise, even if the number of variables is higher than the number of subjects. All predictors are included in the final solution; no variables have to be discarded, unlike in stepwise OLS.

When developing a prediction method, typically, the model is fit for part of the data (the training dataset), and the quality of the fit is judged by how well it predicts the other part of the data (the test set, also called the validation dataset). To evaluate the predictive performance of the prediction equations, the leave-one-out cross-validation method was used. For a more detailed algorithm for the validation method, please refer to previous literature.[25,40-41]

After fitting the equation, the bias was calculated as a mean difference. The difference between the actual result and predicted position was calculated by subtracting the value for the predicted position from the actual position, Y_{actual} - $Y_{predicted}$. Furthermore, the criterion of goodness-of-fit was defined as the mean absolute error, $|Y_{actual}$ - $Y_{predicted}|$.

Language R (Vienna, Austria),[42] which is a free software environment for statistical computing, was used. Detailed codes of the multivariate OLS, modified PLS, and validation algorithm for use with language R is available upon request to the authors.

RESULTS

Table 1 provides further details of the subjects. Three-fourth of the subjects were females, and this predominance in surgical orthodontic samples was found in previous studies.[35] The average time after surgery was ten months. Seventy-five patients underwent a mandibular advancement surgery. Fifty-nine patients had a Le Fort I surgery, and six patients received an anterior segmental osteotomy in the maxilla. The average amount of surgical repositioning at point B was 6 mm anteriorly. The amount of surgical repositioning at point B was comparable to the amount of overjet before surgery. This may be due to the clinicians' aim to produce occlusions with normal overjet and overbite during surgical-orthodontic treatment.

The derived prediction method was successfully cross validated. After fitting the prediction equations in the training dataset, errors (both bias and mean absolute error) were determined to be trivial to none by both the OLS and PLS methods (data not shown).

The reference plane and landmarks chosen in this study were shown in **Figure 2**. The results of the prediction errors after applying the prediction equations in the test dataset from the two methods are summarized in **Tables 2-1 and 2-2**. After applying the prediction equations in the test dataset, the bias (the error with plus/minus sign) did not show a statistically significant difference between the two methods except at stomion. However, a comparison test based on the means between the predicted and the actual soft tissue profile may not have been appropriate since underestimates and overestimates will cancel each other out, showing no significant difference between the means.[20,43-44] Instead, as previously suggested,[20,43] scattergrams and 95% confidence ellipses for several soft tissue landmarks were constructed to compare the error between

the OLS and PLS methods (**Figure 3**, **A-D**). The ellipsoid satisfies $(\mathbf{z} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{z} - \boldsymbol{\mu}) \leq \chi^2(\alpha)_2$, where $\mathbf{z}$ is the two dimensional (x- and y coordinates) vector for the error, $\boldsymbol{\mu}$ is the mean vector for $\mathbf{z}$, $\boldsymbol{\Sigma}^{-1}$ is the inverse matrix of the covariance matrix, and $\chi^2(\alpha)_2$ is the upper 95th percentile of a chi-square distribution with two degrees-of-freedom.[39] The contour of an ellipse indicates the 95% confidence boundary. A negative value indicated the prediction was more posterior in the x-axis or more superior in the y-axis compared to the actual result. If any points are outside the ellipse, they can be called outliers.[44] The size of the 95% confidence ellipses for the OLS method were significantly larger than the ellipse for the PLS method. This showed superior predictive performance of the PLS method over the OLS method (**Figure 3**, **A-D**).

Absolute prediction errors after applying the prediction equation in the test sample showed significant differences for all the soft tissue landmarks between the two methods. The PLS method showed a significantly more accurate and higher predictive performance than the conventional OLS method in all response variables (**Tables 2-1 and 2-2**).

DISCUSSION

We explored the complex relationship between bone and soft tissue responses by invoking an intricate multivariate statistical analysis, the PLS method. Unexplainable individual variations are inevitably always present. Therefore, it is unrealistic to expect perfect predictions. Furthermore, responses after surgery across individuals are not constant. Perfect accuracy is not available in practicality, but some methods are more accurate than others are. Orthodontics has problems with which conventional statistical inferences cannot properly deal. Statistics is an utmost essential tool in finding clinically significant evidences for proper decision making procedures for both clinicians and researchers. Most familiar statistical tests in orthodontics, such as the t test, analysis of variance, and regression analyses are all based on the conventional OLS method. The OLS models basically require the prerequisite condition of independence between the predictor variables as well as normality and equality of variance among them. Orthodontics includes the dentition, skeletal configuration, and soft tissue responses. The relationships among teeth, dentition, jaw bone, and soft tissue are so correlated that a more sophisticated method which would be capable of considering the correlation among variables simultaneously, rather than the ordinary OLS testing method, is needed. Including the amount of surgical skeletal movement anteroposteriorly, the amount of skeletal movement vertically, the direction of the movement, the patient's age, and the patient's gender, there are a number of factors to consider when predicting the soft tissue response following orthognathic surgery. Since anteroposterior skeletal anatomy is significantly related with vertical repositioning and vice versa, these highly correlated variables should be considered before predicting soft tissue results. In this respect, multivariate methods, like the PLS method, enjoy large popularity in a wide range of fields in natural sciences. Partial least squares (PLS) is the preferred method for constructing a prediction equation when the factors are many and highly collinear or correlated. Applying

