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IJIE

http://penerbit.uthm.edu.my/ojs/index.php/ijie
ISSN : 2229-838X e-ISSN : 2600-7916

The International Journal of Integrated Engineering

Decision Tree Algorithm for the Classification of Dental Caries Severity via Saliva

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DOI: https://doi.org/10.30880/ijie.2022.14.03.023
Received 13 December 2021; Accepted 07 June 2022; Available online 20 June 2022

Abstract: Dental caries is one of the most prevalent chronic diseases. Early detection is prominent to avoid the tooth weakening or worst the tooth loss. UV absorption spectroscopy is a non-invasive technique used for the detection of salivary alpha-amylase which are increasing in the presence of caries. Spectrum acquired from patient at Faculty of dentistry, UKM showed significant peak around 260-300 nm which are correspond to the absorption of amino acid found in salivary alpha-amylase. The spectra are preprocesses using autoscale and multiplicative scatter correction (MSC) to optimize the signal. Decision tree algorithm was implemented on the UV absorption spectra. The best model of decision tree obtained when using autoscale preprocessing method. The accuracy, precision, sensitivity and specificity for the validation data obtained were 0.70, 1.00, 0.14 and 1.00 respectively. The decision tree requires more tuning for the robustness for future application.

Keywords: UV Spectroscopy, dental caries, chemometrics, decision tree

1. Introduction

Dental caries is among the most common infectious disease affecting kids and adults. Based on the report from world health Organization (WHO), approximately 60-90% of children age 5-7 years old experienced dental caries [1]. The occurrence of dental caries is due to poor oral hygiene, high sugar diet and plaque. The bacteria inside the mouth work as a break down agent for food but the high carbohydrate intake cause the presence of other bacteria such as Streptococcus mutans [2]. Streptococcus mutans cause the formation of the dental plaque and subsequently will result in the damage to the tooth structure by providing the acid environment inside the mouth.

The early screening for dental caries detection is crucial to reverse the carious process while save the treatment cost and restore the condition of the teeth [3]. The conventional method to detect the presence dental caries such as visual inspection [2] [3], electrical conductance measurement [6] and X-ray imaging [7]. The visual inspection must be done by the certified dentist that follow the International Caries Detection and Assessment System (ICDAS) [8][9]. The

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challenges of the dentist in teeth inspection is differentiation of early stage of the caries (ICDAS score 1 and 2) and identify the proximal caries [10]. The concern on the conventional method are the technique requires sophisticated procedures handled by the expert and require direct examination on the patient thus new method for indirect measurement are crucial.

Ultraviolet (UV) illumination mostly used fluorescence technique [11][12] to detect the presence of the dental caries in teeth. The fluorescence method is a reliable assessment of caries and plaque but it unable to detect the interproximal lesion and equipment need to be handled by the professional [13]. To the extent of author knowledge, there are only few works that adopt UV spectroscopy technique [14] to detect the early sign of dental caries. The concern on the UV spectroscopy techniques is the differentiation of the spectra is very minimal and hardly distinguished by the naked eyes. Chemometrics analysis is required to be coupled with the UV spectroscopy for the qualitative analysis of dental caries. Methods such as multivariate curve analysis-alternating least square [15], linear discriminant analysis [16] and K-nearest neighbor [17] are among the algorithms used in chemometrics analysis to extract the information and build predictive model. Olsen et. al adopt decision tree algorithm form image processing of dental caries system because this algorithm can be used for high dimension data and the nonlinear relationship between the features do not affecting its performance [18].

The objective of this paper is to classify the severity of the dental caries based on the ICDAS score using saliva sample. The sample will be irradiated with UV emission to obtain the UV absorption spectra and the spectra will be preprocess with spectra pretreatment process to enhance the spectra signal. Decision tree will be implemented on the calibration data and the model will be validated with the validation data. The performance measure will be discussed to test the robustness of the decision tree prediction model.

2. Methodology

The saliva collection was carried out at Faculty of Dentistry, UKM with the ethical from Research Ethics Secretariat, Universiti Kebangsaan Malaysia with ethics code UKM PPI/111/8/JEP-2018–441. The saliva was collected by the dentist using saliva collection aid and the teeth was inspected by the professional dentist. The saliva collected with different caries severity ranging from ICDAS 0 to 5. The details for each ICDAS score was explained by Ormond et.al [8]. The lowest ICDAS score 0 indicate normal teeth and the increasing score number shows the increasing caries progresses. A protease inhibitor was added to the saliva as buffer and centrifuged for 30 minutes at 6500 rpm to remove any food detritus.

