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Article

# Classification of vanilla by quality using MOS gas sensors: assessing the effectiveness of wavelet time-frequency analyzer

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**ABSTRACT**

This paper presents an overview of the global vanilla industry, emphasizing vanilla's status as the second most costly spice and the most extensively used flavoring worldwide. To satisfy global demand, there is an increasing reliance on synthetic methods for flavor extraction, raising concerns about quality and health risks due to widespread adulteration with cheaper synthetic vanillin, often misrepresented as "pure." To tackle adulteration effectively and economically, this study proposes employing a single-stage classification model trained using the transient response of an electronic nose (e-nose) equipped with four metal oxide semiconductor (MOS) gas sensors with Principal Component Analysis (PCA) and machine learning classification models to sample vanilla from various countries (Indonesia & Madagascar) and grades (Grade A & B). 33 classifiers were trained and compared based on classification and validation accuracy. Through trial and error, it was determined that the sensor response times at the 20s, 60s, and 90s marks, using Weighted KNN, contributed to 100% classification accuracy and 80% validation accuracy. A second analysis method was attempted where the sensor transient response was processed using the Wavelet Time-Frequency Analyzer. When training classification models using the processed data, the bilayer neural network yielded the highest classification accuracy of 100% and validation accuracy of 70%.

## 1. Introduction

Due Vanilla, the second-costliest spice globally and the most widely used flavoring agent in the food industry, is sourced from orchids within the Vanilla genus, primarily native to Mexico. The primary contributor to global supply, Vanilla Planifolia, dominates production at 80%, mainly cultivated in Madagascar and nearby islands [1]. Despite its value in various sectors, the vanilla market faces substantial supply challenges, exacerbated by the 2018 "vanilla crisis," leading to price surges and criminal activities in producing regions [2, 3]. Synthetic means are increasingly used due to the limited availability and high production costs of natural vanilla [4]. Adulteration with cheaper synthetic vanillin poses health risks and quality concerns [5]. To address these challenges, this study aims to distinguish between natural and synthetic vanilla and enhance the authenticity and traceability of vanilla planifolia. Vanilla samples from Indonesia and Madagascar, categorized into different grades (A and B), have been prepared for this purpose.

In the current phase of the research, a single-stage classification model was created to distinguish between vanilla samples originating from Indonesia and Madagascar, each with varying grades. The training and prediction processes of the classification model were iterated to ascertain precise sample categorizations. Consequently, various methods were employed subsequently to assess the accuracy of these classifications. Additionally, wavelet analysis will be employed to assess its effectiveness in conjunction with the single-stage method. The Continuous Wavelet Transform (CWT) is among the various iterations of the Wavelet Transform frequently utilized to detect patterns or frequencies within a signal, with the specific pattern or frequency corresponding to the chosen wavelet. Continuous analysis often offers easier interpretation due to its redundancy, reinforcing signal traits and enhancing the visibility of all information, particularly subtle details [6].

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## 2. Methodology

### 2.1 Preparation, storage, and sampling of vanilla samples

A total of 68 training samples were gathered as follows:

- 20 Madagascar Grade A (MGA) samples
- 20 Madagascar Grade B (MGB) samples
- 16 Indonesia Grade A (IGA) samples
- 12 Indonesia Grade B (IGB) samples

These samples were utilized to form the training datasets used in training the classification models examined in this investigation. To validate the trained classification models, a total of 20 vanilla samples were prepared as follows and predicted by the trained classification models:

- 5 Madagascar Grade A (MGA) samples
- 5 Madagascar Grade B (MGB) samples
- 5 Indonesia Grade A (IGA) samples
- 5 Indonesia Grade B (IGB) samples

The vanilla samples in this study were stored in individual zip-lock plastic bags, as shown in Figure 1.


**Figure 1.** Indonesia grade A vanilla sample- each sample was stored in a zip-lock plastic bag

Vanilla sampling was conducted by inserting a 2 cm sample into a sensing chamber with four MOS gas sensor models: TGS2600, TGS2602, TGS2611, and TGS2620 for headspace sampling. Table 1 shows the specifications of each MOS gas sensor model. Each sample was inserted into a sample holder before placing it within the sensing chamber. Given the utilization of two distinct grades of vanilla samples, two separate sample holders shown in Figure 2 were employed.