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the PLS method is even possible when the sample size is less than the number of variables.[45-46]

When applying the OLS method, if the number of factors gets too large, it is likely to result in a model with a prediction equation that fits the sampled data perfectly, but will fail to predict new data well. In fact, the OLS method demonstrated perfect accuracy when applied to a training dataset from which the prediction equation was formulated. However, when the prediction equation was applied to a real test dataset, the prediction error showed a significantly larger discrepancy than the PLS method. To restate, the OLS method was excellent when developing a prediction equation, but poor when applied to the real subject. This type of phenomenon is termed overfitting.[25] Overfitting also occurred when we predicted the soft tissue response of single-jaw mandibular setback surgery for Class III patients.[20] The same overfitting occurred for the Class II surgery patients in this study. The PLS method demonstrated significantly more accurate predictions than the conventional OLS method when applied to a real dataset through the leave-one-out validation method (**Tables 2-1 and 2-2**). This may be because the OLS method assumes that all the predictor variables are independent, which is not the case, especially for the numerous dental and facial variables in **X** and **Y** matrices. In practice, this condition of independence will never exactly be met.

Excluding or including an additional surgery, such as a genioplasty or maxillary surgery, has a great impact on the soft tissue profile changes. Therefore, in order to develop an accurate prediction method, most previous papers report ratios of only one specific maxillofacial surgical procedure because the more surgical procedures one adds, the more complex the soft tissue prediction becomes. A surgery, such as a maxillary surgery or a genioplasty, in addition to a mandibular surgery, would be considered to be a

confounding variable that would interfere with an accurate soft tissue prediction.[1,47-48] Our study included both mandibular and maxillary surgery patients, and, nonetheless, showed considerable prediction accuracy. This prediction accuracy benefited from incorporating an increased number of skeletal and soft tissue landmarks.

Compared to Class III surgery studies, the soft tissue response to Class II surgeries seems to behave differently from that of the Class III patients. Several other papers also reported this difference. Due to its stretching of the soft tissue, mandibular advancement surgery has a positive "lifting-effect" on the soft tissue profile. In mandibular advancements, the lower lip followed the hard tissue less so than in mandibular setbacks, 50% in advancements and 100% in setbacks.[1-2,48-49] Previous studies have reported that the predictability of the upper lip position after mandibular setback or advancement is poor and highly variable in both directions.[1,48] On the other hand, other papers have reported that the main area of inaccuracy was the lower lip.[5,7,50] In this study, however, both the upper lip and lower lip areas demonstrated accurate prediction results when compared to the conventional OLS method. This study's results seem to be consistent with a previous report that applied the PLS method to mandibular setback patients.[20] The terminal point and R point were the main areas of inaccuracy. This may be partly because the soft tissue in the neck region is highly movable, or this error may come from the changes in the defined points on the cephalometric tracings and superimpositions. The defined preoperative landmark would not always be at the same location on the soft tissue line after surgery. For example, the preoperatively defined soft tissue pogonion would not always be transferred to be the same 'point' after surgery. When locating the most anterior point of the chin, pogonion, it is likely easier to determine the position on the x-axis coordinate than on the y-axis, thus producing the large vertical variation in the distributions for pogonion. By the same token, since soft tissue menton is the most

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inferior point of the chin, there is greater horizontal variation in the x-axis than in the y-axis. This has been a common problem in reporting cephalometric reliability.[43] Therefore, the landmark definition for several soft tissue landmarks might have contributed to the resultant prediction error.[20]

CONCLUSIONS

- We conclude that the multivariate PLS method is significantly more accurate than the conventional OLS analysis in predicting the soft tissue change after Class II orthognathic surgery. We also envision that, in the future, the resultant prediction algorithm can be used to provide an accurate surgical prediction for virtual planning and soft tissue simulation of Class II orthognathic surgeries.

