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Advanced Mineralogical Classification and Concentration

Estimation in Mining with MATLAB-Powered Hyper-Spectral

Imaging and Machine Learning

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ABSTRACT

The study presents a new technique that combines hyperspectral imaging and machine learning to identify minerals. Overcoming the challenges of processing hyperspectral data, the solution offers a user-friendly hyperspectral analysis tool tailored for constructing datasets and enhancing mineral identification and concentration estimation. The tool integrates hyperspectral data processing with segmentation, simplifying complex operations and making mineral identification accessible to non-experts. The tool's capabilities extend to handling multi-spectral data efficiently, potentially leading to energy-efficient analysis when combined with dimensionality reduction techniques. Presented as a novel approach, it improves geological surveys in mining areas, enabling industrial applications and mineral research.

Keywords: Hyperspectral Imaging, MATLAB, Spectroscopy, Mineral Processing

List of Abbreviations

ROI - Regions of Interest
App- Application
SVM- Support Vector Machine
CNN- Convolutional Neural Network
UI- User Interface

1. Introduction

The technique of material mapping known as hyperspectral imaging has long been employed in both aerial and spaceborne platforms for environmental investigations, change detection, and mapping of minerals and plants [1]. Exploration and sorting of minerals have shown progress with the introduction of hyperspectral imaging. According to Bauer [2], the method can be applied to the sorting of minerals; nevertheless, additional investigation is required to enhance the classification outcomes. Neville [3] discovered striking similarities in the unmixing of fraction images for specific minerals after comparing data from two aerial sensors. A thorough analysis of the application of hyperspectral imaging for mineral mapping was given by Sudharsan, who emphasized the significance of temporal, spectral, and spatial resolution[4]. The authors' previous study on Mineral Processing suggested that mineral species have unique spectral waveforms by using hyperspectral imaging [5]. These studies demonstrate how useful hyperspectral imaging can be for mineral discovery and investigation.

However, there are several difficulties associated with hyperspectral image analysis, such as frequent requirements for calibration, redundant data, and large data volumes [6]. Hyperspectral images are large, difficult to transmit and restore, and require expert analysis due to their distinctive properties [7]. Because of the limited spatial resolution and abundance of information, target recognition in hyperspectral images is challenging [8]. The special qualities of hyperspectral data, namely its high dimensionality and limited ground truth, increase the complexity of analyzing this data [9]. Additionally, aspects such as spectral mixing, degradation mechanisms, and limited spatial resolution further complicate hyperspectral data processing [10]. Despite these obstacles, hyperspectral target identification has a wide range of possible applications, which emphasizes the need for further studies in mining applications [11]. A number of these issues have been resolved by recent developments in deep learning, especially in the fields of transfer learning for multi-source image analysis, unsupervised, semi-supervised, and active learning techniques [12] which require expert analysis.

In the mining industry, hyperspectral image analysis, while with great potential, lacks immediacy and usability due to the above-mentioned challenges. This research thus presents a hyperspectral image analysis tool that could aid in addressing the aforementioned issues and simplify their processing:

(1) Simple dataset creation for machine learning applications:

•Regions of Interest (ROIs) on loaded hyperspectral pictures can be selected to enable interactive labeling, making dataset generation simple.

•This tool makes it easy to label hyperspectral photos, which have a larger data volume than regular RGB images, a task that was previously demanding.

(2) Machine learning processing:

•The MATLAB Machine Learning App is integrated to perform 34 different types of machine learning processing, such as Decision tree, Support Vector Machine (SVM), and other techniques.

•Numerous machine learning strategies can be compared in classification and regression tasks via the combination of deep learning techniques such as Convolutional Neural Networks (CNN), and MATLAB Classification learner and Regression learner. This has made button-driven, and user-friendly UI interactive machine learning processing possible, eliminating the need for specialized experience.

(3) Mineral species identification and concentration estimation:

•A robust system has been developed to aid mining operators in the identification of mineral species and calculation of mineral concentrations by combining the procedures described in (1) and (2).

(4) Band selection for multispectral data processing:

•Although hyperspectral images have a high spectral resolution, there are drawbacks, including the requirement for costly hyperspectral cameras, redundancy, and enormous data volumes.

•In order to address these, this program allows users to select specific wavelengths to construct multispectral data from loaded hyperspectral data. This in principle, allows for the processing of multispectral data, this includes segmentation, machine learning, and dataset construction.

(5) Visualization via Segmentation:

•Segmentation allows for the visualization of the minerals present in examined mineral samples as well as their concentration levels.

2. Tool description

Dealing with the large dimensionality and multitudes of information in hyperspectral image processing poses a significant challenge [13]. Due to its intricacy, machine learning which is good at processing complex data and the creation of user-friendly tools are needed developments [14]. The tool allows users to (1) build and label data sets for machine learning, (2) perform machine learning (classification and regression), (3) compare machine learning performances, and (4) perform segmentation. This tool assists in processing advanced hyperspectral images with a simple button operation that does not require specialized expertise. More specifically, it can determine mineral species and estimate mineral concentrations without tedious complicated processing. A case study using this tool is included in Chapter 3, Experiment and analysis.