**Table 1.** MOS gas sensors specifications

| Sensor Model | Target Gases |
|---|---|
| TGS2600 | Hydrogen, ethanol, smoke, general smoke contaminants |
| TGS2602 | VOCs, ammonia, H2S |
| TGS2611 | Methane, natural gas |
| TGS2620 | Alcohol, organic solvent vapors |

**Figure 2.** Vanilla sample holder

This division is essential to prevent the cross-contamination of vanilla caviar from the two different grades. Upon the conclusion of the sampling procedure, the solenoid valves were unsealed to enable the introduction of the carrier gas. This study utilized the MOS gas sensors module, sampling process, and feature extraction method practiced by Lee et al. in their studies [7-10]. Sensor response is defined as the change in sensor output voltage (voltage across an external load resistor) due to the change in resistance of the sensing material in the sensor. The change in sensor output voltage is calculated as a percentage change by comparing it with the sensor output voltage baseline, which was set to 1.0 V in this study. The complete e-nose circuit configuration is shown in Figure 3. The sensors were preheated before commencing the vanilla sample collection. This was done by adjusting the sensor heater to 5 V and samples with strong aroma, for example, coffee beans, were introduced into the sensing chamber for a duration of 15 minutes. After the 15-minute interval, the coffee beans were removed, and purging was employed until the sensor readings returned to the baseline values, after which the sampling procedure was initiated.

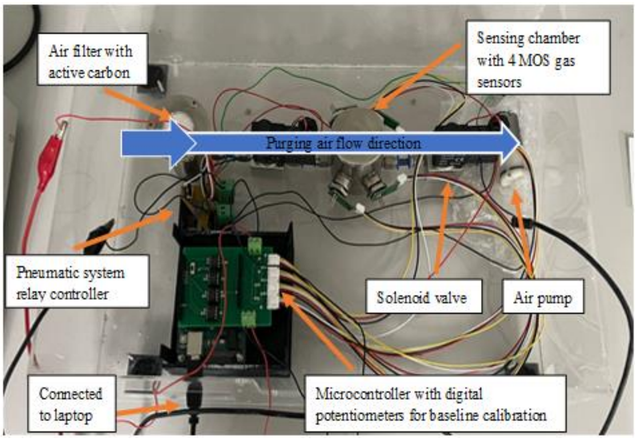


**Figure 3.** Complete e-nose circuit configuration

The sampling process started with a 10-second baseline period, followed by static headspace sampling of vanilla for 120 seconds, a maximum purging duration of 30 seconds, and a maximum recovery interval of 250 seconds. This sums up to a total duration of 410 seconds. For the vanilla sampling process, temperature modulation was employed setting three different levels of heater voltage at different time intervals to produce three different temperatures. The three different sensor temperatures contributed to three distinct sensor sensitivity and selectivity. Table 2 lists the heater voltage corresponding to each sensitivity level in this study. Figure 4 shows the flowchart of the warmup procedure, whereas Figure 5 shows the flowchart of the sampling procedure.

**Table 2.** The heater voltage corresponding to each sensitivity level

| Sensitivity | Heater Voltage |
|---|---|
| 1 | 4.6 V |
| 2 | 4.8 V |
| 3 | 5.0 V |

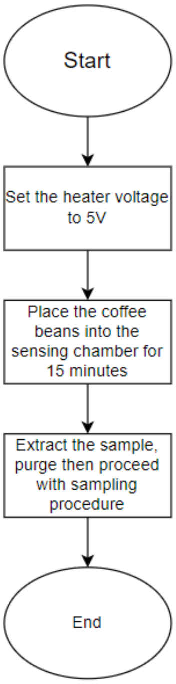


**Figure 4.** Sensor warmup procedure

## 2.2 Sample Data Analysis

Sample data analysis was conducted using the MATLAB software. Data obtained from both the training and validation sets was processed using Principal Component Analysis (PCA) for data visualization and interpretation. This process will reveal distinct PCA scatter clusters corresponding to each grade and country. However, to augment sample classification, the processed data was then used to train and validate 33 classification models from broad categories of decision tree, discriminant analysis, logistic regression classifier, naïve bayes classifier, SVM, k-nearest neighbour (KNN), ensemble classifier and neural network, from which the most accurate models were shortlisted to evaluate the accuracy of sample classification.

