

Decision Support System for Orthognathic diagnosis and treatment planning based on machine learning

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Research Article

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Abstract

Objectives

This study aims to establish a machine learn-based decision support system for the treatment of dental and maxillofacial malformations and verify its feasibility.

Materials and Methods

Between January 2015 to August 2020, 574 patients with spiral CT and have confirmed diagnosis of dento-maxillofacial deformities were used to train the diagnostic model based on five kind of machine learning algorithm. The diagnostic performance of the algorithm was compared with the ground truth and evaluated by accuracy, sensitivity, specificity, and area under the ROC curve (AUC). The adaptive artificial bee colony (aABC) algorithm was used to calculate the orthognathic surgical plan based on cephalometrics in the normal population. The algorithm was used to automatically generate surgical plans for 50 patients and the plans were rated by three experienced maxillofacial surgeons.

Results

The binary relevance extreme gradient boosting model delivered the best overall performance. The final diagnosis success rates on six different kinds of maxillofacial deformities were all over 90%, except for maxillary overdevelopment (89.27%).

Conclusions

The machine learning algorithms show high accuracy and effectiveness in diagnosis and surgical plan design of dento-maxillofacial deformities. The AUC of all diagnostic types was greater than 0.88. The median score for surgical plan was 9. The scheme scores were further improved after human-computer interaction.

Clinical Relevance

The decision support system based on machine learning could be used for automatic diagnosis and surgical design for patients with dento-maxillofacial deformities, which will help improving diagnostic efficiency and provide expertise to areas with lower medical levels.

Introduction

Dento-maxillofacial deformities is a common disease clinically[1]. It could bring appearance and psychology distress to the patient, and may also involve physiological functions such as chew, swallow, and language, significantly reduce the quality of life.[2, 3] Orthodontic- orthognathic surgery is the primary treatment option for this kind of patients. In order to improve the treatment, it is essential to accurately diagnose the deformity and carefully design surgery plan. [4, 5] The process, however, relies heavily on the surgeon's experience and

subjective aesthetic judgments. These surgery decisions may vary between clinicians due to differences in experience with procedures. In particular, clinicians with limited experience have difficulty making such judgments. Inadequate treatment plan may lead to complications or unfavorable results.[6]

As currently there is no standardized criterion for decision-making regarding the need for orthognathic surgery. Some researchers try to build a rule-based expert systems to assist diagnostic decisions.[7, 8] But the application of these systems has a large limitation, and is mainly based on orthodontic treatment decision.

Cephalometric radiographic examination and analysis are important part of dento-maxillofacial deformities diagnosis and Surgical plan design.[9] With these data, researchers achieve dento-maxillofacial deformity classification by means of machine learning.[10, 11] However, these studies use lateral cephalometric data as the basis of their research, which may lead to loss of information.

The purpose of realizing accurate diagnosis of dento-maxillofacial deformity is to guide the design of the surgical plan. However, it is important to note that different orthognathic surgeon can have different plans for a specific case. Clinical surgical plans are also influenced by patients' preferences and the preoperative orthodontic outcomes. Because of the above complex reasons, there has been no report on an auxiliary system that can assist orthognathic surgery design.

In this study we aim to build a decision support system for the treatment of dento-maxillofacial deformities based on machine learning. The decision support system could promptly output dento-maxillofacial deformities of patients according to the inspection results. And output a variety of viable surgical plans based on diagnostic results. The surgical plan proposed by the auxiliary system is interactive and adjustable according to the preferences of surgeons and patients.

Methods

Datum Collection.

This study was conducted in the West China Hospital of Stomatology of Sichuan University and was approved by the Ethics Committee of the West China School of Stomatology, Sichuan University (WCHSIRB-OT-2019-125). The patients included in training diagnose model consisted of 574 cases who visited the Department of Orthognathic and temporomandibular joint surgery, West China Hospital of Stomatology, Sichuan University during the period from January 2015 to August 2020. Exclusion criteria were missing teeth (except third molars), previous orthodontic and orthognathic treatment history, without CT scanning and dento-maxillofacial deformities caused by fracture and tumor. Their medical records before treatment were collected, including demographic information, extraoral photos, intraoral photos and cephalometric measurements. [1, 12]

The demographic characteristics in this study is shown in Table 1. We used 28 commonly features from these clinical records as input features (Supplementary document). The input features were preprocessed to ensure that all of them were quantified before being used for model training. The diagnosis of dento-maxillofacial deformities is determined by orthognathic surgeon (Dr. Luo) with 19 years of clinical experience. All experiments were performed in accordance with relevant guidelines and regulations. The diagnostic types of dento-maxillofacial deformities include maxillary development, mandibular development, maxillary deviation and mandibular deviation.

Table 1
The demographic characteristics in this study

N = 574	Male		Female			
Age mean (SD)	23.4 (7.2)		26.3 (8.5)			
Gender	203 (35.4%)		371 (64.6%)			
Maxillary development	Underdevelopment	201 (35%)	Normal	210 (36.6%)	Overdevelopment	163 (28.4%)
Maxillary deviation	Deviation		208 (36.2%)	Non-deviation		366 (63.8%)
Mandibular development	Underdevelopment	175 (30.5%)	Normal	138 (24%)	Overdevelopment	261 (45.5%)
Mandibular deviation	Deviation		253 (44.1%)	Non-deviation		321 (55.9%)

Diagnose models.

