CALIBRATION TRANSFER IN NEAR INFRARED SPECTROSCOPIC ANALYSIS USING ADAPTIVE ARTIFICIAL NEURAL NETWORK

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To my beloved parents, thank you.

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ABSTRACT

Near Infrared Spectroscopy (NIRS) has been implemented in various areas due to its non-invasive and rapid measurement features. A NIRS calibration model can be transferred among different instruments using calibration transfer methods. According to review paper reported by J. Worksman, the most popular calibration transfer methods of spectra standardization methods require primary and secondary instruments to acquire transfer samples at the same samples. However, if the primary instrument is broken, then the existing model cannot be transferred using these methods. Artificial Neural Network (ANN) that has the capability of adapting new environmental conditions. Thus, this study aims to investigate the feasibility of an adaptive ANN (AANN) as an alternative in transferring models from primary to secondary instruments with transfer samples collected on secondary instruments only. First, ANN was developed and optimized using primary instrument's spectrum. Then, the optimized ANN was adapted to secondary instruments using transfer samples collected on secondary instruments, in which the weights and biases of the ANN were updated. Finding show that the excellent results were obtained using proposed AANN and 20 transfer samples, with the best averaged root mean squared error of prediction (RMSEP) of 0.1017% and the best averaged correlation coefficient of 0.7898, followed by Direct Standardization – Artificial Neural Network (DS-ANN) and Direct Standardization – Adaptive Artificial Neural Network (DS-AANN) in corn oils prediction applications. The proposed AANN outperformed previous works Piecewise Direct Standardization – Partial Least Squared (PDS-PLS) with RMSEP of 0.1321% and 0.1150%, and correlation coefficient of 0.7780 and 0.7785, for m5/mp5 and m5/mp6 respectively. Hence, proposed AANN has the capability to transfer the existing calibration model to secondary instruments without the involvement of primary instrument.

ABSTRAK

Spektroskopi Inframerah Hampir (NIRS) telah dilaksanakan di pelbagai bidang kerana ciri pengukurannya yang tidak invasif dan cepat. Model penentukuran NIRS dapat dipindahkan di antara instrumen yang berbeza menggunakan kaedah pemindahan penentukuran. Menurut kertas kajian yang dilaporkan oleh J. Worksman, kaedah pemindahan penentukuran yang paling popular dari kaedah standardisasi spektrum memerlukan instrumen primer dan sekunder untuk memperoleh sampel pemindahan pada sampel yang sama. Namun, jika instrumen primer rosak, maka model yang ada tidak dapat dipindahkan menggunakan kaedah ini. Rangkaian Neural Buatan (ANN) yang memiliki kemampuan untuk menyesuaikan keadaan persekitaran baru. Oleh itu, kajian ini bertujuan untuk mengkaji kemungkinan ANN suai (AANN) sebagai alternatif dalam memindahkan model dari instrumen primer ke instrumen sekunder dengan sampel pemindahan dikumpulkan pada instrumen sekunder sahaja. Pertama, ANN dikembangkan dan dioptimumkan menggunakan spektrum instrumen primer. Kemudian, ANN yang optimum disesuaikan dengan instrumen sekunder menggunakan sampel pemindahan yang dikumpulkan pada instrumen sekunder, di mana berat dan bias ANN dikemas kini. Hasil kajian menunjukkan bahawa hasil yang sangat baik diperoleh dengan menggunakan cadangan AANN dan 20 sampel pemindahan, dengan nilai purata ralat terkuasa dua min punca daripada ramalan (RMSEP) 0.1017% dan pekali korelasi rata-rata terbaik 0.7898, diikuti dengan Penyeragaman Langsung – Rangkaian Neural Buatan (DS-ANN) dan Penyeragaman Langsung – Rangkaian Neural Buatan Suai (DS-AANN) dalam aplikasi ramalan minyak jagung. Cadangan AANN mengatasi karya sebelumnya Penyeragaman Langsung Sesecebis – Terkuasa Terkecil Separa (PDS-PLS) dengan RMSEP 0.1321% dan 0.1150%, dan pekali korelasi masing-masing 0.7780 dan 0.7785, untuk m5 / mp5 dan m5 / mp6. Oleh itu, AANN yang dicadangkan mempunyai kemampuan untuk memindahkan model penentukuran yang ada ke instrumen sekunder tanpa penglibatan instrumen primer.