## 2.3 Wavelet Time-Frequency Analyzer

A second data analysis method was developed where the sensor transient response (output voltage against time) was analysed using the Wavelet Time-Frequency Analyzer in MATLAB. This analysis aimed to ascertain whether the wavelet technique could improve result accuracy compared to the method in section 2.2. Figure 6 outlines the steps for using the Wavelet Time-Frequency Analyzer.

## 2.4 Vanilla Classification Methods

In this study, multiple techniques (Method A, B, C, D, E and F) were employed to classify the vanilla samples as follows:

a. Method A: Single-stage multi-class machine learning, focusing on distinctions between grades and countries.
b. Method B: Multi-stage two-class machine learning, examining relationships between grades and countries – Madagascar Grade A (MGA), Madagascar Grade B (MGB), Indonesia Grade A (IGA) and Indonesia Grade B (IGB) – as illustrated in Figure 7.
c. Method C: Similar to Method B, specifically comparing the classification and validation accuracy between the two classification approaches in the second stage – (1) MGA vs non-MGA; (2) IGA vs non-IGA.
d. Method D: Similar to Method B, concentrating on the classification of IGA vs non-IGA in stage 2.

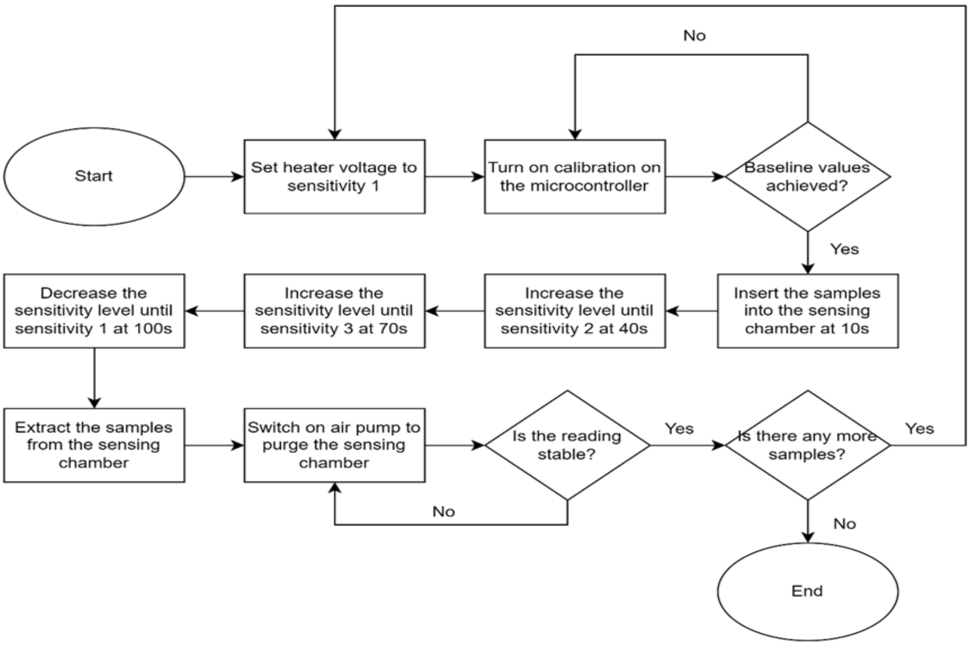


**Figure 5.** Vanilla sampling procedure

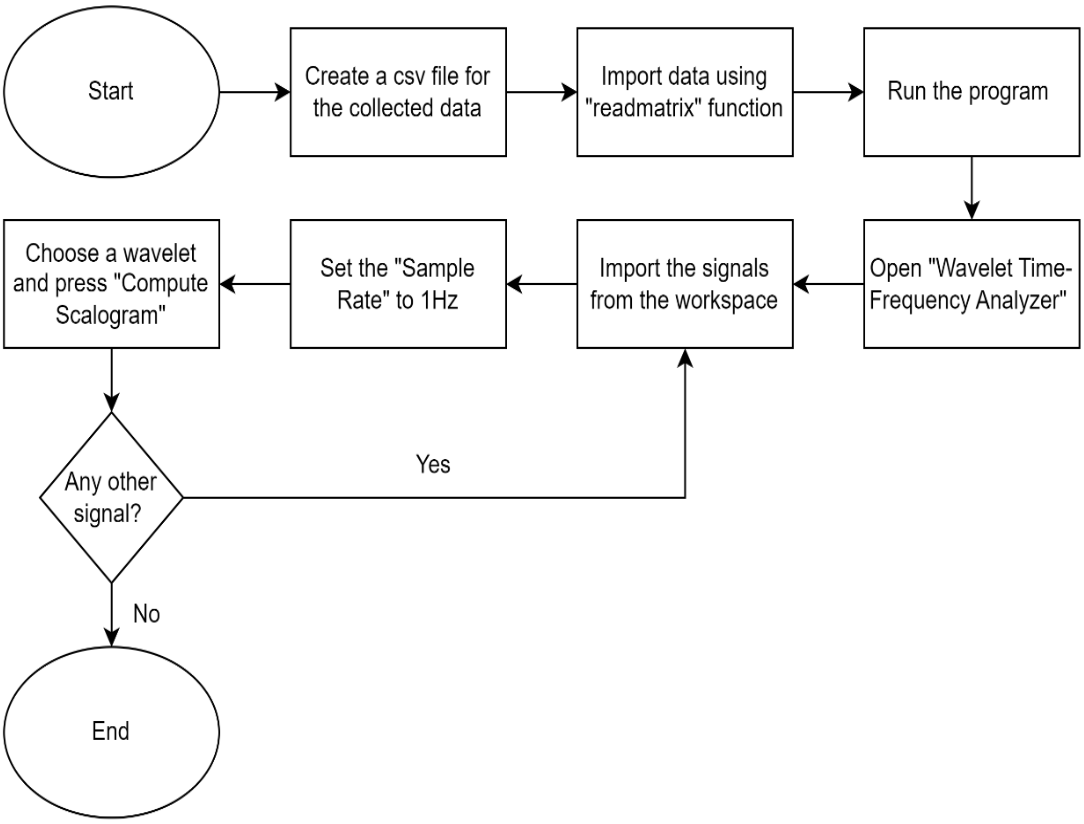


**Figure 6.** Procedure for using the Wavelet Time-Frequency Analyzer in MATLAB

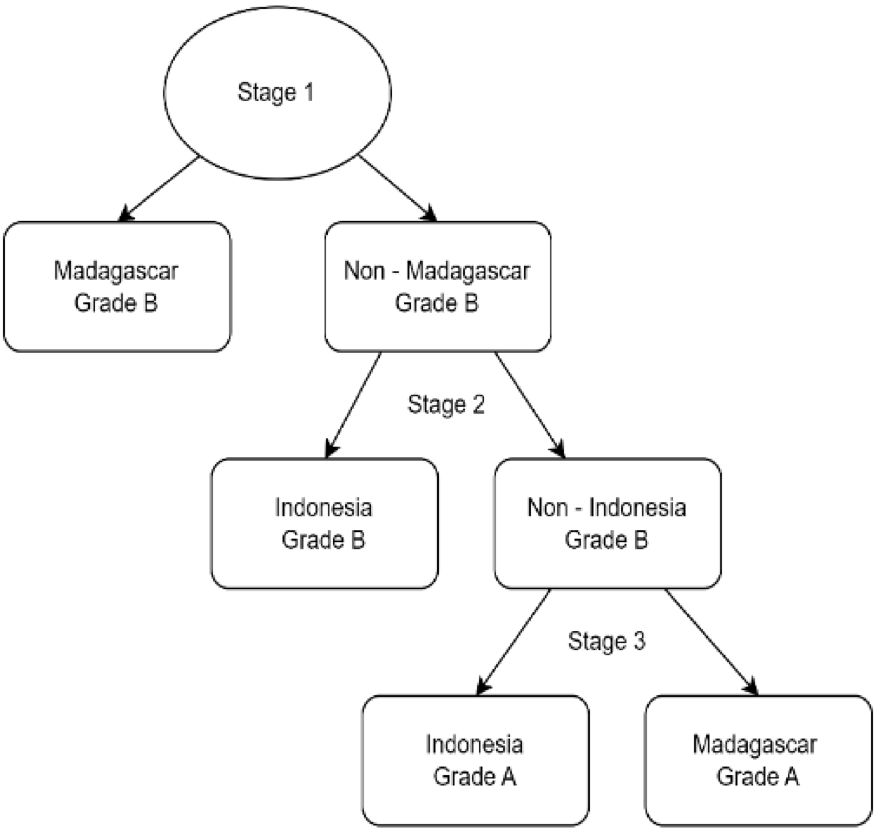


**Figure 7.** Method B of vanilla classification

e. Method E: Single-stage machine learning that classifies the vanilla samples into two classes only – Madagascar or Indonesia.
f. Method F: Similar to method E, except that wavelet time-frequency analysis was used to process the sensor transient response. The processed data was then used to train the classification models.

