

**UNIVERSITI TEKNOLOGI MARA**

**CHEMOMETRICS ANALYSIS FOR  
THE DETECTION OF DENTAL  
CARIES VIA ULTRAVIOLET  
ABSORPTION SPECTROSCOPY**

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## ABSTRACT

The prevalence of dental caries is still high and this has raised a major concern to the society and government. Dental caries is a progressive disease that belongs to the group of non-communicable diseases (NCDs). Currently, dental caries has become the first ranking among the NCDs due to its high prevalence. Methods such as visual inspection by the dentist, imaging and illumination techniques have been widely used by the dentist to diagnose the patient's severity of dental caries. These conventional methods required expert assistance, reagent and were mostly used for diagnostic purpose. Ultraviolet (UV) spectroscopy has a great potential to be an early screening tool for the detection of dental caries. Chemometrics analysis needs to be coupled with UV spectroscopy to correlate with the UV spectra and the caries score based on International Caries Detection and Assessment System (ICDAS). The UV spectra collected in the range 200 – 350 nm shows the absorption at 260-310 nm due to the presence of certain bacteria that cause dental caries. The spectra were split into calibration and validation data using stratified random sampling for each of ICDAS class by a ratio of 80:20. Different preprocessing methods (mean centre, autoscale and Savitzky-Golay smoothing) were applied to the spectra to reduce the noise embedded in the spectra. Classification algorithms such as K-nearest neighbour (KNN), logistic regression (LR), linear discriminant analysis (LDA) and decision tree (DT) were employed to classify the spectra into its ICDAS score. The best performance obtained using Savitzky-Golay smoothing and LDA algorithms after the wavelength selection with the accuracy reported of 0.90. The precision, sensitivity, specificity obtained for the model were 1.00, 0.86 and 1.00 respectively. Artificial neural network (ANN) was performed on the spectra to investigate its feasibility to predict the dental caries. The ANN architecture was optimized by tuning the hyperparameter. The best result of ANN model obtained were 0.85, 0.8, 0.57 and 0.92 for accuracy, precision, sensitivity and specificity. Dimension reduction algorithm such as LDA and CNN were applied on the spectra to reduce the number of variables to be trained. The result obtained has revealed that the combination of LDA-ANN did not improve the performance of the model. The accuracy obtained using CNN was 0.85 for the overall performance of calibration and validation. Model 2 of CNN has maximum performance of validation in terms of accuracy, precision, sensitivity and specificity but the calibration model requires more optimization. The accuracy of the CNN model is comparable with the accuracy of the previous work that utilizing CNN for the imaging data to detect caries (diagnostic tool).

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# CHAPTER ONE

## INTRODUCTION

### 1.1 Motivation

Medical technology has advanced in recent decades due to consumer demand. Furthermore, the growing number of diseases drives the demand for medical technology. Factors such as sedentary lifestyle and poor eating habit has contribute to the growing prevalence of many diseases thus fuelling the growing demand for diagnostic and treatment. Healthcare agencies and research centre from various countries have put an effort to find diagnostic test and procedure for detection of a disease. Based on the market research report from Fortune Business Insight that was published in June 2022, the market for medical devices is expected to increase from USD 495.46 billion in 2022 to USD 718.92 billion in 2029 at a compound annual growth rate (CAGR) of 5.5% over the forecast period of 2022-2029 [1].

Dentistry is one of the fields that require the advancement of medical devices and diagnostic test. The diagnostic in dentistry require in depth examination of teeth, gum, jaw, nerve, and muscle of the patient. Among the disease that effect the oral health are dental caries, periodontal (gum) disease, edentulism (total tooth loss), oral cancer and many more. Based on the report by World Health Organization (WHO), United States spends more than USD 124 billion on dental related expenses annually [2]. Figure 1.1 shows that the estimated total number of cases of oral disease is approximately 1 billion higher than the total number of cases of the five major noncommunicable diseases (NCDs) such as mental disorders, cardiovascular disease, diabetes mellitus, chronic respiratory illnesses, and cancers [2]. NCD is a chronic disease that occurs for a long period. Although the dental caries has high cases, but this disease has less contribution to the number of deaths but can impact the quality of life of an individual. The examples are missing days of school or work due to toothache and possibly of hospital administration due to complications from large dental caries that causes spreading of infections systematically. The dominant effect of the cariogenic diet, poor oral hygiene habits such as not brushing teeth effectively and the use of tobacco has led to the high prevalence of oral disease.