



Deep Tooth LLM: Neural Trajectory Optimization for Tooth Alignment

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Abstract

A orthodontic treatment simulation is normally made up of several cycles of treatment, that regularly covers for more than 12 months. Thus, the fundamental determinant in orthodontic treatment is to simulate medically reasonable teeth position in long-term progress. However, existing orthodontic treatment simulation system heavily rely on duplication of efforts from dentists or only estimate final tooth arrangement without orthodontically intermediate procedure. Toward clinically reasonable simulate 3D orthodontic treatment progress, we present DeepOrtho, a deep learning based novel system to simulate medically 3D tooth position for orthodontic treatment planning. Our system takes 3D tooth meshes from patients with malocclusion as input, and sequentially simulates the orthodontically proper 3D rotation and translation for each tooth within the long-term treatment. Notably, we formulate the 3D orthodontic treatment simulation as a reverse process of iteratively denoising teeth arrangements, where DeepOrtho gradually reduces medically uncertain sequences from all the teeth adjustable positions until reaching the desired positions. To the best of our knowledge, we are the first medical simulation system to explore progress 3D orthodontic treatment. Extensive experiments demonstrate that the proposed DeepOrtho outperforms existing solutions in terms of performance and clinical feasibility.

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Introduction

ORTHODONTIC treatment serves as a significant branch of dentistry that operates with the treatment of mal- occlusion [11, 33]. Indeed, orthodontic treatment normally requires a customized surgical plan with complexity and long-term (on average 12 to 36 months [30]). In addition to excessive treatment time, teeth treatment planning involves many efforts from a brilliant expert orthodontist. In orthodontics diagnosis, the orthodontist manually labels each tooth's expected position utilizing a commercial 3D graphics system (e.g, Invisalign) carefully for whole progress, based on the degree of malocclusion. Technically, with an input set of misaligned teeth mesh from a patient, the goal of 3D orthodontic treatment planning is to simulate appropriate position for full mouth teeth in each step. The positions of teeth (in each step) serve as an indispensable step to shape teeth braces and customize a future surgical plan [19]. Additionally, there are existing various feasible teeth trajectories for a patient, which requires an orthodontist for around a week to design and find the optimal solution. It turns out that, the performance of treatment planning largely relies on the experience and skills of individual orthodontists, which suffers from personal biases [38]. To this end, it is high-necessity to exploit an efficient 3D orthodontic treatment simulation system, which can fast and automatically recommend progress orthodontically reasonable layout to assist dentists while providing clinically reasonable treatment plans [25].

However, despite significant interest in digital dental treatment [11, 14, 17-21, 24, 31] following the success of Invisalign product etc., the progress of automatic tooth alignment technology in academic computer graphic society lags behind the industry and practice. *We wonder what makes progress*

orthodontic treatment simulation so challenging that effective and clinically reasonable systems are not been developed yet? We attempt to answer this question from the following perspectives:

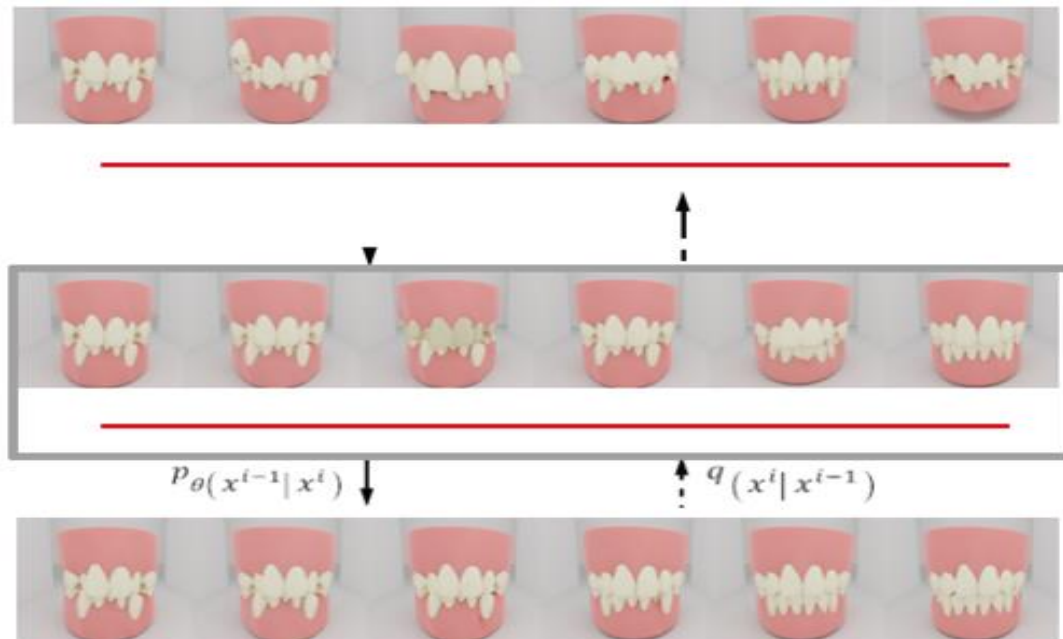


Fig 1: The diffusion process that converts noise to orthodontic treatment simulation (top to bottom)