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Table 1. The subjects′ sex, age, and other characteristics

Variables		N	Mean	SD	Min	Max
Age (years)						
	Female	59	24.3	4.7	19.1	40.4
	Male	21	23.6	4.0	19.8	36.7
Time after surgery (months)		80	9.6	4.1	4.2	26.7
Type of maxillary surgery*						
	None	15				
	Le Fort I	59				
	Anterior segmental osteotomy	6				
Type of mandibular setback*						
	None	5				
	BSSRO	62				
	IVSRO	13				
Genioplasty						
	No	11				
	Yes	69				
Asymmetry (mm)						
	Mandible shift to right	44				
	Mandible shift to left	23				
	None	13				
Overjet before surgery (mm)		80	7.5	2.4	3.6	14.5
Overbite before surgery (mm)		80	2.9	3.0	-6.2	8.4
Amount of surgical repositioning at point A (mm)						
	Anteroposterior repositioning	80	-0.3	2.1	-5.8	3.8
	Vertical repositioning	80	-1.7	3.3	-10.9	7.5
Amount of surgical repositioning at point B (mm)						
	Anteroposterior repositioning	80	5.7	3.8	-0.1	16.9
	Vertical repositioning	80	-0.7	4.7	-17.1	8.8

*BSSRO, bilateral sagittal split ramus osteotomy; IVSRO, intraoral vertico-sagittal split ramus osteotomy.

Table 2-1. Comparison of soft tissue prediction errors between conventional ordinary least square (OLS) and partial least squares (PLS) prediction methods (x-axis)

Variable or coordinate	Bias		P-value	Mean absolute error		P-value
	OLS	PLS		OLS	PLS	
Horizontal (x value [mm])						
glabella	0.83	-0.03	0.8853	6.35	1.22	< 0.001*
nasion	-0.33	-0.04	0.0489	5.91	0.91	< 0.001*
inferior tip of nasal bone	0.79	-0.05	0.7156	5.99	1.37	< 0.001*
deepest point of the nose	1.33	0.13	0.2387	6.90	1.33	< 0.001*
supranasal tip	-0.04	0.25	0.3227	6.84	1.76	< 0.001*
pronasale	0.19	0.11	0.4562	5.01	0.84	< 0.001*
columella-lobular junction	-0.72	0.04	0.4711	7.39	1.65	< 0.001*
subnasale	0.41	0.09	0.2971	6.81	1.18	< 0.001*
cheek point	-1.01	-0.03	0.3085	12.13	2.99	< 0.001*
soft tissue A point	0.58	0.08	0.3814	6.52	1.10	< 0.001*
superior labial sulcus	1.50	0.06	0.7013	7.41	1.35	< 0.001*
labrale superius	0.33	0.04	0.6839	7.70	2.10	< 0.001*
upper lip	0.88	0.06	0.8205	7.09	2.37	< 0.001*
stomion	0.51	0.02	0.0454	11.62	3.00	< 0.001*
lower lip	1.22	-0.15	0.7960	8.73	1.47	< 0.001*
labrale inferius	0.95	-0.17	0.4830	9.13	1.44	< 0.001*
soft tissue B point	-0.19	-0.14	0.7772	9.03	2.31	< 0.001*
protuberance menti	-0.32	-0.13	0.8181	8.68	2.40	< 0.001*
pogonion	-1.49	0.01	0.9608	11.70	3.17	< 0.001*
gnathion	-3.40	-0.13	0.4565	20.73	3.88	< 0.001*
menton	-1.06	0.60	0.3105	28.50	7.99	< 0.001*
menton. a	-0.07	0.56	0.2984	19.35	7.86	< 0.001*
R point	-1.27	0.40	0.2991	20.53	10.87	< 0.001*
terminal point	0.99	0.28	0.2289	21.98	11.51	< 0.001*

* $P < 0.001$, result of paired t test.

Table 2-2. Comparison of soft tissue prediction errors between conventional ordinary least square (OLS) and partial least squares (PLS) prediction methods (y-axis)

Variable or coordinate	Bias		P-value	Mean absolute error		P-value
	OLS	PLS		OLS	PLS	
Horizontal (x value [mm])						
glabella	0.39	0.11	0.3556	13.02	4.69	< 0.001*
nasion	3.15	-0.02	0.3707	9.66	3.72	< 0.001*
inferior tip of nasal bone	0.05	0.02	0.2832	9.03	2.92	< 0.001*
deepest point of the nose	2.52	0.23	0.2948	10.99	2.37	< 0.001*
supranasal tip	-0.32	0.34	0.4368	11.22	2.70	< 0.001*
pronasale	-2.57	0.01	0.613	8.11	1.07	< 0.001*
columella-lobular junction	0.15	-0.04	0.3048	5.25	1.69	< 0.001*
subnasale	-1.46	0.03	0.9878	4.55	0.83	< 0.001*
cheek point	-1.44	-0.06	0.8923	11.87	2.57	< 0.001*
soft tissue A point	-3.60	-0.02	0.6729	13.10	3.13	< 0.001*
superior labial sulcus	-0.79	-0.08	0.3222	14.21	3.23	< 0.001*
labrale superius	-0.47	-0.18	0.9306	11.22	2.24	< 0.001*
upper lip	-4.48	-0.03	0.6378	13.67	2.00	< 0.001*
stomion	-1.01	-0.01	0.7738	7.46	1.19	< 0.001*
lower lip	-1.54	0.21	0.3571	11.99	3.26	< 0.001*
labrale inferius	-1.08	0.32	0.5249	11.90	3.24	< 0.001*
soft tissue B point	-2.47	-0.13	0.8327	13.19	4.13	< 0.001*
protuberance menti	-4.18	-0.13	0.5481	13.99	4.51	< 0.001*
pogonion	-2.94	-0.20	0.3041	19.80	6.26	< 0.001*
gnathion	0.03	0.17	0.7143	16.30	3.22	< 0.001*
menton	-2.74	0.07	0.8026	14.37	2.43	< 0.001*
menton. a	-3.31	0.10	0.5687	11.24	3.50	< 0.001*
R point	-4.44	0.21	0.5888	14.54	5.26	< 0.001*
terminal point	-2.90	0.21	0.6486	16.48	4.49	< 0.001*