In this paper, we use binary relevance extreme gradient boosting (BR-XGBoost) algorithm to process the information of patients' dental and maxillofacial malformations, so as to realize intelligent diagnosis. Similar to the traditional supervised tree model algorithm based on boosting idea, XGBoost integrates several weak classifiers into a strong classifier through multiple rounds of iteration and residual fitting, which has good generalization performance and operation efficiency. In this paper, we model the diagnosis problem as single label two classification models. is the number of labels, and each label represents whether the patient has this kind of disease. For disease , set up a training set $D_j = \{(X_i, y_i) | 1 \leq i \leq n\}$ ($1 \leq j \leq Q$), where is the sample serial number, is the patient's clinical symptom vector, and the variable $y_i \in \{1, 0\}$ indicates whether sample belongs to label . The XGBoost binary classification model is constructed based on D_j training, so that the prediction result y_j of label can be obtained. Then, multiple binary classifiers are combined into BR-XGBoost to output the multi label diagnose result $Y = [y_1, y_2, \dots, y_Q]$.

Considering the difference of patients' clinical symptoms, it is necessary to further study the generalization performance of the proposed algorithm. In this paper, the feature selection of each $XGBoost_j$ is based on the forward sequence selection method. For label , firstly, the importance ranking of all features is obtained based on XGBoost, then the features with the top ranking are added to the feature subset (initially empty set), and the cross-validation classification accuracy of the feature subset is calculated after each addition. If the classification accuracy is improved, the feature is retained, otherwise it is eliminated, and the optimal feature subset of label can be obtained by traversing all features. The performance of the model is not only affected by the training set, but also depends on the selection of its built-in parameters, that is, super parameters. In order to avoid the complexity and uncertainty of manual parameter adjustment, this paper calls the distributed asynchronous hyper parameter optimization module on the Pycharm platform. Based on the Bayesian optimization theory, the cross-validation method is adopted to optimize each XGBoost on the basis of determining the range of hyper parameters, so as to improve the model accuracy of BR-XGBoost.

To evaluate the performance of the artificial intelligence model, the following normal metrics are used.

1. Accuracy: $Accuracy = \frac{TP+TN}{TP+FP+TN+FN}$
2. Precision: $Precision = \frac{TP}{TP+FP}$
3. Recall: $Recall = \frac{TP}{TP+FN}$
4. Specificity: $Specificity = \frac{TN}{FP+TN}$
5. F1score: $F1score = 2 \cdot \frac{Precision \cdot Recall}{Precision+Recall}$
6. AUC: Accuracy and area under the curve

TP: true positive; TN: true negative; FP: false positive; FN: false negative

Basis of surgical plan design.

The system assists orthognathic surgery design is built based on clinical experiences. We screened 19 indicators as restrictions for designing surgical plan. The normal interval of these restrictions is given according to clinical experience. Surgeons can also adjust the range based on personal experience to produce personalized solutions. The imported data were the three-dimensional coordinates of 25-mark points on the preoperative CT. The involved landmarks were shown in the Supplementary Information. The terminal occlusal relationship was recorded by the three-dimensional spatial relationship of three marks on the maxilla and the mandible. Six sets of data were used to accurately describe the three-dimensional movement of the maxilla, mandible and chin respectively according to the commonly used clinical methods. We randomly selected 50 patients from the aforementioned 574 patients and performed expert ratings on the automatic output surgical plan. The subjects included were all patients who had undergone bimaxillary surgery. The objective of the output surgical protocol was to correct the patient's diagnosed dento-maxillofacial deformities. The effectiveness and feasibility of the surgical plan were evaluated by three experienced maxillofacial surgeons. For unsatisfactory surgical plans, the final score will be given by experts after human-computer interaction.

Treatment plan model.

In this paper, the design of surgical scheme is determined based on artificial intelligence. We use the adaptive artificial bee colony (aABC) algorithm to calculate the maxillary movement, mandibular movement and mentum movement. Artificial bee colony algorithm is an intelligent optimization algorithm that simulates bee colony behavior. It was proposed by Karaboga in 2005. Because ABC algorithm has strong global, parallel and can better combine with other intelligent algorithms, it has attracted the attention of the majority of scientific researchers in recent years.

In this paper, the three-dimensional translation and rotation of each part in the surgical scheme constitute the solution space of the artificial bee colony algorithm. All possible solutions in the solution space are expressed by honey source, and the degree of honey source is measured by the value of fitness function. Bees can be divided into three types according to different division of labor: collecting bees, following bees and reconnaissance bees (collecting bees and following bees each account for half of the total number of bees, and the collecting bees corresponding to inferior honey sources are transformed into reconnaissance bees to search for new honey sources). The specific search for honey source is as follows:

1) Algorithm initialization. In a random way, an initial solution is generated according to the following formula, which is the honey source:

$$x_{m,i} = L_i + rand(0,1)(U_i - L_i)$$

1

where the position of each honey source is represented by $x_{m,i}$. U_i and L_i are the upper and lower bounds of the algorithm space. The number of honey sources is equal to the number of bees, and the number of honey source cyclic search is the number of optimization iterations.

2) The investigation bee found the honey source and measured the amount of honey (fitness value). The calculation formula of fitness value is:

$$fit(x_m) = \frac{1}{J + \varepsilon}$$

2

where, is the evaluation function, which is determined by the doctor preference.

3) Neighborhood search. Search for new honey sources through neighborhood search. If the new honey source fitness value is better than the current honey source fitness value, replace the honey source.