## 3. Results and discussion

In this study, sensor data was extracted from three response times – 20 s, 60 s, and 90 s – where each response time corresponded to a unique sensor sensitivity and selectivity. This contributed to greater data dimensionality, which led to better interclass separation of vanilla samples.

### 3.1 Method A

Table 3 discerns that the top three most effective classification models belong to the ensemble classifiers category. These models demonstrated perfect accuracy of 100% with the training dataset. However, in terms of validation accuracy, the performance ranged between 50% and 60%, falling short of satisfactory levels. Consequently, the subsequent section will introduce an approach aimed at enhancing the outcomes.

### 3.2 Method B

In this section, a multi-stage, two-class machine learning technique was employed. This method involved a simpler classification process where samples are divided into two classes rather than four simultaneously. During data training, several classification models attained a perfect classification (training) accuracy of 100%, including Support Vector Machine (SVM), K-Nearest Neighbor (KNN) Classifiers, Ensemble Classifiers, and Neural Network. Tables 4-6 show the best performing classification models in terms of validation results at each stage of Method B. For the validation dataset, Linear Discriminant, Bagged Trees, Trilayer Neural Network, SVM Kernel, and Logistic Regression Kernel demonstrated robust performance in the initial stage, achieving validation accuracies ranging from 80% to 95%. However, in the second stage, none of the models effectively differentiated between samples of Indonesia Grade B and Non-Indonesia Grade B, with the exception of Fine KNN and RUS Boosted Trees, which achieved an accuracy of 73.33%. Progressing to the final stage, three models—Fine Gaussian SVM, Subspace KNN, and Trilayer Neural Network—displayed enhanced proficiency in distinguishing between samples of Madagascar Grade A and Indonesia Grade A.

**Table 3.** Best performing classification models in method A

| Classification Model | Training | | | | Training Accuracy | Validation | | | | Validation Accuracy |
|---|---|---|---|---|---|---|---|---|---|---|
| | IGA | IGB | MGA | MGB | | IGA | IGB | MGA | MGB | |
| Bagged Trees | 16/16 | 12/12 | 20/20 | 20/20 | 100% | 3/5 | 1/5 | 1/5 | 5/5 | 50% |
| Subspace KNN | 16/16 | 12/12 | 20/20 | 20/20 | 100% | 2/5 | 1/5 | 3/5 | 4/5 | 50% |
| RUS Boosted Trees | 16/16 | 12/12 | 20/20 | 20/20 | 100% | 4/5 | 2/5 | 1/5 | 5/5 | 60% |

**Table 4.** Best performing classification models in method B, stage 1 (MGB vs Non-MGB)

| Validation | | | |
|---|---|---|---|
| Classification Model | Stage 1 | | Accuracy |
| | MGB | Non-MGB | |
| Linear Discriminant | 5/5 | 12/15 | 85% |
| Bagged Trees | 5/5 | 14/15 | 95% |
| Trilayer Neural Network | 5/5 | 11/15 | 80% |
| SVM Kernel | 5/5 | 11/15 | 80% |
| Logistic Regression Kernel | 5/5 | 11/15 | 80% |

**Table 5**. Best performing classification models in method B, stage 2 (IGB vs Non-IGB)

| Validation | | | |
|---|---|---|---|
| Classification Model | Stage 2 | | Accuracy |
| | IGB | Non-IGB | |
| Fine KNN | 1/5 | 10/10 | 73.33% |
| RUS Boosted Trees | 1/5 | 10/10 | 73.33% |

**Table 6.** Best performing classification models in method B, stage 3 (IGA vs MGA)

| Classification Model | Validation | | |
|---|---|---|---|
| | Stage 3 | | Accuracy |
| | IGA | MGA | |
| Fine Gaussian SVM | 3/5 | 2/5 | 50% |
| Subspace KNN | 4/5 | 4/5 | 80% |
| Trilayer Neural Network | 3/5 | 3/5 | 60% |