* $P < 0.001$, result of paired t test.
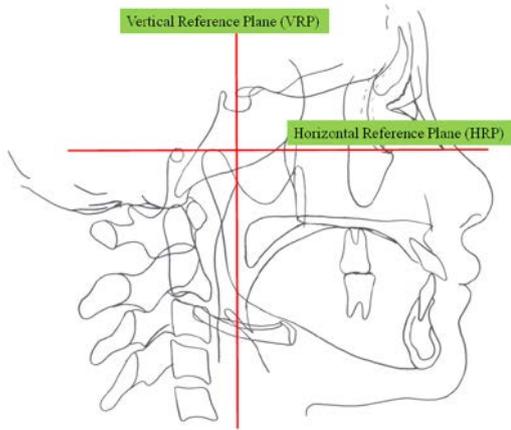
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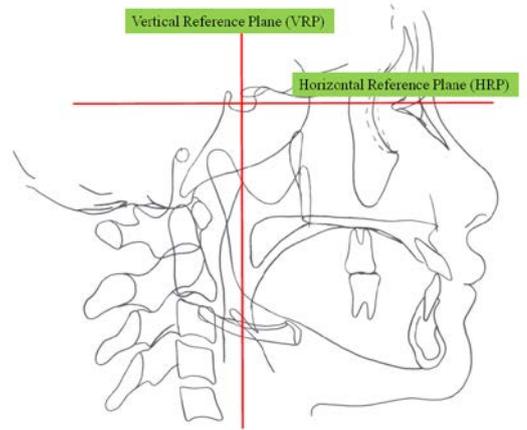
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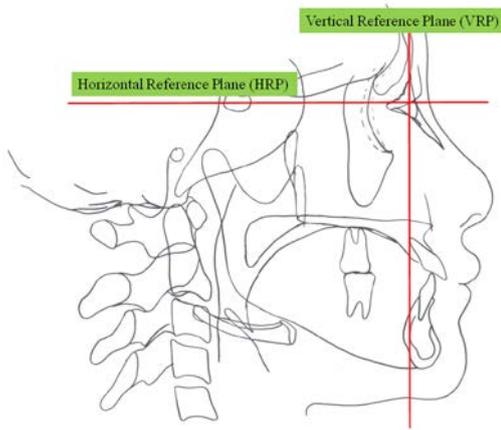
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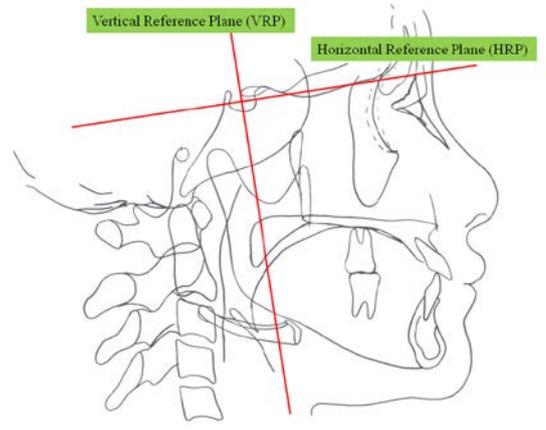