2.1. Operating procedure

Figure 1 shows a flowchart for constructing a dataset for performing machine learning from hyperspectral data, as well as segmentation of the test data. The flowchart shown in Figure 1 can operated with a simple button press after the script is executed. The flowchart description is provided below:

Firstly, when the script is executed, a screen for selecting hyperspectral data to be used for training via machine learning is displayed, and the user selects the data. This operation progresses until the user presses the cancel button, allowing multiple hyperspectral data to be loaded. Next, pre-process the loaded data. The tool selects the wavelength region to be used and defines the mean filter region for the acquired spectral data when selecting the ROI. Although the acquired hyperspectral data may contain noise, the quality of the data can be further improved by combining various noise reduction techniques that have been proposed such as averaging. After pre-processing the imported hyperspectral data, a dialog box will appear requiring the user to process either a hyperspectral or multispectral image. For the case where the user selects a multispectral image, multispectral data will be constructed from the input bands only, the same flow of events is seen for the case where hyperspectral is selected. Thereafter, the user is permitted to choose the machine learning task they wish to perform based on classification or regression as prompted by a dialog. Selecting the classification task will automatically drive toward the identification of mineral species while selecting the regression task will automatically drive toward the estimation of mineral concentrations. The ROI selection screen for creating the training data set is displayed after selecting a machine learning task. This operation completes the labeling of the dataset for machine learning. Once the dataset is built, the user can thus select the machine learning algorithm, either CNN or machine learning. When CNN is selected, the analysis is

126 automatically performed using CNN, and the progress of the model training and validation can be monitored via the
127 learning curve. Hyperparameters can also be easily modified. When machine learning is selected, the MATLAB
128 Classification Learner App is automatically launched for Classification, and the MATLAB Regression Learner App
129 is automatically launched for the case of Regression likewise. Once launched, interactive instructions can be
130 followed, allowing for machine learning hyperparameter tuning. Each app can run multiple machine learning tasks
131 at a given time, allowing the user to pinpoint the best machine learning model. The user then selects a trained model,
132 outputs it to the workspace, and moves on to the next operation. As a final operation, segmentation can be
133 performed in both the Classification and Regression tasks on test data, this being data that has not been used for
134 training the model. Performing this operation provides the user with graphical information that aids in the analysis
135 of results. As indicated above, this system can provide useful support for the analysis of minerals using
136 hyperspectral data by miners without the need for specialists. The visual representation of the execution screen is
137 shown in Figure 2.