**Table 7.** Best performing classification models in method C

| Classification Model | Validation | | | |
|---|---|---|---|---|
| | Stage 2 | | | |
| | MGA | Non-MGA | IGA | Non-IGA |
| Cubic KNN | 0/5 | 10/10 | 4/5 | 6/10 |
| RUS Boosted Trees | 1/5 | 10/10 | 3/5 | 6/10 |
| Medium Neural Network | 1/5 | 5/10 | 4/5 | 5/10 |

**Table 8.** Best performing classification models in method D, stage 1 (MGB vs Non-MGB)

| Classification Model | Validation | | |
|---|---|---|---|
| | Stage 1 | | Accuracy |
| | MGB | Non-MGB | |
| Linear Discriminant | 5/5 | 12/15 | 85% |
| Weighted KNN | 4/5 | 13/15 | 85% |
| Bagged Trees | 5/5 | 14/15 | 95% |
| Medium Neural Network | 4/5 | 12/15 | 80% |
| Wide Neural Network | 4/5 | 11/15 | 75% |
| Bilayer Neural Network | 4/5 | 11/15 | 75% |
| Trilayer Neural Network | 5/5 | 11/15 | 80% |
| SVM Kernel | 5/5 | 11/15 | 80% |
| Logistic Regression Kernel | 5/5 | 11/15 | 80% |

### 3.3 Method C

This section redirects its focus to testing and analyzing samples from Madagascar and Indonesia Grade A, aiming to ascertain which origin offers greater separability from the other classes during classification in the second stage. Table 7 lists the models with the highest validation accuracy for both Madagascar and Indonesia Grade A. Three models showed outstanding performance on the validation dataset for Indonesia Grade A, while none stood out for Madagascar Grade A. Therefore, the decision has been made to differentiate between Indonesia and non-Indonesia Grade A samples in Stage 2 – this was employed in method D.

### 3.4 Method D

Tables 8-10 show the best performing classification models in terms of validation results at each stage of Method D. Validation in stage 1 achieved accuracy ranging from 75% to 95%. Following this, the KNN, RUS Boosted Trees, and Neural Network models produced satisfactory results in stage

2. However, stage 3 yielded notably less favorable results, with these models encountering challenges in differentiating between Indonesia Grade B and Madagascar Grade A. In this context, only one model achieved a validation accuracy of 60%. Conversely, the training dataset showcased strong performance across various classification models.

In conclusion, the most effective models stem from the Neural Network category, achieving a classification accuracy of 100% for the training dataset. Moreover, the Medium Neural Network achieved an 80% validation accuracy in Stage 1 and a 60% validation accuracy in Stage 2, while the Wide Neural Network attained a 75% validation accuracy in Stage 1 and a 53.3% validation accuracy in Stage 2.

**Table 9.** Best performing classification models in method D, stage 2 (IGA vs Non-IGA)

| Validation | | | |
|---|---|---|---|
| Classification Model | Stage 2 | | Accuracy |
| | IGA | Non-IGA | |
| Cubic KNN | 4/5 | 6/10 | 60% |
| RUS Boosted Trees | 3/5 | 6/10 | 60% |
| Medium Neural Network | 4/5 | 5/10 | 60% |
| Wide Neural Network | 3/5 | 5/10 | 53.33% |

**Table 10.** Best performing classification models in method D, stage 3 (IGB vs MGA)

| Validation | | | |
|---|---|---|---|
| Classification Model | Stage 3 | | Accuracy |
| | IGB | MGA | |
| RUS Boosted Trees | 1/5 | 5/5 | 60% |

**Table 11**. Best performing classification models in method E – training accuracy

| Classification Model | Training | | Training Accuracy |
|---|---|---|---|
| | Indonesia | Madagascar | |
| Cubic SVM | 28/28 | 40/40 | 100% |
| Medium Gaussian SVM | 28/28 | 40/40 | 100% |
| Coarse Gaussian SVM | 28/28 | 40/40 | 100% |
| Fine KNN | 28/28 | 40/40 | 100% |
| Weighted KNN | 28/28 | 40/40 | 100% |
| Bagged Trees | 28/28 | 40/40 | 100% |
| Subspace KNN | 28/28 | 40/40 | 100% |
| RUS Boosted Trees | 28/28 | 40/40 | 100% |
| Narrow Neural Network | 28/28 | 40/40 | 100% |
| Medium Neural Network | 28/28 | 40/40 | 100% |
| Wide Neural Network | 28/28 | 40/40 | 100% |
| Bilayer Neural Network | 28/28 | 40/40 | 100% |
| Trilayer Neural Network | 28/28 | 40/40 | 100% |
| SVM Kernel | 28/28 | 40/40 | 100% |
| Logistic Regression Kernel | 28/28 | 40/40 | 100% |