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LIST OF SYMBOLS AND ABBREVIATIONS

NIR	–	Near infrared
NIRS	–	Near infrared spectroscopy
DS	–	Direct standardization
DS-ANN	–	Direct standardization - Artificial neural network
DS-AANN	–	Direct standardization – Adaptive artificial neural network
PDS	–	Piecewise direct standardization
TSR	–	Trimmed score regression
JYPLS	–	Joint-Y partial least squares
CNN	–	Convolutional neural network
ANN	–	Artificial neural network
ACNN	–	Adaptive convolutional neural network
AANN	–	Adaptive artificial neural network
SNV	–	Standard normal variate
MSC	–	Multiplicative scatter correction
MCOD	–	Monte-Carlo outlier detection
SPXY	–	Sample Partitioning set based on joint x-y distance
PCs	–	Principle components
IRLS	–	Iterative reweighted least squares
SVD	–	Singular value decomposition
RMSEC	–	Root mean squared error of calibration
RMSEP	–	Root mean squared error of prediction
Rc	–	Correlation coefficient of calibration
Rp	–	Correlation coefficient of prediction

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CHAPTER 1

INTRODUCTION

1.1 Background of the study

Near infrared spectroscopy (NIRS) is a secondary analytical approach that measures the absorption of electromagnetic radiation consists of wavelengths from 780nm to 2500nm. NIRS measures the absorption according to overtones and combinations of vibrational modes of the C-H, O-H, and N-H chemical bonds [1]. The chemical bonds' vibration was created by emitting the near infrared light. The absorption was recorded through the reflected light back to the sensors and produced the spectra representing important information on the sample. Near infrared (NIR) spectrum is mixed by various interested chemical information and unwanted noises from variant backgrounds [2]. Consequently, a tedious modelling process is needed to optimize a predictive model for a specific NIRS application with specific instruments.

Before modelling process, the near infrared (NIR) spectrum needed to pre-process and sample separation. First, sample selection method was applied to NIRS application to improve the performance of the predictive model because the samples were distributed uniformly and cover the range of the validation. SPXY algorithm were selected for sample selection method compared to KS algorithm because the performance of SPXY was better than KS [3]–[5]. Second, NIR spectrum needed to pre-process with SNV to remove the unwanted noises and baseline shift effect. The SNV has been chosen because SNV easy to implement and performance is better than MSC [6]. After that, PCA was used to compress the data into few numbers of principle and to reduce the dimension of input of the predictive model [7]–[10].

After pre-processing samples, the predictive model needed to optimize. For optimizing the predictive model, the parameter of the predictive model could be tuned such as number of iterations, weights and biases. ANN was chosen as a predictive model because ANN has been widely used in NIRS researches [11]–[15]. Besides, the typical non-linear algorithms (i.e. Artificial Neural Network (ANN), AdaBoost, local algorithm (LA), support vector machine (SVM), and extreme learning machine (ELM)) for NIRS in food analysis was reviewed by M. Zareef et. al. [16]. ANN can be considered as the most popular non-linear algorithm among these algorithms. For instance, ANN coupled with NIRS was used to predict nitrogen content [12], [15], zinc oxide content [13], dry matter content [17], protein content [11], moisture content [18], and blood glucose [14]. Hence, ANN is considered as a popular calibration model in NIRS applications.

Ideally, a reliable calibration model developed with consistent spectra can be re-used in secondary instruments. However, direct use of an optimized calibration model from one (primary) to another instrument (secondary) often caused the performance of the existing model to be invalid or degraded [19], [20] because there are differences among the spectra acquired by primary and secondary instruments [21], [22]. This inconsistency of the spectral response among different instruments could be due to the manufacturing process and measurement environmental conditions.