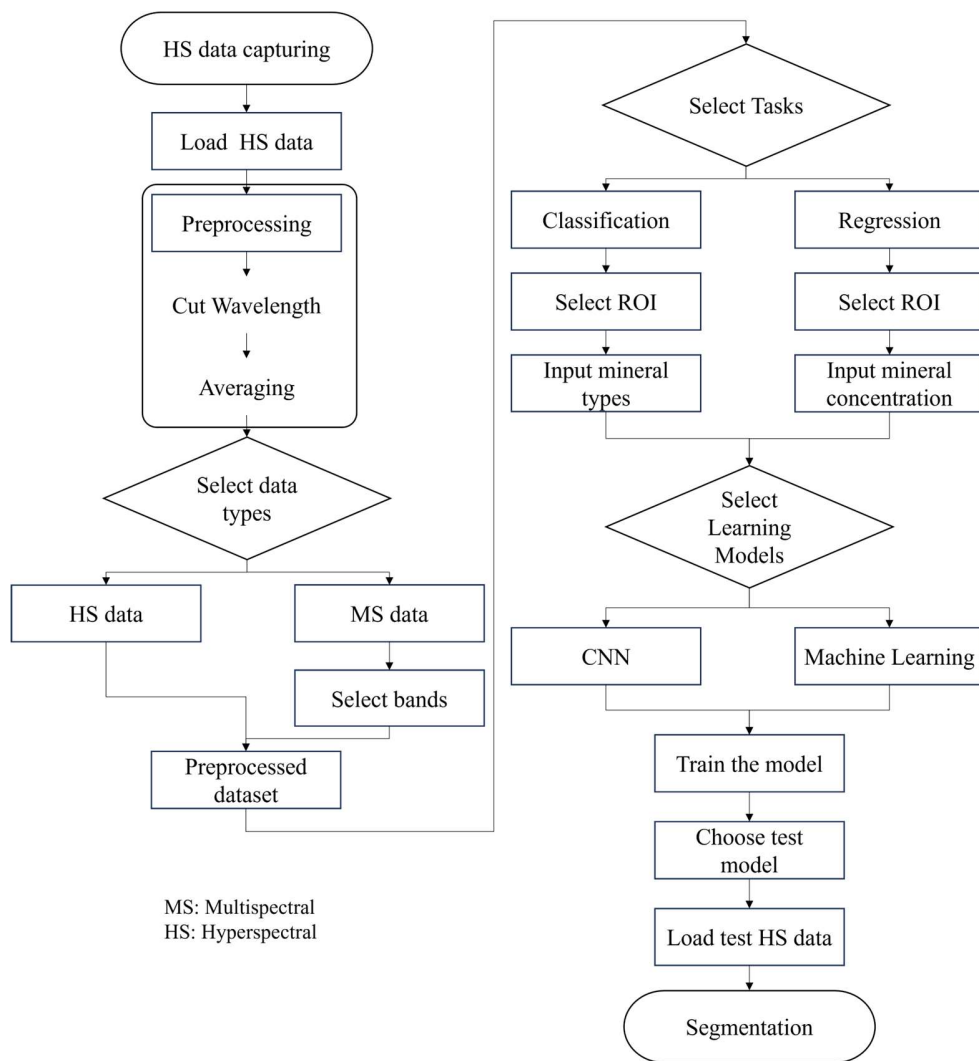


Figure 1 Flowchart of the tool.

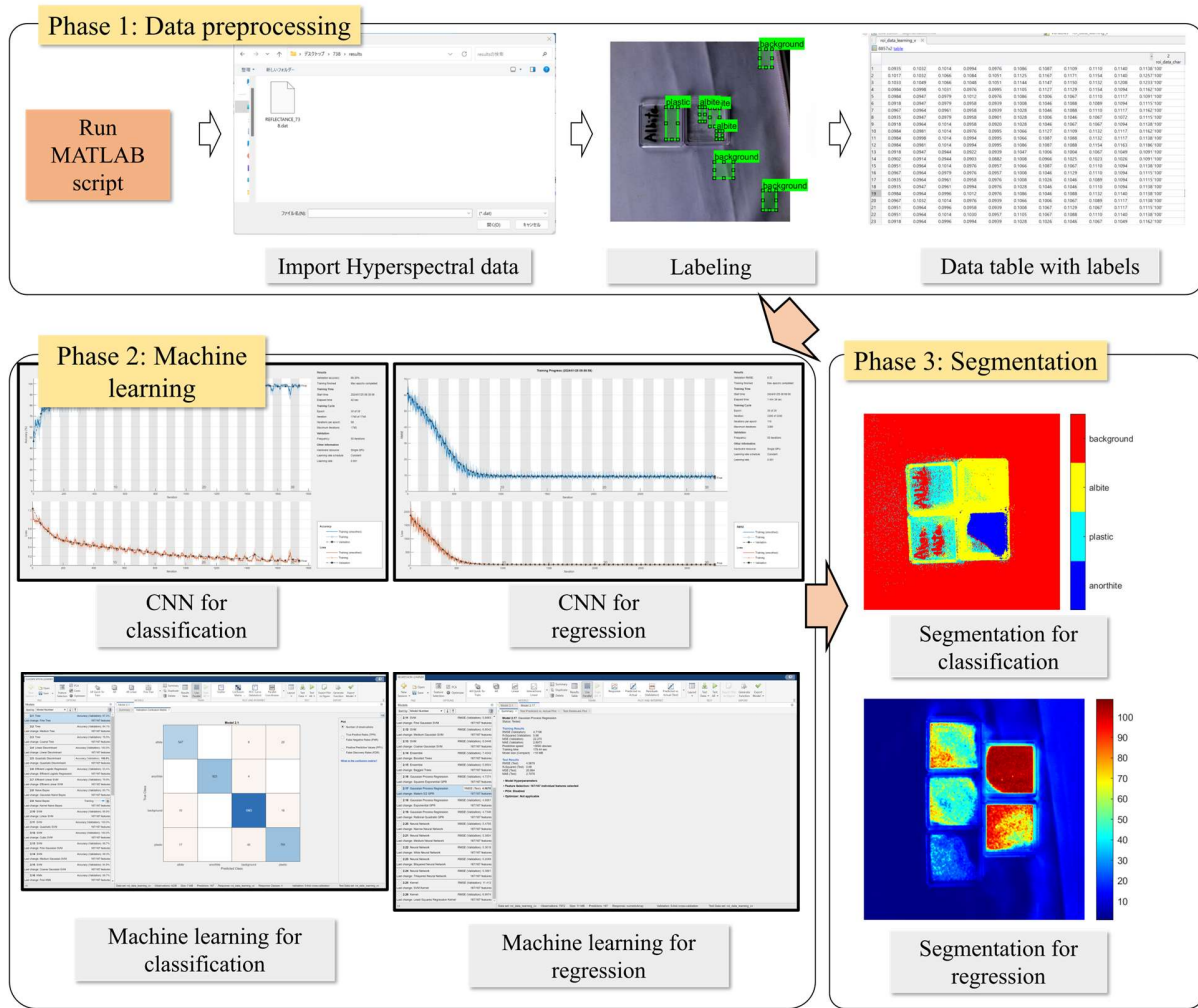


Figure 2 ROI selection and labeling using proposed tool.

