Form 3

Abstract of Thesis

Name (LI HEFEI)	
Title	Development of interpretable AI to explore effective components of CAD/CAM resin composites （CAD/CAM用コンポジットレジンの最適組成探索のための解釈可能なAIの開発）

[Objective]

High flexural strength (FS) of CAD/CAM resin composite blocks (RCBs) are required for successful restorations. However, the conventional *in vitro* approach of modifying materials composition by trial and error is time-consuming and inefficient to elucidate the optimum components for achieving the desired flexural strength. Machine learning (ML) is a subfield of AI which combines traditional experimental methods with intelligent data analysis. It learns meaningful regularities between target properties and related factors from known empirical data, which brings predictions of unknown data. Unlike the opaque explainability of output from deep neural networks, ML allows the implementation of interpretable methods to make the predictions understandable to humans.

The aim of this study was to develop an interpretable AI to predict the FS of CAD/CAM RCBs and investigate the components that affect FS to explore the optimum composition.

[Materials and Methods]

I. <u>ML model development</u>

The composition and flexural strength of 12 commercially available CAD/CAM RCBs were collected. The initial data consisted of 16 attributes (15 input compositional descriptors and 1 label) and 12 samples. Each product had a unique composition; therefore, 1 and 0 were used to represent whether the sample contained the specific descriptor or not, respectively. The descriptor filler content was set to be in the range from 62 to 85 (wt)%. Considering that the input data for each sample were recognized as a multidimensional vector, fluctuation range of 0.1 was decided after evaluation and applied for each vector. Specifically, [0, 0.1] and [0.95, 1.05] was applied for 0 and 1, respectively. The generated sample number was decided by evaluating the model's performance. Then, nine samples were decided and generated within the fluctuation range of 0.1 according to the data of the original sample. Consequently, the training data set was increased to 16 attributes and 120 samples.

The regression algorithms of random forest (RF), extra trees (ET), gradient boosting decision tree (GBDT), and extreme gradient boosting (XGBoost) were used to develop the final ML models. The whole data set was imported and randomly split into two groups: 80% of the data was used for training the model, and the remaining 20% was used for testing. The function "GridSearchCV" was applied to search for the optimal combination of hyperparameters for each model.

The coefficient of determination (R^2), the root mean square error (*RMSE*), the mean absolute error (*MAE*), and the relative error were calculated to assess the regression accuracy of each model, and the values were compared.

II. <u>Feature importance analysis</u>

The feature importance was calculated and compared within the ET and GBDT models. The feature importance analysis determined the contribution of each feature to the targeted properties by assigning a score for each feature.

III. <u>Exhaustive search</u>

The first 14 descriptors were set to 0 or 1, and the 15th descriptor (filler content) was set to be in the range from 62 to 85 (wt)%. An exhaustive search was performed by the best performed ML models to iterate all 214×24 (393,216) combinations of the descriptors and predict 393,216 values of the corresponding flexural strengths. The combinations were then screened, and the impossible combinations were deleted. The combinations of descriptors with the highest and lowest flexural strengths were selected and compared.

IV. Bayesian optimization

The time cost for an exhaustive searching for 393,216 combinations was 48 hours. Therefore, Bayesian optimization (BO) was used to shorten the searching time. Optimization with Gaussian process surrogate model and the expected improvement (EI) acquisition function was conducted. The time to find the highest flexural strength among combinations was compared between the exhaustive search optimized by BO and without BO.

[Results and Discussion]

I. All of the four selected algorithms achieved R^2 values of over 0.9 in terms of prediction accuracy, which indicated the acceptable predictive ability of the developed models for the flexural strength of CAD/CAM RCBs. GBDT was the best performing model with R^2, *RMSE*, and *MAE* to be 0.998, 1.179 MPa, and 0.761 MPa, respectively, closely followed by the ET model. The *RMSE* values for the RF and XGBoost models were 5.643 MPa and 6.639 MPa, respectively, which were greater than GBDT and ET. These results suggest that the RF and XGBoost models yielded uncertainties during the extrapolation process.

II. The feature importance analysis demonstrated that the filler content, TEGDMA, and $ZrSiO_4$ to be the top three important features. According to the ranking, it was found that the filler content and the use of monomers should be adjusted with the highest priority when modifying the composition of CAD/CAM RCBs to improve flexural strength.

III. In the exhaustive search, TEGDMA was found to be contained in 53.5% (shared the highest ratio) of the combinations predicted by GBDT model in the lower flexural strengths predicted group, with filler content ranging from 62 to 69 (wt)%. In the higher strength prediction group, none of the combinations contained TEGDMA or Bis-GMA. Instead, UDMA was one of the most frequently contained monomers, and the filler content ranged from 82 to 85 (wt)%. These findings were consistent with the *in vitro* published results, which indicated the established ML approach performed appropriately. $ZrSiO_4$ had a relatively high frequency in the lower strength prediction group for GBDT (59.2%) model's predictions, which suggest that $ZrSiO_4$ may have effect on the flexural strength of CAD/CAM RCBs, which needs to be further explored. The chemical compositions of RCB with the maximum flexural strength (269.5 MPa) predicted by GBDT were SiO_2; barium glass; methacrylate mixed filler for fillers; and UDMA alone for monomers. Simultaneously, the filler content was indicated to be in the range from 82 to 85 (wt)%.

IV. By applying BO, the average time to find the optimum compositions with the maximum flexural strength was 5.56 hours. This result suggests that Bayesian optimization with EI as an acquisition function could be applied to save the time for searching an effective composition of CAD/CAM RCBs.

[Conclusion]

In this study, the interpretable AI process was established, and flexural strength of CAD/CAM RCBs were predicted with acceptable accuracy. UDMA and filler content were identified by the process to be the major factors to affect the flexural strength during the established process. This technology has great potential as an important tool to help modify various targeting properties for different dental materials, provided an adequate data set is available, which will save time and cost for materials designing.

様式 7

論文審査の結果の要旨及び担当者

氏　名　（　Li Hefei　）			
論文審査担当者		（職）	氏　名
	主 査	教授	今里　聡
	副 査	教授	池邉　一典
	副 査	准教授	野崎　一徳
	副 査	講師	峯　篤史

論文審査の結果の要旨

本研究は、CAD/CAM 用コンポジットレジンの構成要素と強度の既知情報を用いて解釈可能な人工知能モデルを作成し、所望の強度を達成するための最適な構成要素を探索するツールとしての有用性を評価したものである。

その結果、アンサンブル学習を採用することで高性能な人工知能モデルを作成でき、それを用いた網羅的探索により、UDMA とガラスフィラーの含有率が曲げ強さに影響を及ぼす主な要素であることが明らかになった。さらに、ベイズ最適化を応用することで、上記の探索に要する時間を大幅に短縮することに成功した。

以上の研究成果は、CAD/CAM 用コンポジットレジンを含む、さまざまな歯科材料の設計を支援するツールとして有用な人工知能モデルの開発に成功したことを示すものであり、本研究は博士（歯学）の学位授与に値するものと認める。