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Article 1 Utilization of Machine Learning Methods for Predicting Ortho2 dontic Treatment Length 3

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ABSTRACT

Treatment duration is one of the most important factors that patients consider when deciding 20 whether to have orthodontic treatment or not. This study aimed to build and compare Machine 21 Learning (ML) models for prediction of orthodontic treatment length and to identify factors affect-22 ing the duration of orthodontic treatment using the ML approach. Records of 518 patients who suc-23 cessfully finished orthodontic treatment were used in this study. 70% of the patient data was used 24 for training ML models, and 30% of data was used for testing these models. We applied and com-25 pared nine machine-learning algorithms: Simple Linear Regression, Modified Simple Linear Regres-26 sion, Polynomial Linear Regression, K Nearest Neighbor, Simple Decision Tree, Bagging Regressor, 27 Random Forest, Gradient Boosting Regression, and AdaBoost Regression. We then calculated the 28 importance of patient data features for the ML models with the highest performance. The best over-29 all performance was obtained through Bagging Regressor and AdaBoost Regression ML methods. 30 The most important features in predicting treatment length were age, crowding, artificial intelli-31 gence case difficulty score, overjet, and overbite. Without patient information, several ML algo-32 rithms showed comparable performance for predicting treatment length. Bagging and AdaBoost 33 showed the best performance when patient information, including age, malocclusion, and crowd-34 ing, was provided. 35

Keywords: Artificial Intelligence; Machine Learning; Orthodontic Treatment Length

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1. Introduction

Treatment duration is one of the most important factors that patients consider when 39 deciding whether to have orthodontic treatment [1]. An exact and accurate prediction of 40 the duration of the total orthodontic treatment might motivate patients or prepare them 41 for what to expect (Mavreas and Athanasiou, 2008) [2]. Additionally, a reliable idea of the 42 treatment duration helps the orthodontist to better plan the overall treatment and the se-43 quence of appointments (Fink and Smith, 1992; Mavreas and Athanasiou, 2008) [1,2]. Ear-44 lier studies reported that orthodontic treatment employing fixed appliances typically lasts 45 14 to 33 months (Kafle et al., 2019; Tsichlaki et al., 2016) [3,4] with a mean around 22 to 24 46

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Copyright: © 2022 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (https://creativecommons.org/licenses/by/4.0/). months, depending on the discrepancy being treated (Aljehani and Baeshen, 2018; Simister, 2007) [5]. 47

Factors influencing the duration of orthodontic treatment are manifold. They range from general malocclusion, anatomic/biologic factors (like bone morphology, patient age, and disease), the type of treatment (extraction versus non-extraction), to the planned treatment technique (Bhikoo et al., 2018) [6]. A further aspect might be patient cooperation, which is closely related to socio-economic factors and education (Kafle et al., 2019; Mavreas and Athanasiou, 2008; Tsichlaki et al., 2016) [2–4].

As teeth have to be moved through the bone, one decisive factor influencing the speed 55 of orthodontic tooth movement and thus treatment duration is bone metabolism, i.e. the 56 ability of bone to remodel as a result of the applied force systems (Abbing et al., 2020) [7]. 57 Bone metabolism depends, in part, on age, the bony structure itself, and/or systemic dis-58 ease (Abbing et al., 2020; Kaur and El-Bialy, 2020; Landin-Ramos, 2020) [7–9]. One could 59 approach the prediction of treatment duration via bone morphology. Here, the bone struc-60 ture and density, the thickness of the cortical bone, and the structure of the spongious 61 bone would have to be analyzed in detail. An approach using fractal analysis of panoramic 62 x-ray images has recently been presented (Cesur et al., 2020) [10], while more classical 63 approaches use indices of severity, such as The American Board of Orthodontics Discrep-64 ancy Index (ABO-DI), to give an answer to patients' frequent question, "When do I get my 65 braces off?" (Aljehani and Baeshen, 2018) [5]. 66

Artificial intelligence (AI) is bringing a paradigm shift to healthcare, powered by the increasing availability of healthcare data and the rapid progress of analytics techniques [11]. Machine learning (ML) is a subset of AI techniques, used to determine complex models and extract knowledge. In clinical practice, ML predictive models can assist the clinician in decision-making regarding individual patient care [12,13].