### 3.5 Method E

In this section, samples are segregated based on their respective countries, regardless of their grades. It is evident that several classification models exhibited exceptional performance on the training dataset, achieving an accuracy of 100% as shown in Table 11. However, Table 12 shows that only two models, Cosine KNN and Weighted KNN achieved satisfactory validation accuracy of 80%. By summarising the results from Table 11 and 12, Weighted KNN emerged as the most effective model in distinguishing samples based on their countries, displaying a training dataset accuracy of 100% and a validation accuracy of 80%.

### 3.6 Method F

In this stage, both the training and validation datasets underwent a transition from transient response to time-frequency analysis. Specifically, data from the TGS2602 sensor is selected for this analytical process. The sample rate is fixed at 1 Hz, considering that the entire sampling process lasts approximately 130 seconds with a 1-second interval. The "bump" wavelet is opted for this analysis. Subsequently, a magnitude scalogram is generated as shown in Figure 8, aiding in the precise identification of data at designated timestamps. In this scenario, the data are isolated at 20, 60, 90, and 100-second intervals to extract the RGB frequencies.

The data extracted from the magnitude scalogram was used to train and validate classification models. Table 13 presents the training accuracy, whereas Table 14 presents the validation accuracy. Noteworthy is the attainment of 100% accuracy by several classification models, while five models achieve validation accuracy ranging between 65% and 70%.

### 3.7 Comparison between Method E and F

Tables 12 and 14 were used to compare the validation accuracy between methods E and F using their best-performing classification models. It is apparent that method E surpassed the performance of method F, attaining a superior validation accuracy of 80% in contrast to the latter's maximum accuracy of 70%. However, there is a noticeable discrepancy in data distribution between methods E and F. For instance, in method E, the Linear SVM model correctly identified only 1 out of 10 samples from Indonesia and 9 out of 10 from Madagascar.

Conversely, when utilizing the wavelet time-frequency analyzer (method F), 6 out of 10 samples from Indonesia and 4 out of 10 samples from Madagascar were predicted correctly at validation stage. This observation suggested that employing different signal processing methods resulted in classification of samples from different perspectives.

**Table 12.** Best performing classification models in method E – validation accuracy

| Classification Model | Validation | | Validation Accuracy |
|---|---|---|---|
| | Indonesia | Madagascar | |
| Cosine KNN | 7/10 | 9/10 | 80% |
| Weighted KNN | 7/10 | 9/10 | 80% |