Figure 1 shows the UV spectroscopy technique was applied to the saliva sample in transflectance mode. The deuterium lamp (Oriel,63163) with wavelength range from 200-350 nm was used for the spectra measurement. The saliva was put in 10 x 10 mm UV-vis quartz cell. Mirror reflector was used to reflect the light back to the silicone detector. The UV spectrometer used bifurcated fiber optic for the UV transmission path.

Python software (version 3.8.8) was utilized to perform the chemometric analysis for the classification of UV spectra. The spectra obtained from the detector was split into calibration and validation in a ratio of 80:20 using stratified sampling method. Preprocess method such as autoscale and MSC smoothing were implemented to enhance the spectra signal. Decision tree algorithm was implemented to classified the UV spectra based on the ICDAS score.

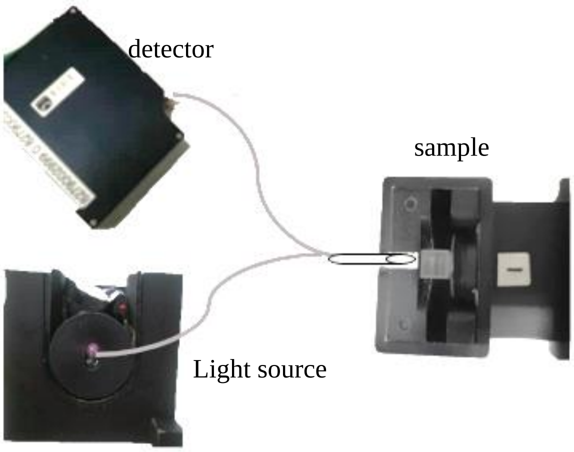

Fig. 1 - The setup of UV spectroscopy measurement using saliva sample.

3. Result and Discussion

The UV spectra as shown in figure 2 shows there are some outlier presence in the data. After the spectra visualization, the outlier was removed to avoid the misclassification of the prediction model by using the z-score removal method. The spectra was focused in the range 250-340 nm due to the high noise in the early stage of the spectra (figure 2b). Based on the spectra obtained, the peak absorption was observed in the range 260 – 310 nm. The peak absorption was due to the presence aromatic amino acids, tyrosine and tryptophan in salivary alpha amylase [19]. These molecules works as a source of receptor to the oral bacteria [20]. The work reported by Singh et. al [21] stated that the alpha amylase concentration was higher for caries patient compared to the non-caries patient.