To our knowledge, ML has not been used to predict orthodontic treatment length. 72 Therefore, our study aimed to build and compare ML models to predict orthodontic treatment length and to identify factors affecting the duration of orthodontic treatment using 74 a ML approach. 75

2. Materials and Methods

We retrospectively evaluated the records of 631 patients who completed orthodontic77treatment at All Care Orthodontics, Chicago, IL. Ethical approval (IRP Number 20193360)78for this study was obtained from the research ethics committee of WIRB-Copernicus. All79experiments were done in accordance with approved guidelines.80

The inclusion criteria were as follows: Patients who had 1) comprehensive orthodontic 81 treatment; 2) successfully finished their orthodontic treatment without disruption during 82 the treatment period; 3) a complete set of standard orthodontic records pre-treatment and 83 at de-bond appointment; 4) treatment by a board-certified orthodontist. The exclusion cri-84 teria were patients who had: 1) limited orthodontic treatment; 2) phase 1 orthodontic treat-85 ment; 3) treatment disrupted and, consequently, increased treatment length; 4) more than 86 four failed appointments; 5) treatment under Medicaid coverage; and 6) craniofacial syn-87 dromes. A total of 518 patients met the inclusion and exclusion criteria, and their records 88 were used in this study. 89

The following parameters were collected for each patient: 1) Gender, race, and age 90 when treatment started; 2) commute distance to the orthodontic office in miles; 3) overjet, 91 overbite, maxillary and mandibular arch crowding calculated in mm; 4) malocclusion classification (I, II and III); 5) actual treatment length, in months, starting from bonding to 93 debonding appointment; 6) estimated treatment length determined by an orthodontist; 7) 94 treatment difficulty estimated by artificial intelligence (AI Score: 1, Easy to 5, Very Difficulty using a deep learning model, previously published by Talaat et al. 2021[13].

Implementation of Machine Learning Models

A total of nine machine learning algorithms were tested. These included: 1) Simple 98 Linear Regression (Baseline Model); 2) Modified Simple Linear Regression; 3) Polynomial 99

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Linear Regression; 4) K Nearest Neighbor (KNN); 5) Simple Decision Tree; 6) Bagging 100 Regressor; 7) Random Forest; 8) Gradient Boosting Regression; and 9) AdaBoost Regres-101 sion[14]. 102

The cases corresponding to each of the possible outcomes were divided into two 103 groups: 70% of cases were used for ML training and the remaining 30% for ML testing. 104 The same training and testing sets were used with every model to ensure fair comparison. 105 After each model was trained and optimized using 70% of the patient sample, the remain-106 ing 30% of cases served as the testing dataset to evaluate the model's predictive ability. 107 We compared all models using three indicators: mean squared error (MSE) on training 108 data, MSE on testing data, and coefficient of determination (R2) of the model on the entire 109 dataset. Ideally, the testing MSE should be as low as possible. A training MSE that is much 110 lower than testing MSE usually indicates model overfitting on the training dataset. In ad-111 dition, a higher R2 score is desirable, representing the proportion of the variance for the 112 dependent variable (actual treatment time) that's explained by independent variables in a 113 regression model. Furthermore, we analyzed residual values according to the statistical 114best practices and generated feature Importance and Permutation Importance for each 115 model. 116

3. Results

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This study used data from 518 patients, 281 females and 237 males. The mean patient 118 age was 17.49 +/- 8.15 years, and the mean patient treatment time was 26.10 +/- 8.15 months; the mean crowding was 3.18 +/- 3.64 mm for the maxillary arch and 2.79 +/- 3.56 120 mm for the mandibular arch (negative crowding represents spacing); Class I malocclusion was present in 299 cases, Class II in 145, and Class III in 74. The mean treatment difficulty 122 estimated by AI Score = 2.53 +/- 0.81. The mean patient commute distance to the orthodon-123 tic office was = 3.44 + - 4.979 miles (Table 1) (Figures 1 and 2). 124

Table 1. Description of Patient Demographic Data								
ual						1		
tment			Maxillary	Mandibular		F		