2.2. Software specifications and tool functionalities

The tool was self-developed using MATLAB R2023a, thus its application with previous versions has not been validated for compatibility. Noteworthy toolboxes integrated into the development include Computer Vision Toolbox, Deep Learning Toolbox, Image Processing Toolbox, Parallel Computing Toolbox, and the Statistics and Machine Learning Toolbox. Given the substantial computational demands inherent in its operations, one must employ a processing machine equipped with a high-performance Graphics Processing Unit (GPU) for optimal performance.

The tool facilitates the loading of hyperspectral data, establishes a machine-learning-ready dataset, conducts machine learning procedures, and subsequently conveys the results visually through segmentation. This entire

workflow is executed seamlessly with a single button press, eliminating the necessity for expert intervention. The machine learning process is firmly integrated with MATLAB's interactive tools, enhancing user efficiency and workflow optimization.

3. Experiment and analysis

3.1. Dataset descriptions

In pursuit of mineral species classification and the estimation of mineral concentrations, we prepared the following samples. For the classification task case study; type of mineral, two distinct samples were employed: pure albite ($\text{NaAlSi}_3\text{O}_8$) and pure anorthite ($\text{CaAl}_2\text{Si}_2\text{O}_8$). The challenge lies in their shared white color, rendering visual discrimination nearly impossible. The primary objective is to employ hyperspectral imaging to ascertain the ability to distinguish between these visually indistinguishable samples. Simultaneously, for the regression task, a series of powder samples were prepared and systematically adjusted in 20% increments of the mass ratio between ilmenite and albite ($\text{NaAlSi}_3\text{O}_8$). The sample was mixed by manually shaking the sample container. Regression analysis is used to estimate the mineral grade attributable to this careful preparation. The HS camera captured images of the sample in a darkroom environment, as depicted in Figure 3. The sample was illuminated from two directions using halogen lights to prevent shadows, and images were taken directly from above using the HS camera. The technical specifications of the camera are Spatial sampling is 512 pix and F/number is 1.7. The accompanying Table 1 provides meticulous documentation of the specific composition breakdown in terms of area percentage and offers a comprehensive insight into the composition differences throughout the powder samples that were created. The reason for adjusting for area ratio rather than weight ratio is that the segmentation results need to be evaluated areal. These powder samples size distribution are arranged 150-250 μm using a testing sieve. Wavelength of these samples are depicted in Figure 4 and Figure 5. Furthermore, we have employed this technique to study a number of other minerals, resulting in the publication of several papers reporting the outcomes of applying this method to a diverse range of minerals [5], [15]. These studies have validated the efficacy of our technique for a multitude of minerals.

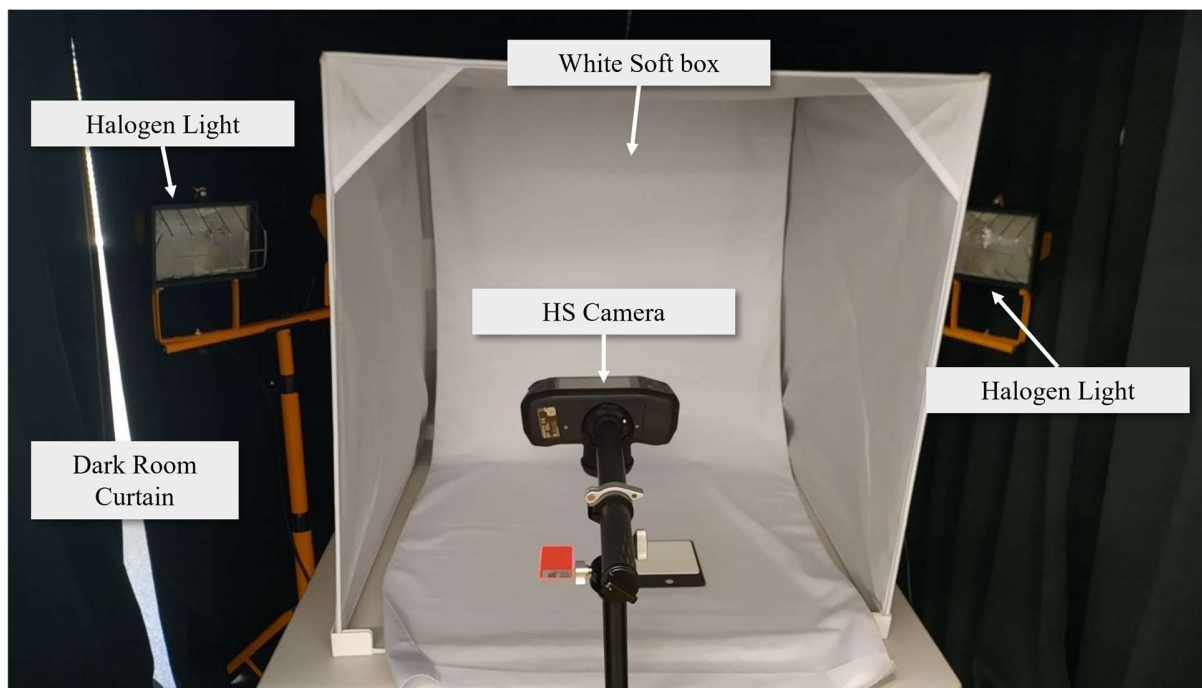


Figure 3 HS camera shooting environment.