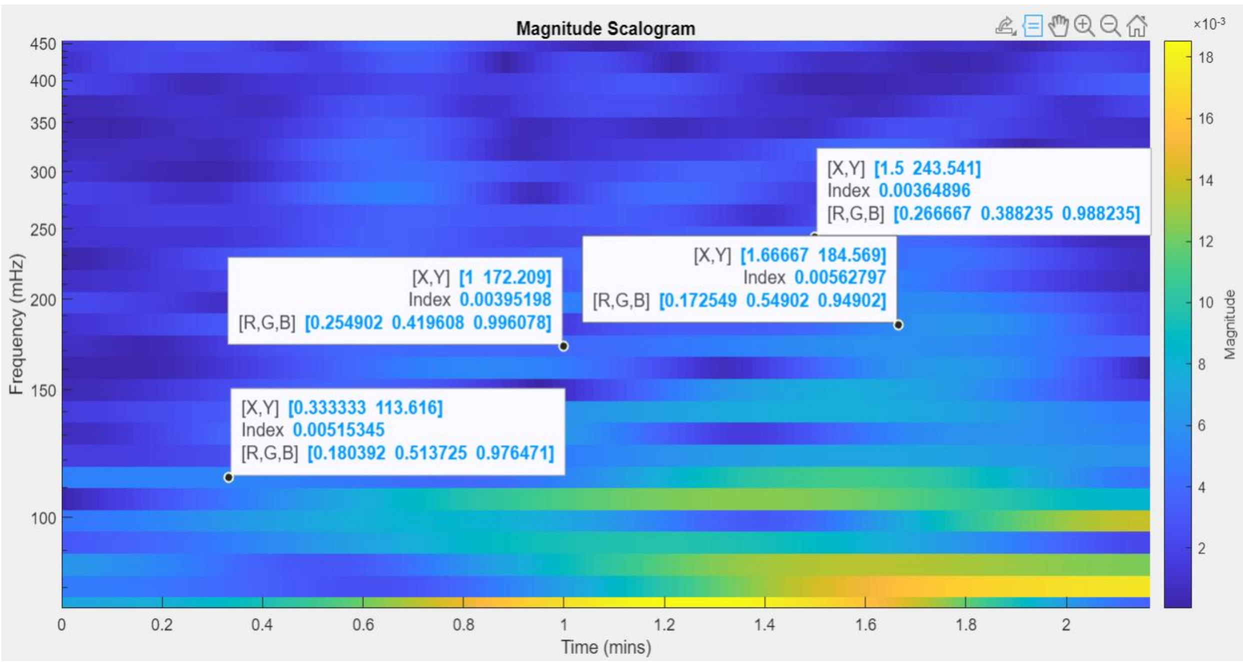


**Figure 8**. Magnitude scalogram

**Table 13.** Best performing classification models in method F – training accuracy

| Classification Model | Training | | Training Accuracy |
|---|---|---|---|
| | Indonesia | Madagascar | |
| Cubic SVM | 20/20 | 20/20 | 100% |
| Coarse Gaussian SVM | 20/20 | 20/20 | 100% |
| Fine KNN | 20/20 | 20/20 | 100% |
| Weighted KNN | 20/20 | 20/20 | 100% |
| Bagged Trees | 20/20 | 20/20 | 100% |
| Subspace KNN | 20/20 | 20/20 | 100% |
| Narrow Neural Network | 20/20 | 20/20 | 100% |
| Medium Neural Network | 20/20 | 20/20 | 100% |
| Wide Neural Network | 20/20 | 20/20 | 100% |
| Bilayer Neural Network | 20/20 | 20/20 | 100% |
| Trilayer Neural Network | 20/20 | 20/20 | 100% |
| SVM Kernel | 20/20 | 20/20 | 100% |
| Logistic Regression Kernel | 20/20 | 20/20 | 100% |

**Table 14.** Best performing classification models in method F – validation accuracy

| Classification Model | Validation | | Validation Accuracy |
|---|---|---|---|
| | Indonesia | Madagascar | |
| Wide Neural Network | 7/10 | 6/10 | 65% |
| Bilayer Neural Network | 7/10 | 7/10 | 70% |
| Trilayer Neural Network | 6/10 | 7/10 | 65% |
| SVM Kernel | 6/10 | 7/10 | 65% |
| Logistic Regression Kernel | 6/10 | 7/10 | 65% |

## 4. Conclusion

Based on the aforementioned discoveries, it is apparent that Method A, which employs single-stage multi-class machine learning to differentiate between grades and countries, achieves a training dataset accuracy of 100% and a validation dataset accuracy of 60%. Meanwhile, Method B, utilizing multi-stage two-class machine learning, demonstrates a training dataset accuracy of 100%, with validation accuracies of 95%, 73.33%, and 80% for Stages 1, 2, and 3, respectively. Furthermore, Method D, which also employs multi-stage two-class machine learning but focuses on Indonesia Grade A as Stage 2, indicates that the Medium Neural Network yields the optimal classification model, achieving validation accuracies of 80% and 60% for Stages 1 and 2, respectively, albeit Stage 3 yielding unsatisfactory results. Additionally, Method E, similar to Method A but aimed at distinguishing samples between countries, yields satisfactory outcomes, particularly with the Weighted KNN model achieving 100% for training and 80% for validation. Lastly, Method F, utilizing the wavelet time-frequency analyzer, demonstrates a training accuracy of 100% and a validation accuracy of 70% for the bilayer neural network. In summary, it is evident that Method E produces the most favorable results for the samples.

### Ethical issue

The authors are aware of and comply with best practices in publication ethics, specifically with regard to authorship (avoidance of guest authorship), dual submission, manipulation of figures, competing interests, and compliance with policies on research ethics. The authors adhere to publication requirements that the submitted work is original and has not been published elsewhere.

**Data availability statement**
The datasets analyzed during the current study are available and can be given upon reasonable request from the corresponding author.

**Conflict of interest**
The authors declare no potential conflict of interest.

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