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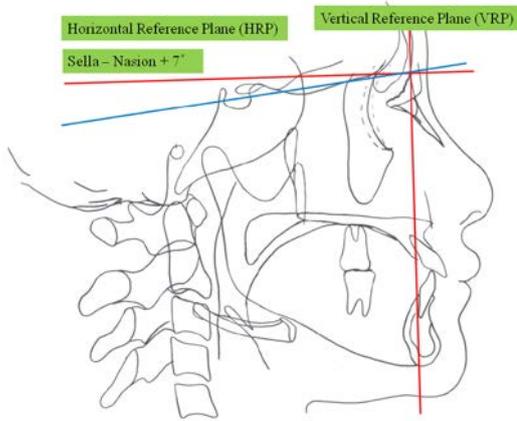
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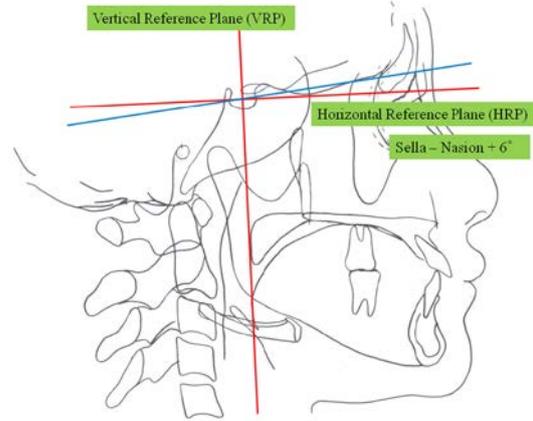
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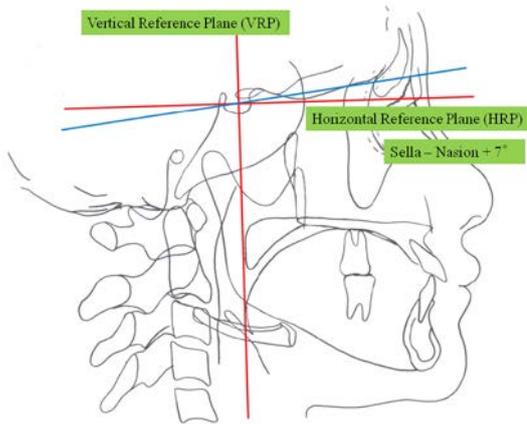