Table 1 Area% of samples for regression task.

Ilmenite Area%	Ilmenite Weight(g)	Albite Weight(g)
0	0	0.698888
20	0.250746	0.55911
40	0.501491	0.419333
60	0.752237	0.279555
80	1.0022982	0.139778
100	1.253728	0

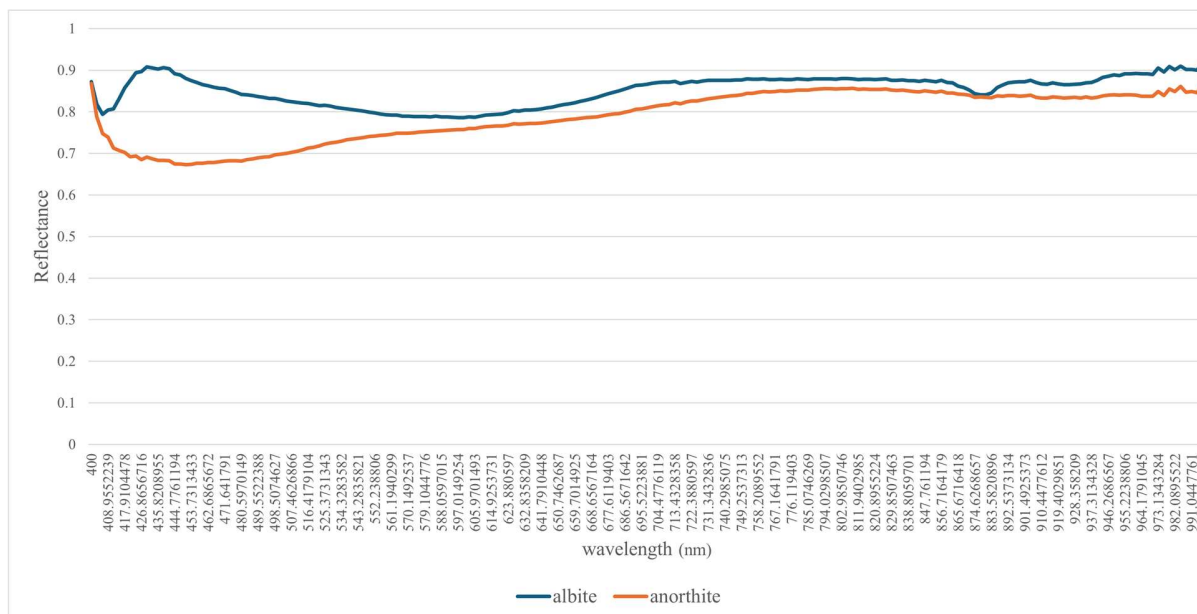


Figure 4 Average reflectance spectra of albite and anorthite.

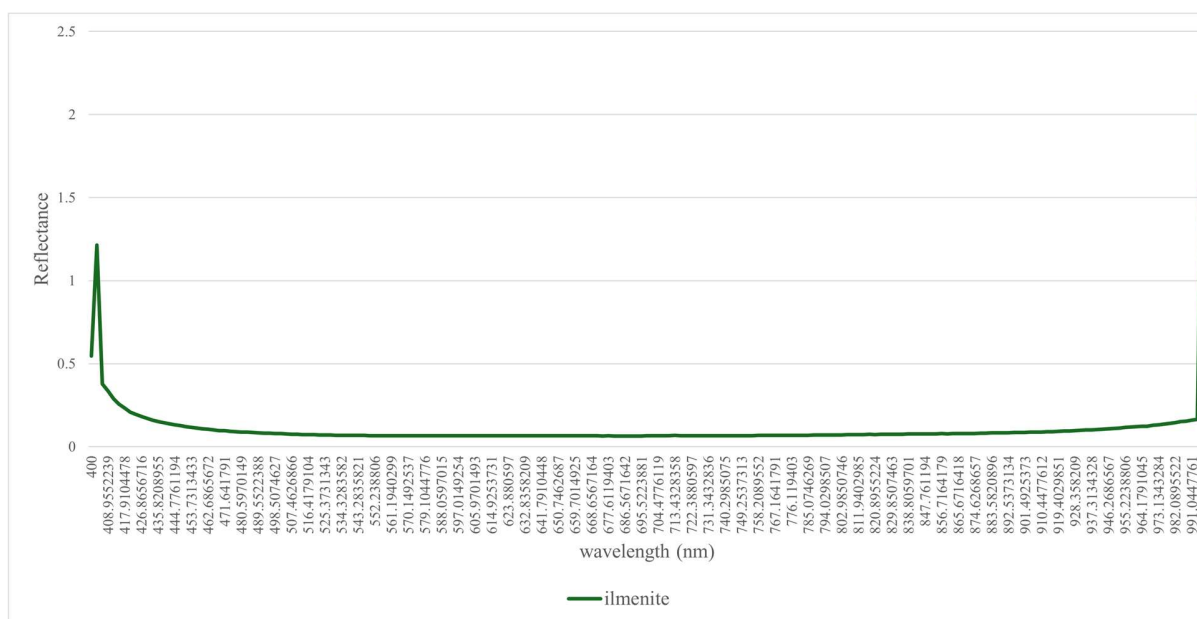


Figure 5 Average reflectance spectra of ilmenite.