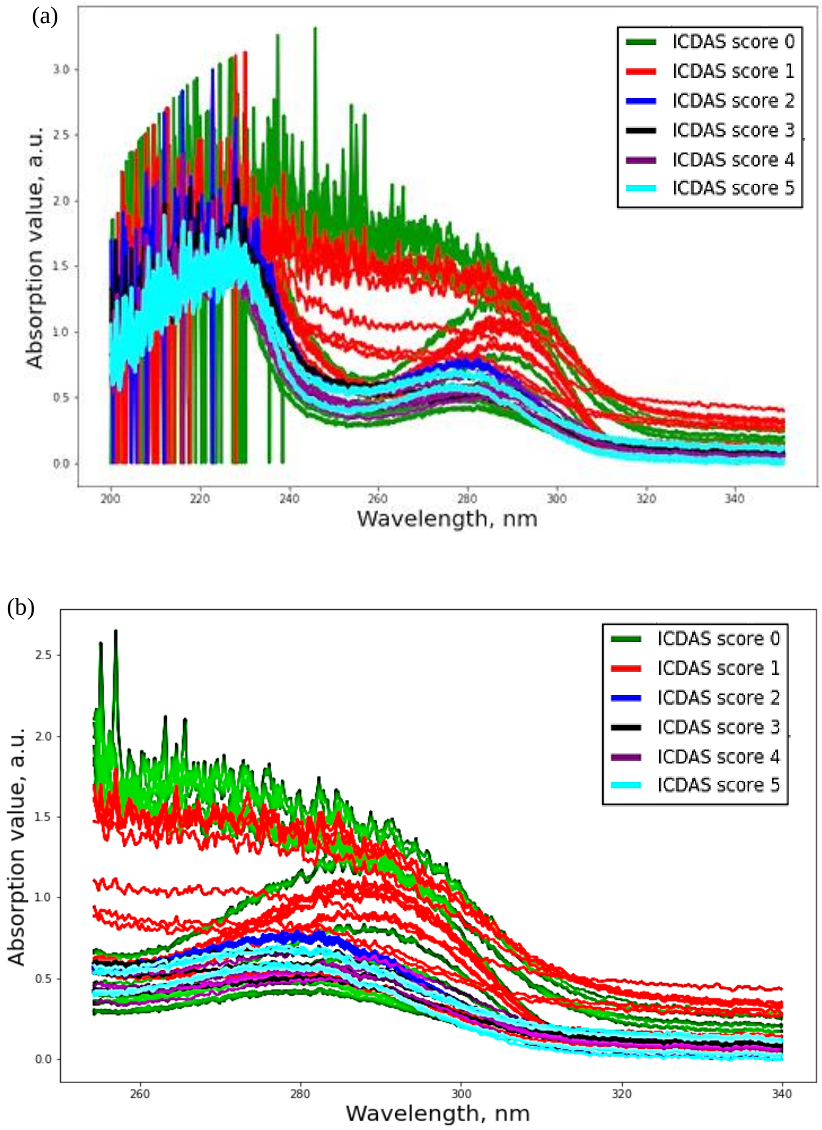

Fig. 2 -The UV absorption spectra for different ICDAS score for (a) 561 and (b) 320 variables

The spectra acquired has no trends based on the ICDAS score thus it is difficult to differentiate the spectra using naked eyes. Chemometrics analysis is crucial to cope this problem because the analysis will trained the calibration data to differentiate the spectra to its respective ICDAS score. The chemometrics analysis will be performed on the spectra data with 561 variables (200-350 nm) and 320 variables (250-340 nm). The performance of these 2 chemometric analysis will be compared in terms of the accuracy, precision, sensitivity and specificity.

Decision tree algorithm is one of the supervised classification analyses that can be used for the classification analysis. The decision tree classifies the spectra based on the ICDAS score using absorption at each wavelength points as the attribute as illustrated in figure 3. The highest node of the decision tree has the highest normalized information gain which in this study is 259.96 nm. The normalized information gain is calculated for each level of the decision tree until the depth of tree is reached.