The neighborhood location search formula adopted by the classical artificial bee colony algorithm is:

$$v_{m,i} = x_{m,i} + \varphi_{m,i}(x_{m,i} - x_{k,i})$$

3

It can be seen that the randomness of neighborhood search makes the classical artificial bee colony algorithm have strong exploration ability, but the development ability is poor, and there are some problems such as slow convergence speed and poor search accuracy. To solve this problem, this paper introduces the adaptive coefficient to improve the neighborhood location search equation of the classical artificial bee colony algorithm.

$$\begin{aligned} v_{m,i} &= x_{m,i} + u(t)(x_{j,i} - x_{k,i}) + \alpha\psi_{m,i}(V_{g,i} - x_{m,i}) \\ \alpha &= (1 - u(t)) \\ u(t) &= 1 - rand^{(1-t/\maxcycle)^2} \end{aligned}$$

4

The global optimal solution under the current cycle is represented by ; \maxcycle is the maximum number of cycles; is the adaptive coefficient ; is current number of cycles. With the increase of the number of cycles of the algorithm, the weight between algorithm exploration and development is constantly changing. When the cycle starts, the algorithm has a high weight in exploration, and the global search ability is strengthened, so it is not easy to fall into local optimization; With the continuous increase of the, the value of the adaptive coefficient decreases gradually. At this time, the algorithm tends to develop the region guided by the global optimal solution, which improves the convergence speed and accuracy of the algorithm.

4) For the following bee, the calculated probability value selects the honey source and carries out neighborhood search to generate a new solution, and selects the honey source with better fitness value.

5) If no better honey source is found within the limited number of times, give up the honey source and randomly generate a new honey source.

6) Save the optimal honey source (global optimal solution) found by all bees, and judge the termination condition of the algorithm (maximum number of iterations). If the conditions are met, the optimal surgical scheme is returned and the algorithm is terminated. Otherwise, return to the first step to continue the algorithm.

The overall process of the Decision Support System is shown in Fig. 1.

Results

We compared the performance of five different types of machine learning algorithms in diagnosis of dental-maxillofacial deformities, among which XGboost algorithm showed the highest accuracy and sensitivity in the classification of different diagnosis types. (Fig. 2)

As shown in Fig. 3, the receiver operating characteristic (ROC) curve illustrated the performance of the XGBoost on the diagnosis of dento-maxillofacial deformities. The model yields an area under the curve (AUC) from 0.881 to 0.982. Among them, the diagnosis of deviation showed better diagnosis results. Followed by the mandibular overdevelopment and maxillary underdevelopment. The diagnostic model classified the possible maxillary and mandibular deformities respectively. The combination of diagnostic of the maxillary and mandibular means the final dento-maxillofacial deformities. As is shown in Fig. 4, the proposed algorithm still has good performance in noisy environment.

Performance of treatment plan system

For different patients, the system can output personalized surgical plan. (Fig. 5) The output results contain six three-dimensional parameters representing rotation and movement of maxilla, mandible and chin respectively. The movement of maxilla and mandible take the corresponding incisor point as the movement center. The chin uses pogonion point as the movement center and is reduced to have movement only. The system will output a general surgical plan according to the preset reference range, and doctors can interact with the system to adjust the surgical plan according to their own preferences. The effectiveness and feasibility of intelligently designed surgical procedures were rated on a scale of 1 to 10. The scoring results are shown in Table 2. Iterations of ABC algorithm is shown in Fig. 6.

Table 2
Evaluation of surgical effect and feasibility

Effect of surgery												
score	1	2	3	4	5	6	7	8	9	10	median	Mean ± SD
	(unsatisfactory)					(satisfactory)						
Preliminary plan	0	0	0	0	6	3	9	21	69	42	9	8.8 ± 1.21
Revised plan	0	0	0	0	0	3	3	36	45	63	9	9.08 ± 0.97
Surgical feasibility												
score	1	2	3	4	5	6	7	8	9	10	median	Mean ± SD
	(unsatisfactory)					(satisfactory)						
Preliminary plan	0	0	3	0	9	9	18	33	27	51	9	8.34 ± 1.69
Revised plan	0	0	0	0	0	3	18	30	36	63	9	8.92 ± 1.14

Discussion

In this study, we propose an aABC-based decision support system for orthognathic diagnosis and treatment planning. The system could diagnose dento-maxillofacial deformities based on cephalometric measurements and output an interactive and personalized surgical option by analyzing patients' medical records and preference of both surgeon and patient. The results of clinical application show that the system can effectively assist clinicians in the diagnosis of dental and maxillofacial malformations and surgical design.

In previous studies, scholars have reported many different standards and methods for the diagnosis of maxillofacial deformities according to different races, aesthetics and diagnostic habits. The diagnosis of maxillofacial deformities is a complex process determined by multiple factors. Traditional methods are difficult to summarize such complex problems, and rely heavily on the experience of doctors.

Choi et al.[11] used artificial neural networks to construct a model for orthognathic surgical diagnosis. This model can realize the classification of what type of orthognathic surgery should be accepted, and whether tooth extraction treatment is needed. The overall accuracy rate is over 90%. However, the sample size of the study is relatively small, and half of the patients only need orthodontic treatment, which further reduces the sample size that can be used for the diagnosis and classification of maxillofacial deformities. The model proposed in this study was also unable to diagnose facial asymmetry malformation. In addition, the research only uses artificial intelligent model with neural network. Although the results show high diagnostic accuracy, neural network algorithms usually converge to the local minima, and the convergence of each training is different, which means there is uncertainty in each diagnosis.[13] This is unfavorable for clinical diagnosis and treatment. XGBoost is a new machine learning algorithm. Its algorithm operation process is divided into two parts: learning and reasoning. The goal of the learning machine is to minimize the loss function, that is, when the complexity of the decision tree is as low as possible, the prediction error is required to be as small as possible. In the construction