Calibration transfer can solve the inconsistency of the spectra response among different instruments by standardizing the spectrum or updating the model. Calibration transfer is a method to transfer the model from one instrument to other instruments using similar samples and measurement conditions. The technique of recent calibration transfer methods was reported by J. Worksman [21]. According to that review paper, calibration transfer methods were focus to correct the spectrum of the secondary instruments according to the spectrum of the primary instrument e.g. Direct Standardization [9], Piecewise Direct Standardization [23], and canonical correlation analysis (CCA) [24]. However, the existing model cannot be transferred using spectra standardization methods if the primary instrument is broken. Hence, an existing model can be directly transfer to secondary instruments with only transfer samples collected on secondary instruments is worthy to be studied.

On the other hand, the adaptive capability of ANN has been demonstrated in pretrained models. There are two steps to implement this algorithm. First, an ANN is optimized using primary datasets to produce a trained model. Second, adaptive algorithms are used so that the trained ANN can be adapted to other applications. This approach adapts the existing model to suit other applications using various algorithms e.g. transfer learning [25], Adaptive Convolutional Neural Network (ACNN) [26], and pretrained algorithm [27].

Consequently, the learning and optimization costs of ANN can be substantially minimized. A trained ANN from a primary instrument may be applied to secondary instruments using adaptive algorithms as an alternative transfer calibration strategy. Since the adaptive ability of ANN in NIRS applications has not been studied, this study aims to investigate the feasibility of the ANN adaptive algorithm in a NIRS transfer model application.

1.2 Problem statement

To transfer calibration model among different instruments, the instrument that used for calibration is called primary instrument, while the other instruments are the secondary instruments. One of popular calibration transfer method is to standardize the spectra from the secondary instruments to align with the primary spectra [28]. When a calibration model is used in secondary instruments, the calibration model will be invalid. This is because the changes among different instruments and different conditions will degrade the prediction accuracy of the model. Most of the calibration transfer methods require the primary and secondary instruments to acquire transfer samples at the same samples. However, if the primary instrument is broken, then the existing model cannot be transferred using spectra standardization methods. Therefore, an alternative that can directly transfer an existing model to secondary instruments without transfer samples collected on primary instrument is worthy to be investigated.

1.3 Hypothesis

Adaptive Artificial Neural Network (AANN) has a comparative performance achieved by ANN that trained using the calibration dataset and existing calibration transfer i.e. Direct Standardization - Artificial Neural Network (DS-ANN).

1.4 Aim

The adaptive ability of Artificial Neural Network (ANN) can apply to near infrared spectroscopic analysis i.e. corn data. Adaptive ANN (AANN) has the comparative performance achieved by the existing calibration transfer method i.e. DS. Corn data was chosen because the corn data was used for calibration transfer research. The corn data set comprises NIR reflectance spectra and oil content from 80 corn samples. Three instruments scanned each sample. Each instrument acquired 80 spectra. Hence, the total spectra were 240 spectra. The spectra were acquired in the range 1100-1498 nm at each instrument.

1.5 Objectives

This research work embarks on the following objectives:

1. To establish the relationship between the acquired NIR spectra and corn oil values using Artificial Neural Network among different instruments.

2. To construct Adaptive Artificial Neural Network with and without Direct Standardization for transferring the model among different instruments.

3. To evaluate the calibration transfer performance among different instruments based on root mean squared error of prediction, the correlation coefficient of prediction, and the number of transfer samples used.

1.6 Scopes of study

To fulfil the stated objectives, the scope of this project will be divided into three according to objectives:

1. To establish the relationship between the acquired NIR spectra and corn oil values using Artificial Neural Network for different instruments.
    a) The dataset consisted of NIR spectra measured using three NIRS instruments (namely, m5, mp5, and mp6) on 80 corn samples (http://software.eigenvector.com/Data/Corn/index.html).
    b) SNV and SPXY were used for data pre-processing and data separation, respectively.
    c) Artificial Neural Network (ANN) model was used.

2. To construct Adaptive Artificial Neural Network with and without Direct Standardization for transferring the model among the different instruments.
    a) Direct Standardization - Artificial Neural Network (DS-ANN) and Adaptive Artificial Neural Network (AANN) were used to transfer the model from primary to secondary instruments.