3.2. Data pre-processing, data construction for machine learning

Numerous studies highlight the value of high-quality data in machine learning. Franchina and Khoshgoftaar emphasize the importance of having error-free data that is appropriate for analysis [16], [17]. Ding offers a unique

method for validating datasets to emphasize the significance of data quality for machine learning model accuracy [18]. Building on this, Feurer introduces a robust automated machine learning method that demonstrates its usefulness in a variety of applications by accounting for historical performance on similar datasets [19]. Together, these studies highlight how important reliable, high-quality data is for the success of machine learning.

As such, this tool can perform several simple processes to improve the quality of data.

(1) ROI Selection and labeling for learning data creation

Through the extraction and labeling of targeted segments within the loaded hyperspectral data, this tool possesses the capability to formulate a training dataset characterized by minimal noise, particularly suitable for diminutive entities such as minerals. Users can pseudo-display the loaded hyperspectral data in the form of an RGB image, as illustrated in Figure 2. This presentation facilitates the designation of any specific region as the ROI, enabling the construction of a pertinent training dataset. Notably, within this tool, the chosen ROI undergoes concurrent labeling throughout the selection procedure, thereby eliminating redundant steps within the workflow, hence establishing a seamless and efficient operational process. In its ultimate manifestation, the tool generates an output in the form of a table containing the extracted spectra from the designated ROI, complete with their corresponding label names which are used for machine learning.

(2) Averaging process in the xy-plane of the spectrum

The obtained hyperspectral data is comprised of wavelength data with spectral divisions exceeding 100 bandwidths along the z-axis (depth), in conjunction with two-dimensional planar data extending in the x and y directions (length and width). Within this dataset, the tool offers an averaging process, as depicted in Figure 6, wherein averaging occurs between adjacent pixels within the xy-plane. This computational operation serves to mitigate spectral irregularities, diminish noise, and enhance spatial uniformity.

Let D be the hyperspectral data of the region selected by the ROI, the size of D is $x * y * band$, and to average this to A , the data of $1 * 1 * band$, the following operation is performed for each band k .

$$A_k = \frac{1}{xy} \sum_{i=1}^x \sum_{j=1}^y D_{i,j,k}$$

And where $D_{i,j,k}$ is the value of the k th band for the (i,j) pixel in D . The values of all pixels in each band are then summed and divided by the number of pixels to obtain the average spectrum A .

$$A = (\frac{1}{xy} \sum_{i=1}^x \sum_{j=1}^y D_{i,j,1}, \frac{1}{xy} \sum_{i=1}^x \sum_{j=1}^y D_{i,j,2}, \dots, \frac{1}{xy} \sum_{i=1}^x \sum_{j=1}^y D_{i,j,band})$$