process of decision tree, firstly, all qualified tree structure schemes are enumerated by greedy method, and the node splitting or pruning termination splitting is carried out by combining gain value and user-defined threshold as the basis of node splitting; Secondly, calculate the scores of nodes in all schemes and the scores of decision tree, and update the decision tree sequence; Finally, the prediction results of each sample, that is, the sum of the scores of each decision tree, are calculated to obtain the probability that the sample belongs to each category. [14–16] XGBoost algorithm shows unique advantages in dealing with diagnostic problems: it is famous for parallel operation and can run large-scale data quickly; It can automatically optimize split nodes and is good at dealing with irregular data with many outliers and missing values; The model is interpretable and flexible. [17, 18] XGoost algorithm has the advantages of difficult over fitting, higher accuracy of loss function solution, support sparse data processing and so on. Compared with the sample data in the industrial field where artificial intelligence is widely used, the maxillofacial diagnosis problem studied in this paper can obtain less sample size, so it is very consistent with the characteristic that XGoost has less demand for sample size. XGBoost can maintain excellent diagnostic performance with a small sample size. In this study, XGBoost achieved the best overall performance, and the overall accuracy rate was over 90%. Considering that some patient data are collected manually, there is a certain deviation noise. This paper considers the performance of diagnosis algorithm in noisy environment. It can be seen that the proposed algorithm can still have good detection performance when the deviation conforms to the normal distribution.

Some recent studies suggest that the cephalometric process cannot fully describe the facial features in patients. The lateral radiographs of patients with different types of dento-maxillofacial deformities were used to train convolutional neural network (CNN). [19–21] The models in those reports can realize preliminary diagnosis of artificial intelligence assisted dento-maxillofacial deformities. However, dento-maxillofacial deformities are always shown and needed to be corrected in three-dimensional directions. In addition, deep learning of three-dimensional data requires a much larger sample size, which is more difficult to implement than three-dimensional cephalometric data based on clinical experience.

The data input the model in this research are three-dimensional cephalometric measurements. The number of these measurements is large. This will lead to great obstacles to the clinical application of the model. At present, many researches trying to use artificial intelligence technology to identify 3D landmarks and perform cephalometric measurement automatically.[22, 23] These researches could make up for the shortcomings and lay the foundation for the follow-up clinical promotion of the model. In addition, cephalometric measurement is only one of the methods to evaluate maxillofacial deformities. Simply using it to evaluate maxillofacial deformities will inevitably reduce the diagnostic accuracy. However, the diagnostic accuracy rate in this study is acceptable. Except for mandibular underdevelopment, AUC of all diagnostic problems was greater than 0.9, showing high accuracy. The AUC of mandibular underdevelopment was 0.881. The overall diagnostic accuracy of dento-maxillofacial deformities is over 90%.

In clinical practice, orthognathic surgical scheme design is very difficult. This procedure requires consideration of the patient's bony deformity, soft tissue condition, occlusal relationship, the patient's chief complaint and the physician's aesthetic preference, so it is difficult to have objective criteria for evaluation. At present, the research in this area is relatively few, and no one has attempted to explore the design of surgical plan by means of artificial intelligence. The essence of dento-maxillofacial deformities is that the relative position of tooth and bone is not coordinated. In this study, some cephalometric indicators commonly used in clinical were used as limitations. It is hoped that the surgical plan will be designed to correct the patient's abnormal cephalometric

indicators to the normal range. The operation plan determines the movement of the upper and lower jaw bones, and also corresponds to the changes of cephalometric indicators. The calculation of this process is complicated, and there may be multiple schemes meeting the requirements at the same time. Therefore, we design an interface for human-computer interaction for the system, and the output scheme can be adjusted or selected according to the preferences of doctors and patients. The results of the scoring showed that the modified procedure achieved higher scores. It is proved that this design can improve the effect of surgical plan design by auxiliary doctors.

Artificial bee colony (ABC) algorithm is a bionics adaptive artificial intelligence technique for solving extremum problem.[24, 25] The ABC has natural advantages in solving function optimization problems, and it is also the most applied field at present, but there are almost no reports on its application in the medical field. This algorithm can be used to solve the multivariable function problem. In order to further improve the efficiency of the algorithm, we choose to use the aABC.[26, 27] The aABC can adaptively change the weight of each influencing factor in the search equation, so that the algorithm has good exploration and development ability at the same time. The aABC algorithm increases the operation speed by about 30%, and the single operation time of one data is about 30s.

In order to simplify the algorithm, patients who completed preoperative orthodontics and planned to undergo surgery were selected as the research objects for surgical plan design.[28] At present, there is no effective method to predict the impact of dentition movement on soft tissue facial shape.[29] There are also many studies trying to obtain soft tissue through artificial intelligence, and the influence of tooth position on soft tissue surface shape with the tensile change of bone movement.[30] In the future, we may take these factors into account and develop orthognathic-orthodontic therapy at the time of initial diagnosis.

The results of the Evaluation of surgical effect and feasibility showed that the outputted surgical plan was generally good. The score of the surgical plan was further improved after revision, indicating that the interactive function could optimize the final result. However, there are still some problems in the surgical plan of individual cases, especially in the feasibility of surgery, which need further verification and expert intervention.

At present, the system reported in this article has some limitations and is an exploratory attempt. In the future we may take these factors into account and develop orthognath-orthodontic therapy at the time of initial diagnosis. But we believe that the application and popularization of this technology is the inevitable trend of the discipline.