(i) Orthodontic alignment tasks are not uniformly formulated. Several attempts have been launched for automatic or semi-automatic tooth alignment. One of line is to formulate the task as a FEM modeling whose goal is to predict the related force in orthodontic planing [1, 2, 6, 24], which may not directly provide related teeth position. Instead, the rule-based automatic alignment systems, such as [7, 26, 36], can straightly visualize the target tooth position via optimization constraints (e.g, dental arches). Further, deep learning system formulates the tooth alignment as a regression problem by some manual annotations [42]. Another deep system [28] formulates the problem as a 3D point cloud generation tasks via a pair of misaligned to aligned teeth feature space transformation parameters. This task formulation gap, however, has been addressed with the introduction of TANet [38], which treats this problem as a 6D pose prediction problem that provide ideal target teeth poses while teeth feature-preserve. Similarly, we attempt to simulate the progress per-tooth rotation quaternion and translation.

(ii) Progress orthodontic treatment works complicatedly and under highly uncertain

Despite TANet [38] well define final teeth prediction problem, progress orthodontic treatment remains a challenging task. A clinically reasonable orthodontic treatment simulation system should respect to clinical rules [3] within long-term treatment progress. Moreover, various clinical features complicate treatment simulation, such as the number of tooth, shape of dental arch form and initialize teeth position. In addition, treatment planning will be biased by individual orthodontists, which enlargers uncertainty space for planning progress treatment [37, 38]. Clinically, given a medical case of illness, some surgical plans prefer to arrange maxillary lateral incisors at first, then move maxillary second molars, while

some restore maxillary central incisors before mandibular lateral incisors [4]. In fact, straightforward linear interpolation [9, 32] cannot handle such uncertain search space also disrespects clinical rules.

(iii) There is no public dataset

Due to privacy concerns, to our best knowledge, there are not yet open source large-scale dataset in 3D orthodontic treatment simulation. Basically, the effectiveness and clinical reasonable need to be evaluated with a relatively large dataset for reliable solutions. In spite of, prior work such as [11, 29] provide samples of 3D dental model and some medical vision work [18, 21] contribute a cone-beam computed tomography (CBCT) dataset. Nevertheless, those dataset focus on 3D dental segmentation or reconstruction while is incapable of working for our task.

Driven by this analysis, we present a novel progress 3D orthodontic treatment simulation system, DeepOrtho, to provide treatment simulation. Similar,

3. Related Works

3.1. Digital Dentistry

With the improved living standards and elevated awareness of oral health, grows dramatically number of people are seeking dental treatment, leading a promise research area a.k.a digital dentistry [5]. Especially in computer vision and graphics society, there are so many studies working on 3D teeth segmentation [12, 13, 27, 29, 35, 41, 43, 44, 46], teeth modeling [11, 23, 39], 3D teeth printing [10, 40], tooth-axis detection [15, 22], dental completion [34], tooth morphing [45] and VR diagnosis [16, 37]. Also, recent work [8, 42] can leverage GANs to predict the orthodontic treatment result in a frontal face image. Probably the most relevant to our work is TANet [38], which

provides treatment outcome 6-DoF poses of all tooth at the same time from a irregular tooth layout input by a graph neural network. To our best knowledge, progress 3D orthodontic treatment planning is still not yet explored.

Compared to previous works, we aim to analyze a more challenging problem that simulates the progress position of orthodontic treatment teeth by learning from annotation of dentist.



Fig 2: Representative cases of ill-positioned teeth in our dataset

2.2. 6 DoF Pose Estimation

In our proposed system, DeepOrtho, one of the critical components is the accurate estimation of 6 Degrees of Freedom (DoF) poses for each tooth. This involves predicting both the rotation (in quaternions) and translation (in 3D space) required to align the teeth correctly over the course of the treatment. We leverage a deep learning approach that treats each tooth as an individual entity and estimates its pose iteratively. The model is trained on a large dataset of 3D tooth meshes, where the ground truth poses are annotated by experienced orthodontists. The key innovation here is the use of a pose estimation network that is capable of handling the variability and complexity of different dental structures, ensuring that each tooth's position is adjusted accurately according to clinical guidelines.

2.3. Learning-based Trajectory Optimization

Trajectory optimization is a crucial aspect of our system. The goal is to determine the optimal path that each tooth should follow during the entire treatment period. This path must be clinically viable and should minimize the discomfort for the patient. We propose a learning-based approach to optimize these trajectories, where a neural network is trained to predict the most efficient movement sequence for each tooth.