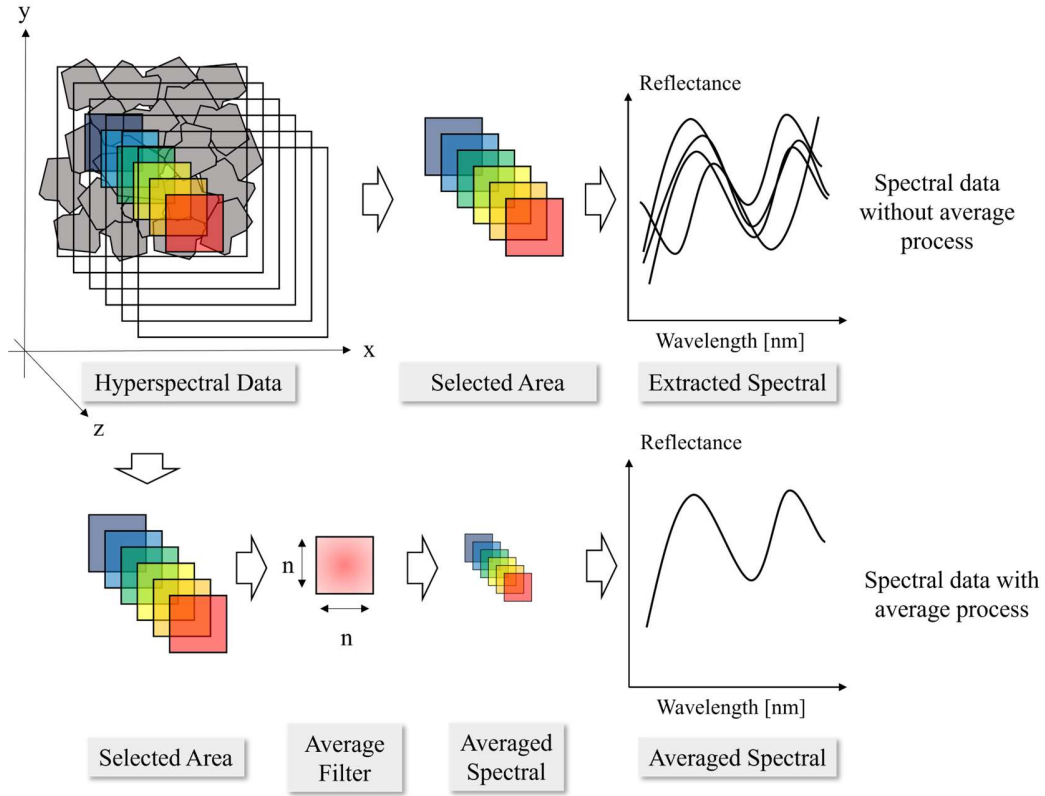


Figure 6 Schematic diagram of averaging of hyperspectral data.

3.3. Multispectral data processing

There is sufficient proof of the difficulties presented by the high dimensionality and large amount of hyperspectral data. Burger [24] and Mohan [20], [21] both emphasize the necessity of reducing the computing load; Burger focuses on data handling, while Mohan concentrates on image interpretation. Aranki [22] highlights data compression even more, especially when considering the processing chain. In his thorough analysis of hardware-accelerated compression techniques, Altamimi [23] emphasizes the significance of maintaining data quality even in the face of processing and storage constraints.

What these studies highlight is how important it is for hyperspectral imaging researchers to have effective data processing and compression methods. The reduction of the dimensionality of hyperspectral data, which typically

consists of hundreds of wavelength bands, to that of multispectral data, characterized by tens of wavelength bands, holds the potential for substantial reductions in both computational resources and economic costs. Other common methods for dimensionality reduction of hyperspectral data include UMAP and PCA [24], [25]. However, since they summarize the data into several dimensions, they are unable to perform wavelength selection. Nevertheless, they are effective in reducing the computational load, and therefore, UMAP and PCA are not used in this tool. Especially in the case of minerals where the wavelength band required for identification is limited according to a previous study by Sinaice et al [26]. Through the utilization of this tool, data processing has been achievable solely through the wavelengths designated by the user. Various methods for the dimensionality reduction of hyperspectral data have been proposed, and integrating this technique into this tool facilitates the processing of multispectral data composed of user-desired wavelength bands. Upon executing the program, an interactive dialog will prompt the user to select between processing hyperspectral data or multispectral data. Opting for multispectral data enables the processing of data with only the predetermined bands, as specified by the user.

3.4. Machine learning descriptions

After hyperspectral data ROI selection and labeling by the user, machine learning is then performed using the created data table. These operations are performed seamlessly. The tool proposed in this paper uses a 1D-CNN model developed by the authors, and the machine learning model embedded in MATLAB's Classification Learner App and Regression Learner App. A description of their architecture is given below.

3.4.1. 1D-CNN

A 1D CNN was viable for this tool since the spectral data handled by this tool is 1D data, making a low-cost implementation possible. The 1D architecture for the classification task is shown in Table 2. The initial layer serves as the input layer, allowing for the initiation of 1-dimensional sequence data. Subsequently, convolutional layers follow suit. In Conv1, 32 convolutions of size 10 are performed with a stride of 1 and padding set to 'same'. Let the input signal x be of length n and the convolution kernel w be of length k . Furthermore, if the stride is s and the bias is b , the i -th element of the output y is computed as

$$y_i = \sum_{j=0}^{k-1} w_j x_{i:s+j} + b$$

Batch normalization and ReLU activation functions are applied to the output of Conv1. Conv2, the subsequent layer, conducts 64 convolutions of size 10 with the same stride and padding configuration. Batch normalization and ReLU activation follow Conv2. Letting z be the output of ReLU, the formula is shown below.

$$z_i = \text{ReLU}(y_i) = \max(0, y_i)$$

Then, in the pooling layer, the Max pooling process is performed, and p is output.

$$p_i = \max_{j=0, \dots, k-1} z_{i:s+j}$$

The model then employs a 1-dimensional global average pooling layer, leading to a final output layer consisting of two fully connected layers. The output of fully connected layers is shown below. Here W is weight of fully connected layer and b is bias.

$$\sigma_j = \text{activation}(\sum_i W_{ji} g_i + b_j)$$

The output layer applies a softmax activation function, and the model performs classification tasks using cross-entropy loss.

$$\hat{y}_j = \frac{\exp(o_j)}{\sum_k \exp(o_k)}$$

The regression task, as shown in Table 3, adopted the same architecture except for the last layer.