In conclusion, we constructed an intelligent system that can be used for the diagnosis of patients with dento-maxillofacial deformities and the design of orthognathic surgery plan through XGBoost and ABC algorithm. The system showed high accuracy and effectiveness in pre-clinical application and may assist clinicians in clinical diagnosis and treatment.

Declarations

Authors Contribution

Wen Du	Data collection, analysis of data and writing of the manuscript
Wenjun Bi	Building and training the model, writing of the manuscript
Yao Liu	Data collection
Zhaokun Zhu	Data collection
Yue Tai	Data collection
En Luo	Analysis of data and writing of the manuscript

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Ethics approval

All the procedure was approved by the Ethics Committee of the West China School of Stomatology, Sichuan University (WCHSIRB-OT-2019-125) and was conducted in accordance with the relevant guidelines and regulations. This study has been registered in the Chinese Clinical Trial Registry (Registration number: ChiCTR1900027586).

Informed consent

For this type of study, formal consent is not required.

Conflict of Interests

The authors declare no competing interests.

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Figures

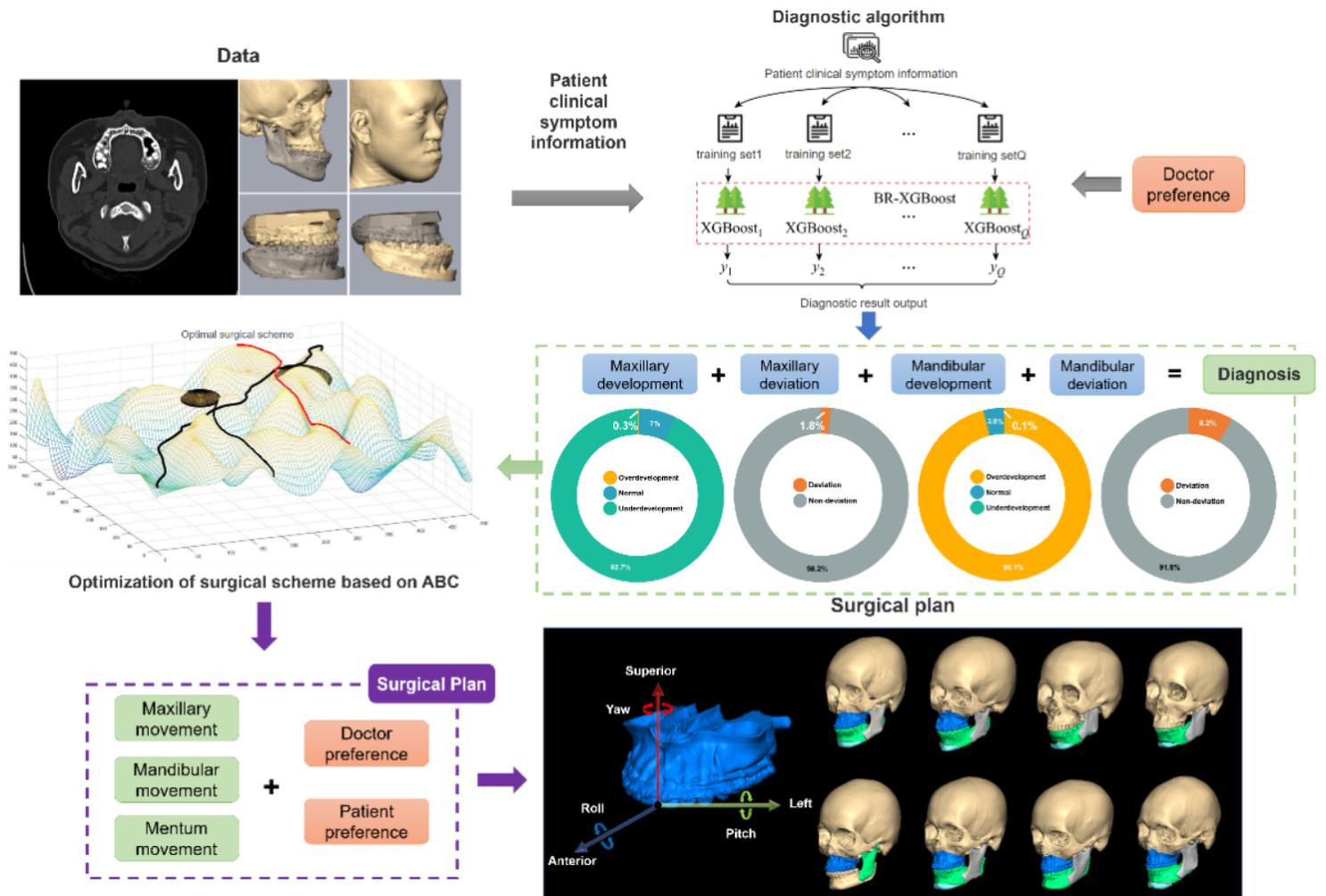


Figure 1

The pipeline of our proposed Decision Support System for Orthognathic diagnosis and treatment planning.