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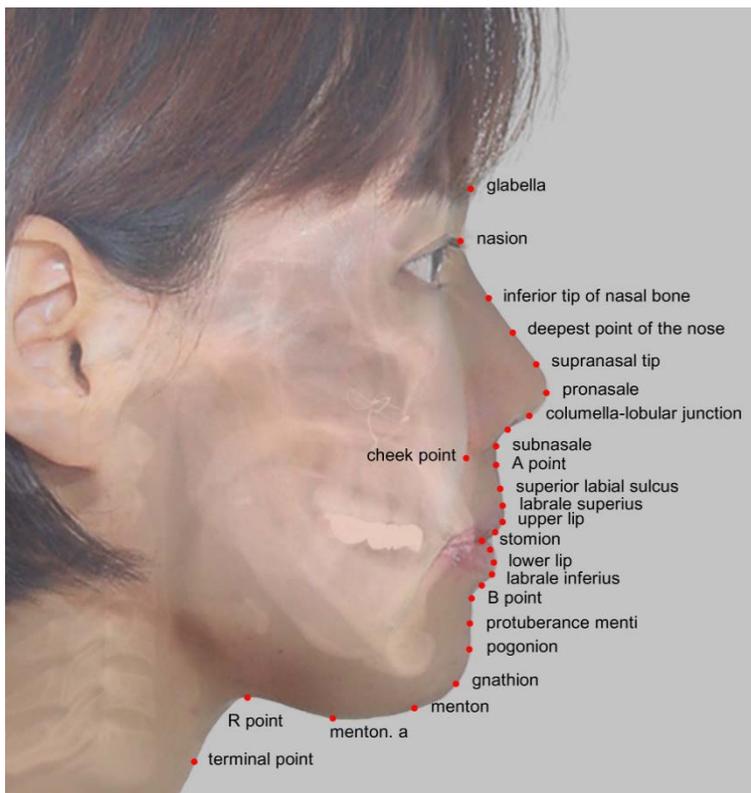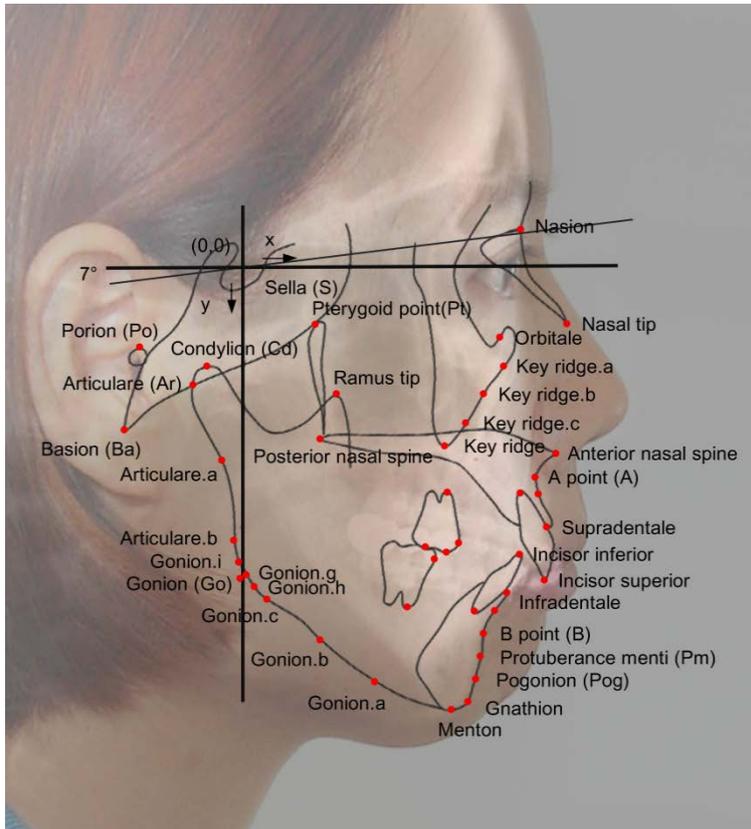
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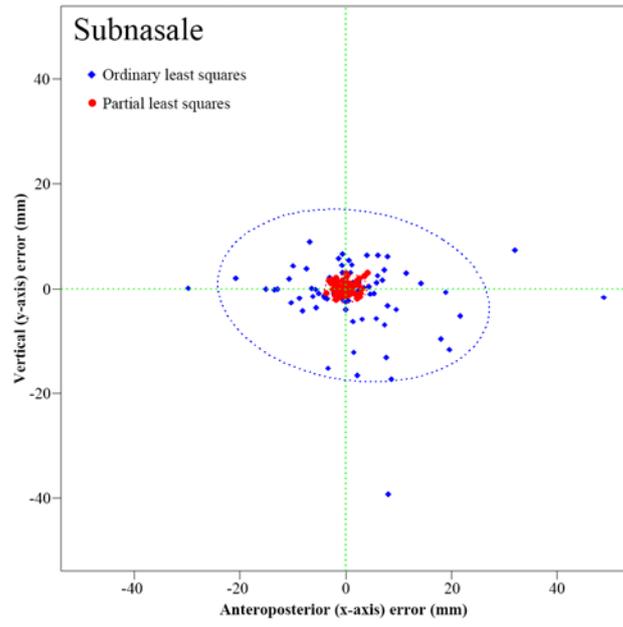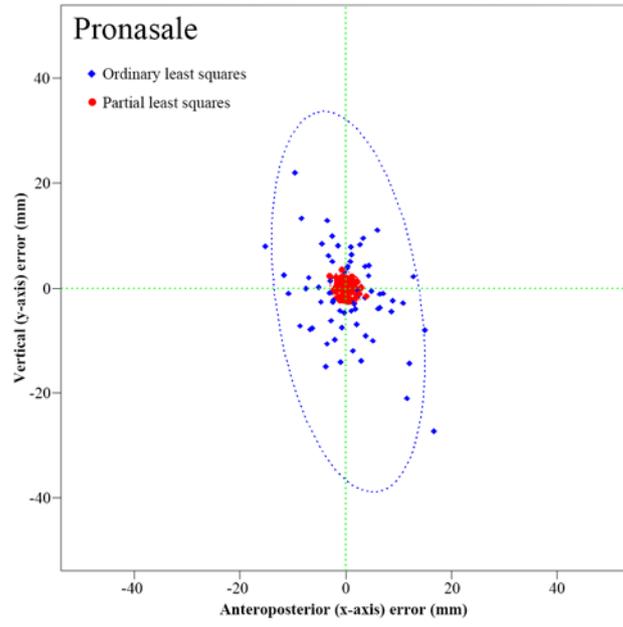
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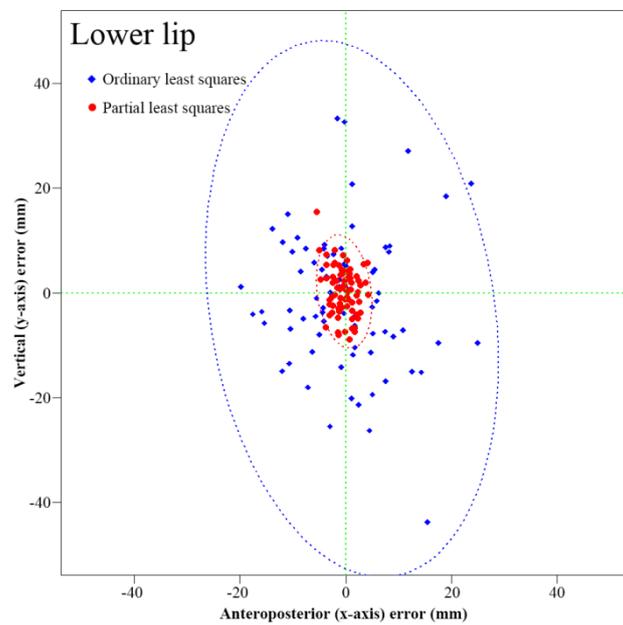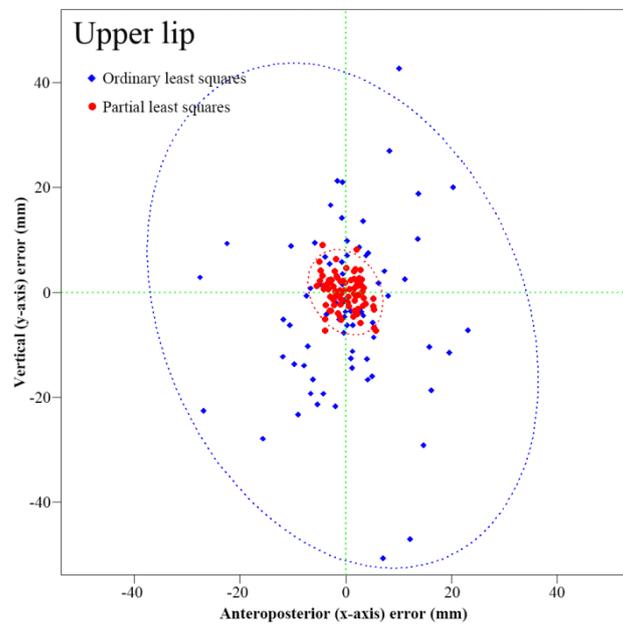