3. To evaluate the calibration transfer performance among different instruments based on root mean squared error of prediction, the correlation coefficient of prediction, and the number of transfer samples used.
    a) All methods were created by using MATLAB toolbox (2018a).
    b) Evaluate the models' performance by calculating the root mean square error of prediction (RMSEP), the correlation coefficient of prediction, and the number of transfer samples used.

1.7 Research contribution

This research contributes to the calibration transfer in NIRS by using Adaptive Artificial Neural Network (AANN). AANN can reduce the computing cost and sample preparation by updating the trained model's weight and bias and without rerun the 100 times process for each number of hidden neurons. AANN only needed a set of transfer samples of secondary instruments to transfer the trained model. The proposed AANN transferring a model from primary to secondary instruments achieved the best averaged RMSEP of 0.1017%, followed by Direct Standardization – Artificial Neural Network (DS-ANN) and Direct Standardization – Adaptive Artificial Neural Network (DS-AANN) of 0.1114% and 0.1149 %, respectively.

1.8 Outline of the thesis

Chapter 1 shows the problem of NIRS. This thesis investigates the feasibility of the ANN adaptive algorithm in a NIRS transfer model application. Chapter 2 explains the background and motivation of the calibration transfer in NIRS. The calibration transfer process and the calibration transfer methods were discussed in Chapter 2. Chapter 3 describes the process to develop ANN and the calibration transfer method i.e. Direct Standardization – Artificial Neural Network (DS-ANN) and Adaptive Artificial Neural Network (AANN). Chapter 3 also discussed the procedure to evaluate the calibration transfer methods' performance. Chapter 4 shows the root mean squared error of prediction, the correlation coefficient of prediction, and the number of transfer samples used for calibration transfer method, AANN, DS-ANN, and DS-AANN. Lastly, Chapter 5 concludes the result of this experiment and recommends some interesting research for future work.

CHAPTER 2

LITERATURE REVIEW

2.1 Overview

This chapter discusses the calibration transfer review is discussed in this chapter, i.e. motivation of the calibration transfer, calibration transfer between different conditions, same instruments, and different instruments. After that, the trend of ANN and adaptive algorithm with ANN are discussed and explained the reason to proposed the adaptive algorithm with ANN. Lastly, corn dataset and NIRS applications and problems are also discussed in this chapter.

2.2 Calibration transfer

Calibration transfer methods can be classified into two categories i.e. calibration transfer between instrument and calibration maintenance as reported by J. Worksman [21]. Calibration transfer is to transfer the model from one instrument to another using similar samples and measurement conditions shown in Figure 2.1. Calibration maintenance uses the same calibration model to adapt to new measurement and sample conditions as shown in Figure 2.2.

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APPENDIX A

LIST OF PUBLICATIONS

1. X. Y. Yap and K. S. Chia, "A Comparison Between Local and Global Models Among Different Near Infrared Spectroscopy Instruments for Corn Oils Prediction," *17th IEEE International Colloquium on Signal Processing & Applications (CSPA 2021)*, 2021. (Scopus proceeding)
2. X. Y. Yap, K. S. Chia, and H. A. G. Al-kaf, "Investigating the Feasibility of a CMOS Camera in Developing a Shortwave Near Infrared Spectroscopy," *Int. J. Integr. Eng.*, vol. 12, no. 8, pp. 212–221, 2020. (Scopus indexed)
3. X. Y. Yap, K. S. Chia, H. A. Rahman, and V. Teh, "A non-destructive oil palm fruit freshness prediction system with artificial neural network," *Int. J. Integr. Eng.*, vol. 11, no. 8, pp. 159–163, 2019. (Scopus indexed)

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1. K. S. Chia and X. Y. Yap, "A portable pid control learning tool by means of a mobile robot," *Int. J. Online Eng.*, vol. 12, no. 6, 2016. (Scopus indexed)
2. K. S. Chia, X. Y. Yap, and E. S. Low, "A badminton robot - serving operation design," ARPN J. Eng. Appl. Sci., vol. 11, no. 6, 2016. (Scopus indexed)