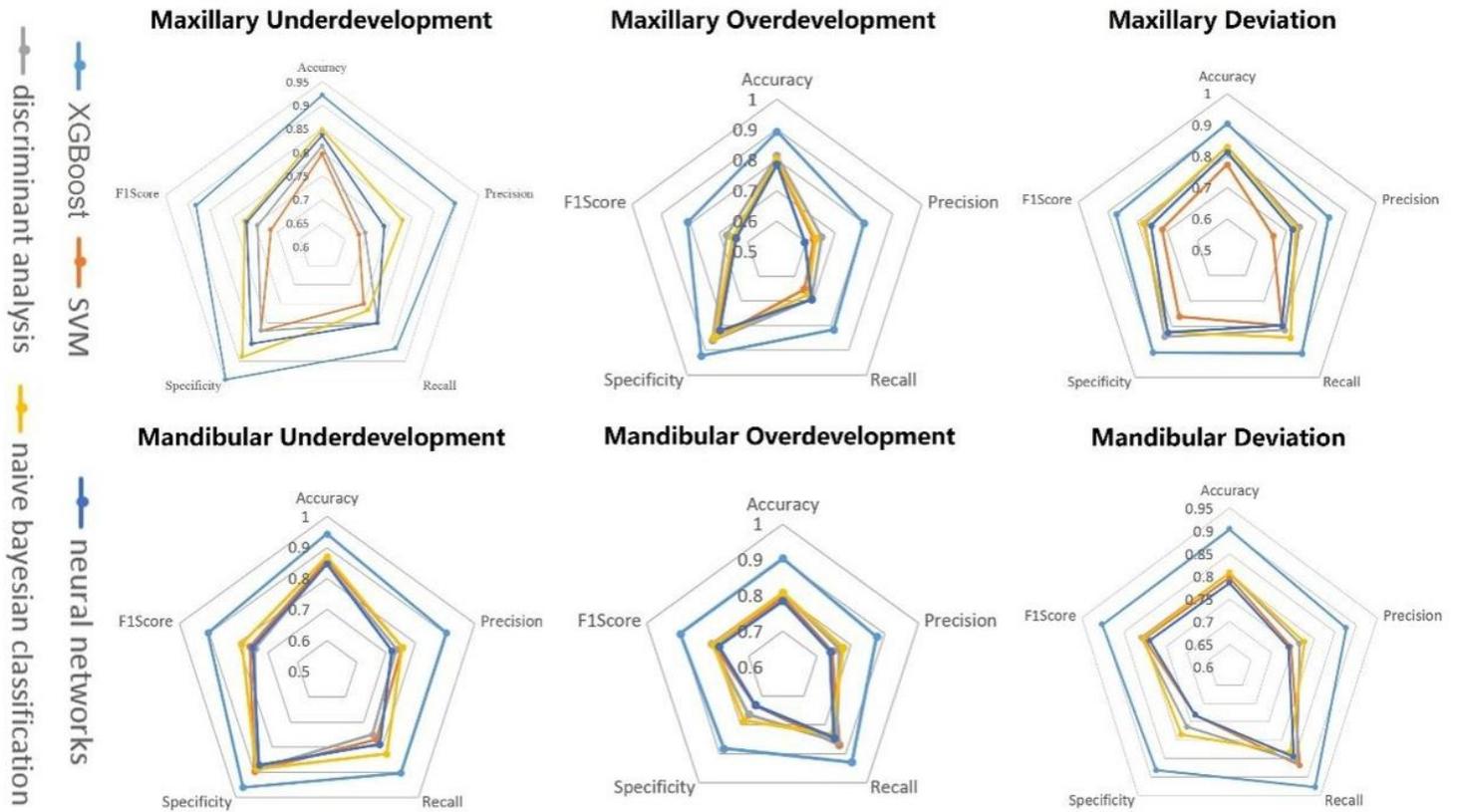


Figure 2

The accuracies of the diagnosis model with XGBoost.