N = 518	treatment time (months)	Overjet (mm)	Overbite (mm)	Maxillary crowding (mm)	Mandibular crowding (mm)	AI score	Patient age (years)	office (miles)
Mean	26.101	2.49	2.844	3.178	2.792	2.527	17.49	3.445
STD	8.146	2.699	1.752	3.644	3.56	0.808	8.15	4.979
Min	2.6	-12	-6	-10	-16	2	8.48	1.06
25%	20	1	2	1	1	2	12.59	1.06
50%	25.6	2	3	3	3	2	14.23	1.41
75%	31.575	4	4	5	5	3	19.977	3.77
Max	47.8	14	8	18	15	5	62.12	34.11

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Distance to







Figure 2. Histograms showing (a) actual treatment time distribution and (b) actual treatment time based on malocclu-133sion Class. (c) Boxplot showing malocclusion versus actual treatment time.134



Figure 3. Heat map showing the correlation between variables.

The correlation between variables shown in Figure 3 reveals that the overbite and over-138 jet values were highly correlated (0.43). In addition, both maxillary and mandibular 139 crowding values are highly correlated (0.51). All other pairs did not show significant cor-140 relations. 141

Different ML models behave differently when processing the inputs. Accordingly, the 142 performance of these models also varies. For the ML algorithms evaluated, the following 143 was observed: Bagging and AdaBoost are the best models, with much lower MSE values 144for both training and testing datasets and a higher R2 score to explain the variances (Table 145 2) (Figure 4 and 5).

ML Model	Training MSE	Testing MSE	R2 Score
Simple Linear Regression	59.65	66.76	0.067
Modified Simple Linear Model	58.85	65.21	0.082
Polynomial Linear Regression	48.85	79.25	0.124
KNN (best k = 9)	79.40	81.25	-0.266
Decision Tree (w/AI score)	51.99	71.97	0.124

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Decision Tree (w/o AI score)	55.65	58.20	0.148
Bagging (w/AI score)	40.86	60.95	0.308
Bagging (w/o AI score)	43.08	55.31	0.276
Random Forest (w/AI score)	47.02	58.65	0.237
Random Forest (w/o AI score)	50.29	54.32	0.222
Gradient Boosting (w/AI score)	59.85	54.08	0.122
Gradient Boosting (w/o AI score)	61.76	54.80	0.100
AdaBoost (w/AI score)	38.55	58.10	0.329
AdaBoost (w/o AI score)	42.38	55.08	0.302

MSE, mean squared error; R2, coefficient of determination

The charts shown in the following figures identify the importance of each indicator in 149 the ML models through Feature Importance and Permutation Importance. The R2 scores 150 of between 0.27 and 0.33 are significantly larger than the chance level, making it possible 151 to subtract individual feature importance and permutation importance to probe which 152 features are most predictive. 153

Feature importance, as the name suggests, shows the importance of each feature vari-154 able in the model. For a complex such as Bagging, Random Forest, or AdaBoost, feature 155 importance is the average of all sub-models. Permutation importance measures the de-156 crease in a model score when a single feature value is randomly shuffled. This procedure 157 breaks the relationship between the feature and the target. Therefore, this drop in the 158 model score indicates how much the model depends on the feature. 159

With or without AI scores, the feature importance shows that patient age, maxillary 160 crowding, and mandibular crowding are the three most predictive components in the Bag-161 ging model (Figure 6). Overjet, overbite, and race identification also have quite significant 162 feature importance. 163



165 Figure 4. scatterplots comparing actual treatment time vs predicted treatment time for 166 bagging model.

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Figure 5. scatterplots comparing actual treatment time vs predicted treatment time for AdaBoost model.



Figure 6. Feature importance for the Bagging model.



Figure 7. Permutation importance for the Bagging model

We can see that patient age, maxillary crowding, and mandibular crowding are also 181 the top predictive variables measured by permutation importance in the Bagging model 182 (Figure 7). In addition, figure 5 shows that the AI score played an important role in the 183 model including the AI score as a predictive variable. 184





With results very similar to the Bagging model, the feature importance of the AdaBoost 187 model (with or without AI score; Figure 8) shows that patient age, maxillary crowding, 188 and mandibular crowding are the three most predictive components. Overjet, overbite 189 and race identification also have significant feature importance.