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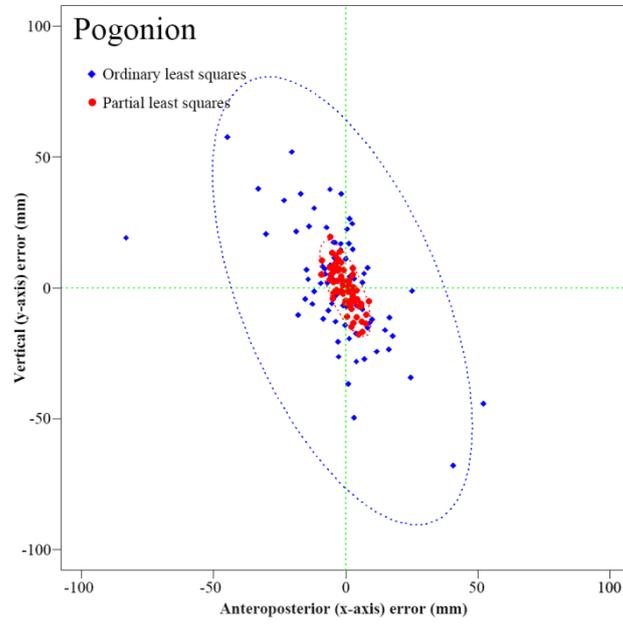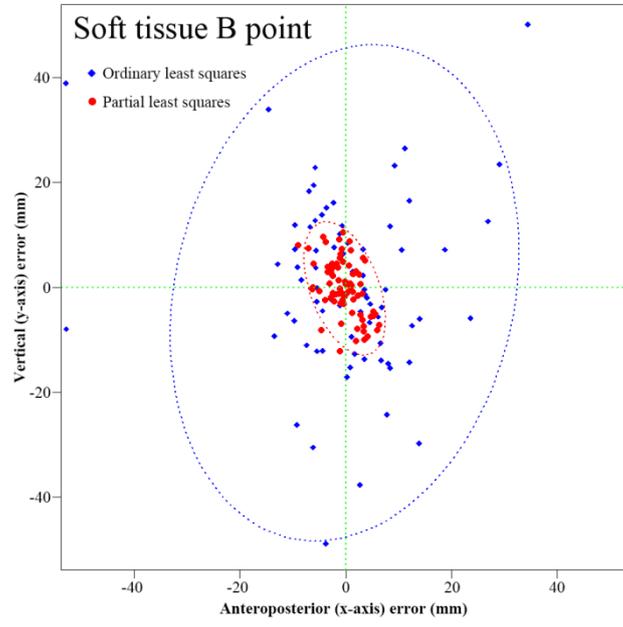
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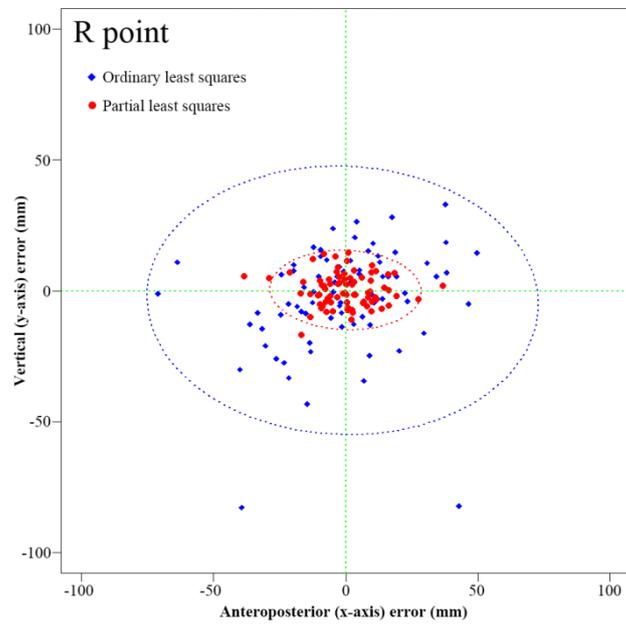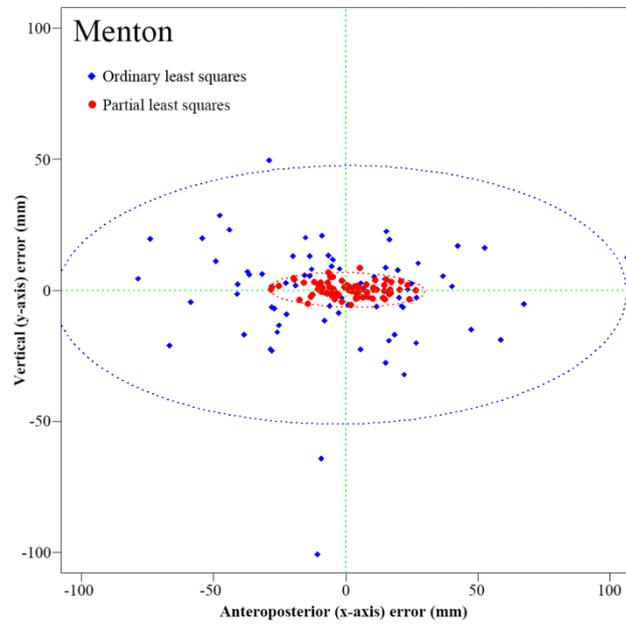
Figure 3, *D*