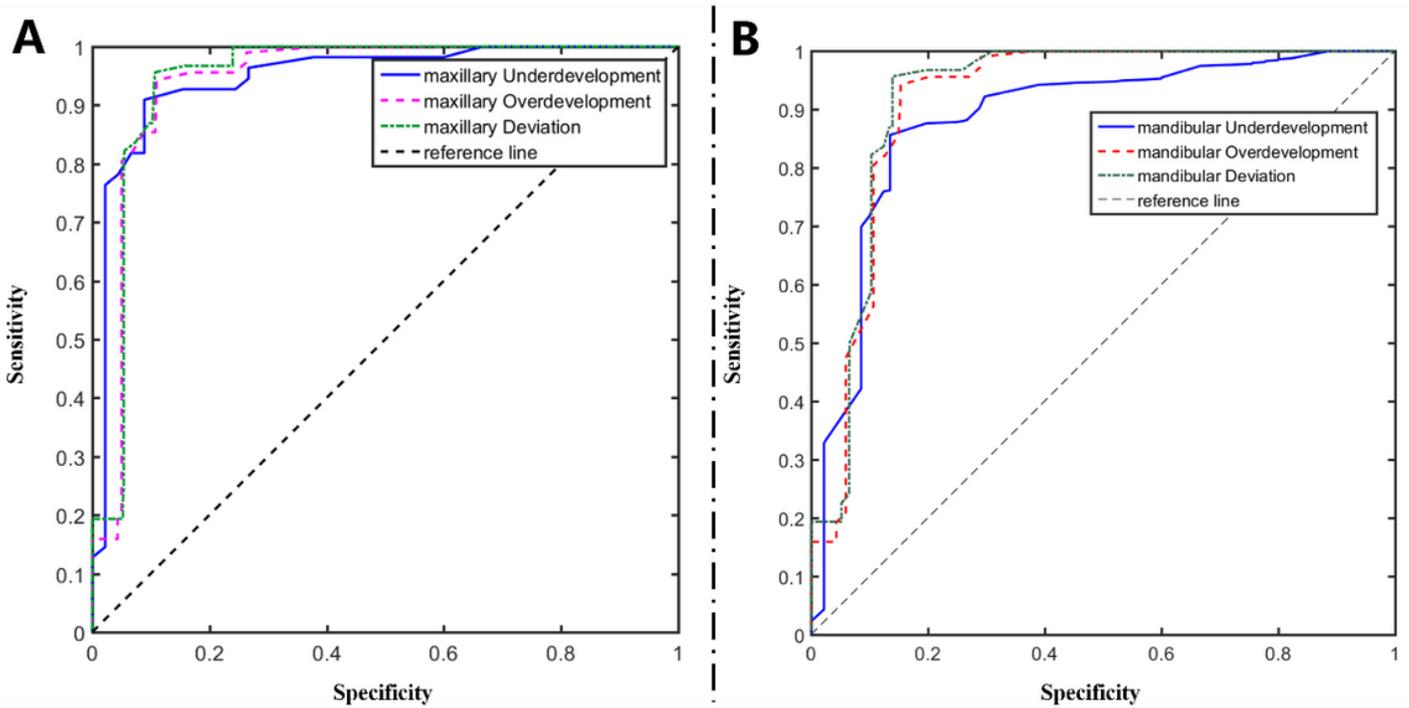


Figure 3

The ROC curve of the XGBoost model to perform diagnosis.

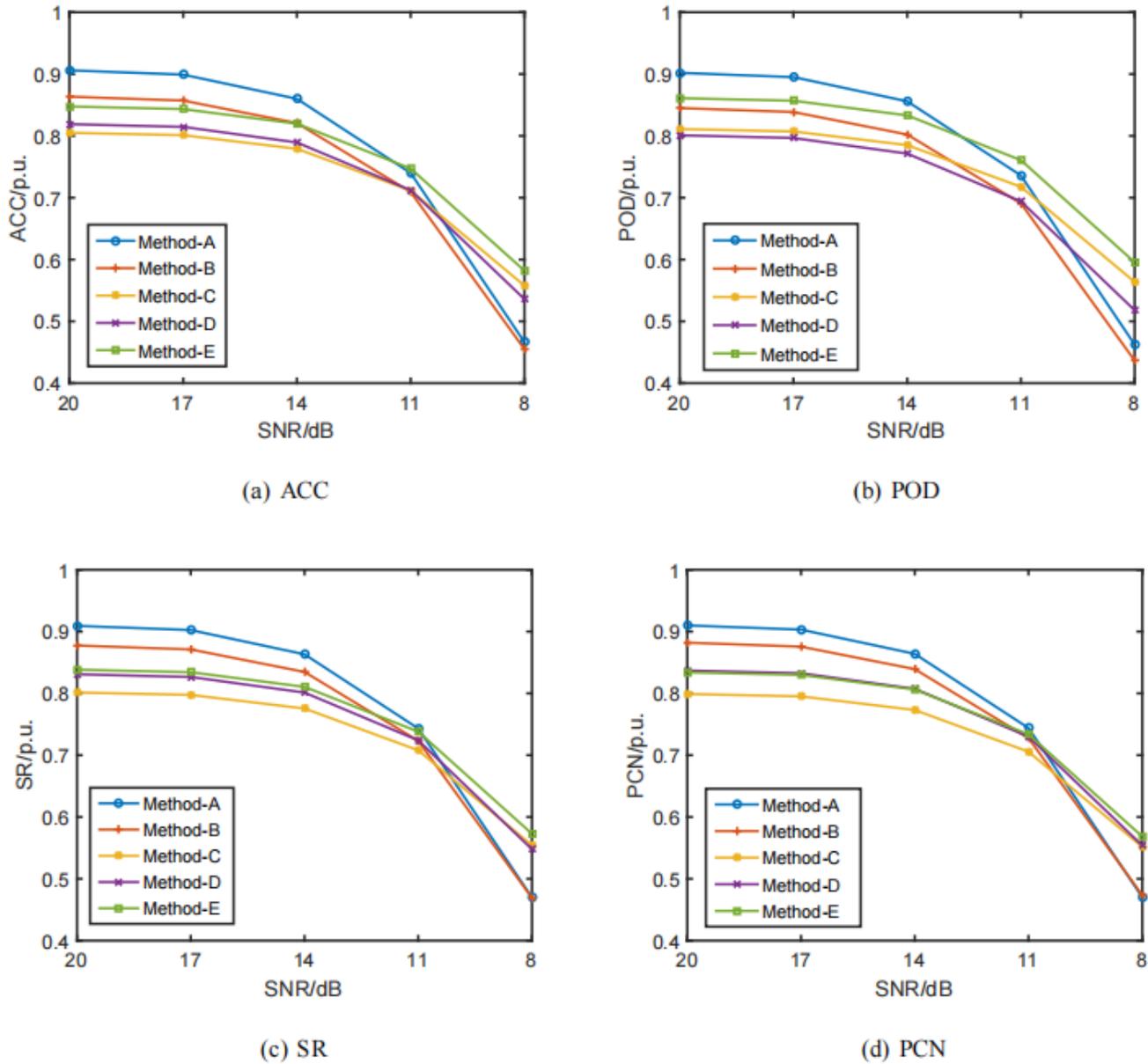
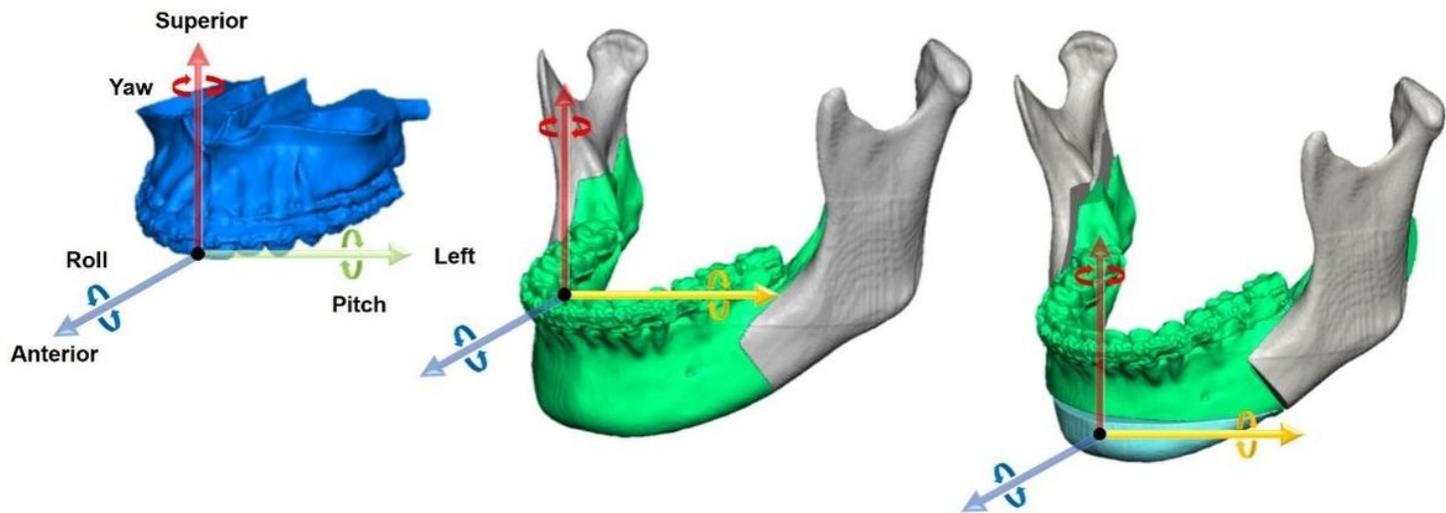