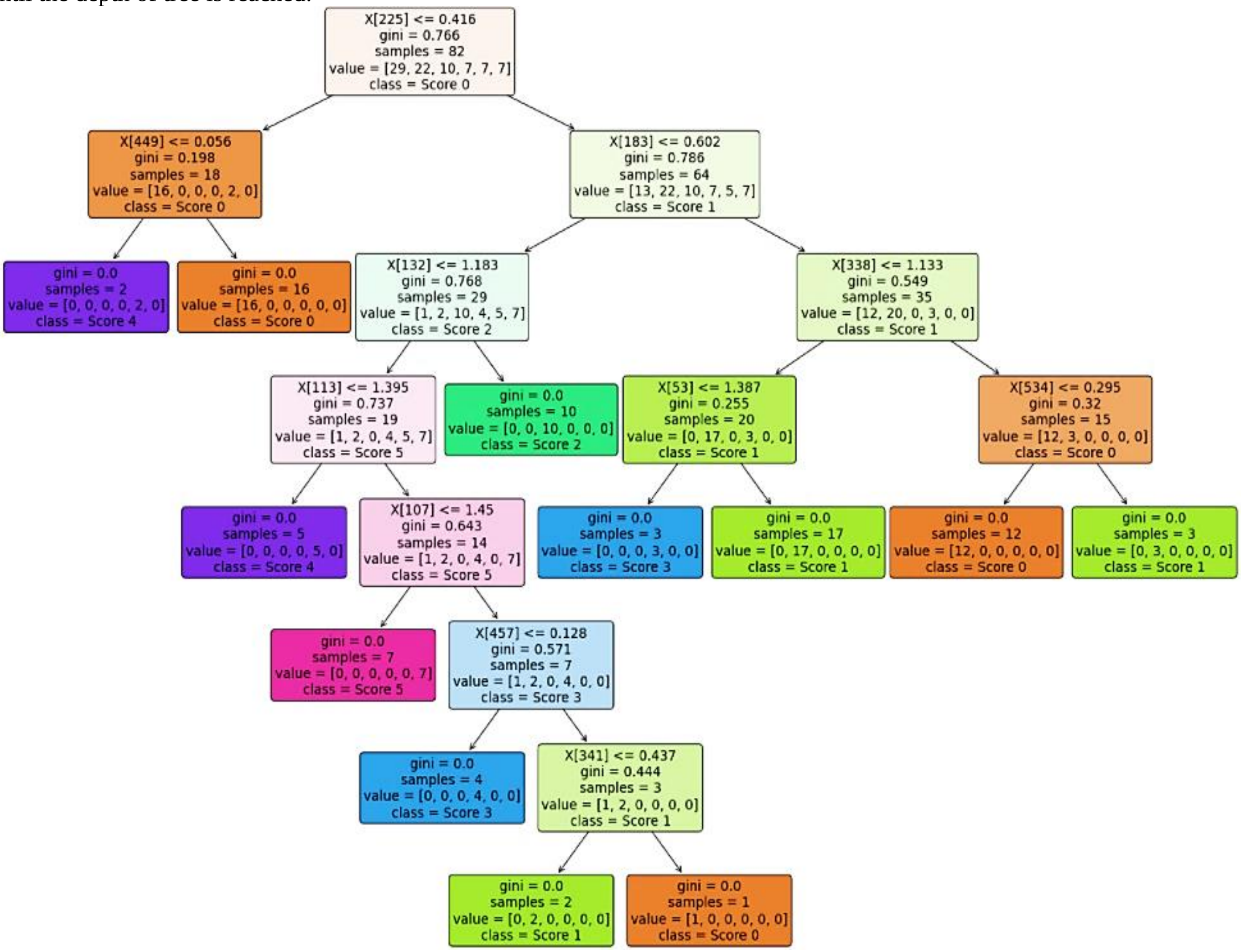

Fig. 3 - The decision tree for the classification of UV spectrum based on ICDAS score

Different methods of preprocessing were applied to the UV spectra to determine the optimized prediction model. The performance measure of the prediction model was accuracy, precision, sensitivity and the specificity based on the calculation used by the previous work [22]. The calibration data performance has shown the optimized performance for the accuracy, precision, sensitivity and specificity for each type of preprocessing method. The accuracy of 561 variables for the validation data obtained for no preprocessing, autoscale and MSC were 0.60, 0.65 and 0.50 respectively. The precision using no preprocessing and autoscale methods has shown the highest value of 1.00 meanwhile MSC method has 0.50 precision. The sensitivity of the prediction model is the capability of the decision tree to predict the normal teeth correctly whereas the specificity is the capability of the model to correctly classified the spectra for the ICDAS score above 0. The autoscale method exhibit the highest sensitivity value of 0.29 compared to the no preprocessing and MSC. The specificity obtained for none preprocessing and autoscale are 1.00 but the MSC has specificity of 0.92. The autoscale exhibit better performance compared to MSC because the absorption value of the spectra data has been standardized in autoscale compared to MSC that only detrend the spectrum based on the reference spectrum [23].

Table 1- The result of decision tree model for calibration and validation data for different preprocessing method

Variables	561			320		
Preprocessing	None	Autoscale	MSC	None	Autoscale	MSC
Accuracy calibration	1.00	1.00	1.00	1.00	1.00	1.00
Accuracy validation	0.60	0.65	0.50	0.55	0.70	0.70
Precision calibration	1.00	1.00	1.00	1.00	1.00	1.00
Precision validation	1.00	1.00	0.50	1.00	1.00	1.00
Sensitivity calibration	1.00	1.00	1.00	1.00	1.00	1.00
Sensitivity validation	0.14	0.29	0.14	0.14	0.14	0.14
Specificity calibration	1.00	1.00	1.00	1.00	1.00	1.00
Specificity validation	1.00	1.00	0.92	1.00	1.00	1.00

The decision tree is built for 320 variables after the removal of region with high noise within range 200-250 nm. The same preprocessing method is applied on the spectra data to check the performance of the decision tree model. Based on the result in table 1, the accuracy of the model for none preprocessing has reduced from the 0.60 to 0.55 but for autoscale and MSC preprocessing method, both accuracy is improved to 0.70. The precision for validation data using MSC preprocess method has significantly increase from 0.50 to 1.00. The sensitivity of the autoscale method has reduced from 0.29 to 0.14 because the model has difficulty to differentiate ICDAS score 0 and 1. Most of the validation data predict ICDAS score 0 with ICDAS score 1.

4. Conclusion

Decision tree with autoscale method has shown the best result for overall performance based on the accuracy, precision, sensitivity and the specificity obtained. The decision tree method with different spectra preprocessing capable to detect the spectra from the caries teeth due to the high specificity obtained and differentiate the spectra based on the ICDAS score. Therefore, the result shows the incorporation of UV spectroscopy and decision tree algorithm using saliva can be used to predict the dental caries based on ICDAS score. The performance of the decision tree model can be refined by normalizing the distribution of the spectra data for each ICDAS score to overcome the problem of the overfit and biased tree.

Acknowledgement

This work is supported by Universiti Teknologi MARA under internal grant known as Geran Penyelidikan Khas(GPK) 600-RMC/GPK 5/3 (091/2020).

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