FIGURE LEGENDS

Figure 1, *A*. The Frankfort horizontal (FH) plane was used as the horizontal reference plane (HRP) and a line perpendicular to HRP through sella represented the vertical reference plane (VRP).

Figure 1, *B*. A line parallel to the FH through sella was used as the HRP and a line perpendicular to HRP through sella represented the VRP.

Figure 1, *C*. FH plane as the HRP, while a line perpendicular to the FH plane passing Nasion (N) was used as the VRP.

Figure 1, *D*. Sella-Nasion plane registered at Sella as HRP and a line perpendicular to HRP through sella represented the VRP.

Figure 1, *E*. Sella-Naion +7˚, with its origin at Nasion.

Figure 1, *F*. Sella-Naion +6˚, with its origin at Sella.

Figure 1, *G*. Sella-Naion +7˚, with its origin at Sella.

Figure 2. Diagram showing the reference planes and cephalometric landmarks used in this study. An image composed of the preoperative radiograph with the hard tissue landmarks. Soft tissue landmarks on the follow up cephalogram (red dots). Concerning the hard tissue landmarks upper-case letters were used. As for the soft tissue landmarks, lower-case letters were used.

Figure 3, ***A-D***. Scattergrams and 95% confidence ellipses for the bias that were obtained from the OLS (blue) and PLS (red) prediction methods. The plots clearly indicate that the bias in both x- and y-axes was greater in OLS than in PLS methods. Application of the equations to individuals may give rise to errors to this extent in 95% probability.

감사의 글

학문적으로 미숙한 제게 석사 과정의 기회를 주시고 학위를 마칠 수 있도록 도와주신 이 신재 교수님, 많은 도움 말씀과 성원하여 주신 김 태우, 백 승학, 안 석준, 임 원희, 양 일형 교수님, 교정학교실 동료 및 선후배 님들께 깊은 감사를 드립니다.

본 연구를 위해 귀중한 연구시간을 할애하여 편의와 도움을 주신 플로리다 대학의 Dr. Richard E. Donatelli 교수님과 논문 심사를 맡아주신 박영석 교수님께 감사드립니다. 많은 시간동안 차트와 자료를 정리하는데 공헌해주신 김 상기 선생님, 윤 경식 선생님, 이 형석 군의 노고에 진심으로 감사드립니다. 연구의 주제에 대한 영감을 주시고, 바쁘신 와중에도 늘 기쁜 마음으로 통계 프로그래밍을 도와주신 박사 이윤식 선생님과, 생소한 통계학의 개념을 배울 때 힘든 고비마다 제게 도움을 주신 박사 서희연 선생님께도 감사드립니다. 늘 한결같이 저의 정신적 안식처가 되어준 친구 류 경국, 박 동원, 서 지형, 신 우열, 윤 성운, 조 영훈에게도 고마움을 전합니다.

평생 물심 양면으로 저의 교육에 헌신 해주신 부모님과 부족한 저의 공부를 위해 홀로 아들 휘성이를 돌보며 묵묵히 후원해준 아내 은경에게 이 논문을 바칩니다.

2013년 12월

저자 씀.