Figure 4

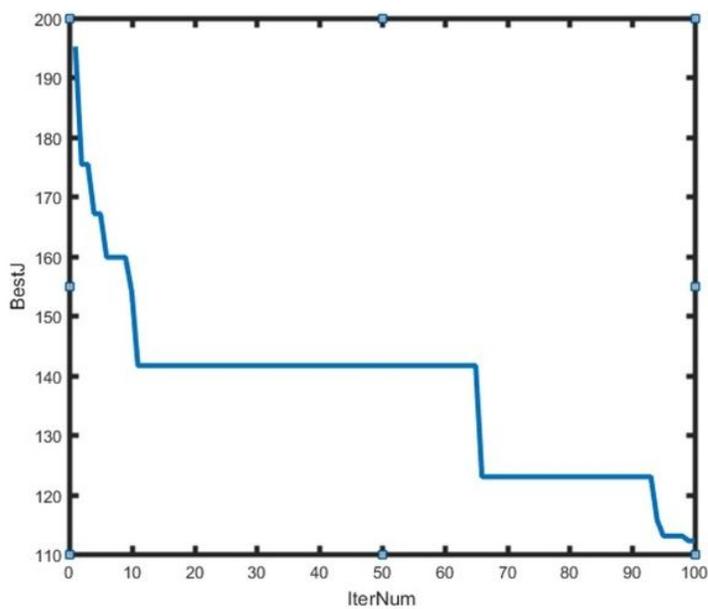
Performance of diagnosis algorithm under different noise levels.



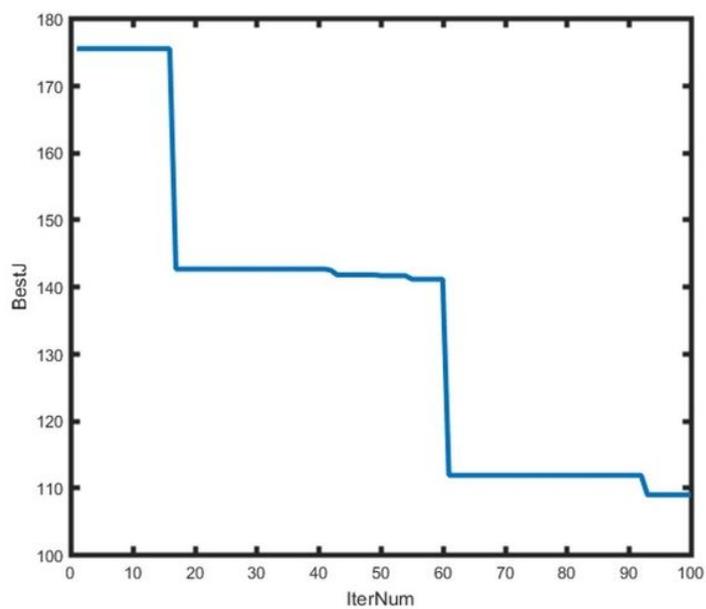
	Anterior- Posterior(mm)	Left-Right (mm)	Superior- Inferior(mm)	Pitch(°)	Yaw(°)	Roll(°)
Maxilla	3.87	1.7	1.61	-1.56	-1.42	0.15
Mandible	-5.06	0.57	-2.57	-2.73	0.19	-0.08
Chin	4.87	1.52	0.12	-	-	-

Figure 5

Personalized surgical plan designed by the system for a skeletal class III malocclusion patient.



(a) Iterations of ABC



(b) Iterations of aABC

Figure 6

Iterations of ABC algorithm.

Supplementary Files

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- [Supplementaryinformation.docx](#)