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Figure 9. Permutation importance for AdaBoost model.

The permutation importance results of AdaBoost (Figure 9) show results similar to 195 those of the Bagging models, with patient age, maxillary and mandibular crowding being 196 more significant than other variables. In the AdaBoost model without AI score, overjet stood out as the second most important variable.

Discussion 4.

The ML models built in this study were used to predict the orthodontic treatment 200 length based on multiple factors, including patient demographics, types of malocclusions, 201 and measures of malocclusion severity such as crowding, overjet and AI score for treat-202 ment difficulty. When we evaluated the performance of different ML models, we found 203 that the Bagging and AdaBoost models had better performance than the other ML models 204 tested. Bagging, or Bootstrap Aggregating, is based on the decision tree model. It gener-205 ates multiple samples of training data via bootstrapping, training a deeper decision tree 206 on each sample of training data, then outputs the averaged results of all models, i.e., ag-207 gregating. Compared to regular decision tree models, bagging enjoys the benefits of high 208 expressiveness and low variances. AdaBoost is a complex boosting decision tree regres-209 sion model that uses multiple subsequent trees of residuals to build a combined, e.g., 210 boosting. AdaBoost assigns larger weights to outliers in each iteration of the boosting 211 model building. This makes AdaBoost especially efficient compared to other boosting 212 methods [15]. We tested the performance of the ML models with and without the AI score 213 [13] Adding the AI score improves the ML models' performances, especially evident with 214 the Bagging and AdaBoost models. The AI score is based on malocclusion detection and 215 assessment by AI from clinical images, including crowding, spacing, deep bite, open bite, 216 and crossbite [13]. AI score is a novel method for assessing the case difficulty, confirming 217 that the more difficult the case, the longer the treatment duration. 218

We assessed the feature importance for the ML predictive models; patient age, max-219 illary crowding, and mandibular crowding were the top features. Patient age could be a 220 contributing factor due to the biological differences between adolescents and adults. 221 Vayda et al. in 1995 reported significant differences in treatment length between adults 222 and adolescents [16]. Other studies reported no significant differences in treatment length 223 between adults and adolescents [17]. Additional parameters contribute to treatment 224 length prediction by ML. For example, crowding, overjet, overbite, and AI score are all 225 measures for the severity of the malocclusion; previous studies found that quantitative 226 malocclusion indices, such as peer assessment rating (PAR) and the objective grading sys-227 tem (OGS), correlated with treatment length [3]. Other factors were found to have less 228 contribution, such as gender, race, and malocclusion classification into Class I, II, and III; 229

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this aligns with previous findings [1,3,7]. Unexplored factors may also contribute to treat-230 ment length, including orthodontic technique employed, the operator skill and experi-231 ence, and patient compliance. However, the impact of these factors is unknown and needs 232 to be examined. 233

The scope of this study was to build a predictive model that can be used at initial 234 patient screening or consultation. Other parameters can be used for fine-tuning of the ML 235 models in the future. Furthermore, individual/subjective issues create more variations 236 than the quantifiable factors presented in the study. However, we can perform additional 237 studies to correlate those numeric variables to better understanding of impact on treat-238 ment length. A clinical application of the ML predictive models presented in this study 239 could be a software or a mobile application with a graphical user interface (GUI) that can 240 be used during the orthodontic screening or consultation to provide helpful information 241 for both the patient and the orthodontist (Figure 10). Furthermore, these ML models could 242 be integrated with orthodontic software currently available. 243

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Figure 10. Graphical user interface for mobile application for treatment length prediction.

5. Conclusion	246		
We achieved our objective of developing predictive models-based ML methods. Bagging	247		
and AdaBoost ML methods provided good predictability for orthodontic treatment length	248		
when patient information, such as age, malocclusion, and crowding, was provided. Fur-	249		
ies should be done on large diverse datasets to include more variables and improve the	250		
performance of ML models for understanding orthodontic treatment length.	252		
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