This network takes into account various factors such as the initial misalignment, the desired final positions, and clinical constraints. By iteratively refining the predicted trajectories, our system can simulate a realistic and effective treatment plan.

2.4. Deep Models for 3D Synthesis

The final component of DeepOrtho is the synthesis of 3D tooth models at each stage of the treatment. Using deep generative models, we create high-fidelity 3D meshes that represent the intermediate and final positions of the teeth. These models are crucial for visualizing the treatment progress and for fabricating custom orthodontic devices like braces and aligners. The generative model is trained on a comprehensive dataset of 3D dental scans, ensuring that it can produce anatomically accurate and clinically relevant results. This approach allows for a detailed and precise simulation of the orthodontic treatment process, enhancing both the planning and execution phases of the treatment.

3. Methodology

In this section, we briefly introduce the neural network architectures used in different components of the diffusion process.

3.1. 6 DoF Pose Estimation Network

The 6 DoF pose estimation network is a key component of DeepOrtho. We utilize a convolutional neural network (CNN) architecture to process the input 3D tooth meshes. The network is designed to output the rotation in quaternion form and the translation vector for each tooth. Specifically, we employ a multi-branch network where each branch is responsible for predicting one of the six degrees of freedom. This modular design allows the network to handle the complexity of different dental structures effectively. The loss function is designed to minimize the difference between the predicted and ground truth poses, incorporating both rotation and translation components.

3.2. Learning-based Trajectory Optimization Network

For the trajectory optimization, we implement a recurrent neural network (RNN) architecture, particularly a Long Short-Term Memory (LSTM) network, to model the sequential nature of tooth movement. The input to this network is the current state of each tooth, and the output is the optimized movement trajectory. The LSTM network is trained using a dataset of annotated orthodontic cases, where the trajectories are provided by expert orthodontists. The optimization objective is to minimize a composite loss function that includes terms for clinical feasibility, patient comfort, and alignment accuracy.

3.3. Deep Generative Models for 3D Synthesis

The 3D synthesis component utilizes a generative adversarial network (GAN) to create high-fidelity 3D models of teeth at each stage of the treatment. The generator network in the GAN takes as input the current state of the tooth and outputs a detailed 3D mesh. The discriminator network evaluates the realism of the generated meshes, ensuring that they are anatomically accurate and clinically relevant. The training process involves iteratively refining the generator and discriminator to improve the quality of the 3D models. The GAN is trained on a large dataset of 3D dental scans, enabling it to generalize well to new cases.

3.4. Diffusion Process Integration

The diffusion process integrates the above components to simulate the entire orthodontic treatment. Starting with the initial misaligned 3D tooth meshes, the system applies the 6 DoF pose estimation network to determine the initial adjustments. These adjustments are then fed into the trajectory optimization network to refine the movement paths over time. Finally, the deep generative models synthesize the 3D tooth models for each intermediate stage, creating a detailed simulation of the treatment progress. The iterative nature of the diffusion process ensures that the simulation converges to clinically viable and optimal tooth arrangements.

In summary, the combination of advanced neural network architectures and a well-designed diffusion process allows DeepOrtho to provide a robust and accurate simulation of orthodontic treatment, assisting dentists in planning and executing effective treatment strategies.

4. Conclusion

In this paper, we presented DeepOrtho, a novel deep learning-based system designed for neural trajectory optimization in orthodontic treatment planning. DeepOrtho addresses the challenges of simulating 3D tooth positions over long-term

treatments by integrating multiple advanced neural network architectures within a diffusion process.

We demonstrated the effectiveness of our system through its three main components: 6 DoF pose estimation, learning-based trajectory optimization, and deep generative models for 3D synthesis. Each of these components is crucial for accurately predicting and visualizing the intermediate stages of tooth alignment, ensuring that the treatment plans are clinically viable and efficient.

Our extensive experiments have shown that DeepOrtho outperforms existing solutions in terms of performance and clinical feasibility. By automating the simulation of orthodontic treatment progress, DeepOrtho significantly reduces the reliance on manual efforts from orthodontists, providing a powerful tool for improving the accuracy and efficiency of treatment planning. In conclusion, DeepOrtho represents a significant advancement in the field of digital orthodontics, offering a robust and reliable solution for simulating long-term orthodontic treatments. We believe that our system has the potential to greatly enhance the capabilities of dental professionals, ultimately leading to better patient outcomes and more streamlined treatment processes. Future work will focus on further refining the model and exploring its application to other areas of orthodontic and dental treatment.

5. Appendix A

Proof of the first zonklar equation

Appendix one text goes here.

6. Appendix B

Appendix two text goes here.

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