280

281 **Table 2 1D CNN architecture for classification task.**

Name	Descriptions	Type
InputLayer	Sequence input with 1 dimension	Sequence Input
Conv1	32 10 convolutions with stride 1 and padding 'same'	1-D Convolution
BN1	Batch normalization	Batch normalization
ReLU1	ReLU	ReLU
Conv2	64 10 convolutions with stride 1 and padding 'same'	1-D Convolution
BN2	Batch normalization	Batch normalization
ReLU2	ReLU	ReLU
GlobalAvgPool	1-D global average pooling	1-D global average pooling
OutputLayer	2 fully connected layer	Fully Connected
Softmax	Softmax	Softmax
ClassOutput	crossentropyex	Classification Output

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285 **Table 3 1D CNN architecture for regression task.**

Name	Descriptions	Type
InputLayer	Sequence input with 1 dimension	Sequence Input
Conv1	32 10 convolutions with stride 1 and padding 'same'	1-D Convolution
BN1	Batch normalization	Batch normalization
ReLU1	ReLU	ReLU
Conv2	64 10 convolutions with stride 1 and padding 'same'	1-D Convolution
BN2	Batch normalization	Batch normalization
ReLU2	ReLU	ReLU
GlobalAvgPool	1-D global average pooling	1-D global average pooling
OutputLayer	2 fully connected layer	Fully Connected
RegressionOutput	Mean-squared-error	Regression Output

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288 3.4.2. MATLAB Classification Learner App and Regression Learner App

289 MATLAB Classification Learner App and Regression Learner App (MATLAB R2023b) are equipped with machine
290 learning models listed in Table 4 and Table 5. The model type may differ depending on the version. By integrating
291 with the proposed tool, the constructed training data can be analyzed seamlessly. High-speed computation is made
292 possible by the ability to compute numerous machine learning models simultaneously when the Parallel Computing
293 Toolbox is utilized. The capacity to handle data in parallel greatly improves the overall computing workflow's
294 efficiency. A noteworthy aspect is the freedom users have in choosing training models, which enables the extraction
295 and training of certain models that are best suited for the given task. The smooth interaction with the MATLAB
296 environment is a significant advantage. This feature makes it possible for learned models to be relatively easy to
297 produce, which allows for further segmentation procedures that are covered in the section that follows. Users can
298 apply segmentation by simply exporting the trained models to the MATLAB workspace. This simplifies the entire
299 analytical pipeline and promotes a unified workflow in the deployment of machine learning models. Detailed
300 operating procedures are shown in the next and subsequent sections.

Table 4 Machine learning models in MATLAB Classification Learner App.

Name	Name	Name	Name	Name
Fine Tree	Gaussian Naïve Bayes	Coarse Gaussian SVM	Boosted Trees	Wide Neural Network
Medium Tree	Kernel Naïve Bayes	Fine KNN	Bagged Trees	Bilayered Neural Network
Coarse Tree	Linear SVM	Medium KNN	Subspace Discriminant	Trilayered Neural Network
Linear Discriminant	Quadratic SVM	Coarse KNN	Subspace KNN	SVM Kernel
Quadratic Discriminant	Cubic SVM	Cosine KNN	RUSBoosted Trees	Logistic Regression Kernel
Binary GLM	Fine Gaussian SVM	Cubic KNN	Narrow Neural Network	
Logistic Regression				
Efficient Linear SVM	Medium Gaussian SVM	Weighted KNN	Medium Neural Network	

305

306 **Table 5 Machine learning models in MATLAB Regression Learner App.**

Name	Name	Name	Name	Name
Linear Regression	Coarse Tree	Coarse Gaussian	Rational Quadratic	SVM Kernel
		SVM	GPR	
Interactions Linear	Linear SVM	Boosted Trees	Narrow Neural	Least Squares
			Network	Regression Kernel
Robust Linear	Quadratic SVM	Bagged Trees	Medium Neural	
			Network	
Stepwise Linear	Cubic SVM	Squared	Wide Neural	
		Exponential GPR	Network	
Fine Tree	Fine Gaussian SVM	Matern 5/2 GPR	Bilayered Neural	
			Network	
Medium Tree	Medium Gaussian	Exponential GPR	Trilayered Neural	
	SVM		Network	

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3.5. Visualization and segmentation

The trained model was trained using user-generated training data as described in the previous section. The trained model is then used to perform analysis based on test data that was not used for training. The procedural sequence unfolds with the execution of a MATLAB script, initiating the loading interface for hyperspectral data. Upon user selection and loading of the designated test dataset, the analysis process seamlessly progresses to its inference. Meticulous attention to detail is imperative, ensuring that the loaded test data aligns with the dimensions of the data previously employed for training.

3.5.1. Segmentation results for classification task

Table 6 presents the outcomes of the validation of the machine learning model for segmentation. A total of 4239 spectral data were utilized for training, while an additional 470 were reserved for validation purposes. The data breakdown is as follows: 80% training data, 10% validation data, and 10% test data. The data was classified using cross-validation on the same data set. As shown in Table 6, the highest performance was achieved with Quadratic Discriminant, which classified the validation data with 100% accuracy. It is crucial to recognize that choosing the right model parameters can have a big impact on how well training goes. Users are recommended to carefully tweak hyperparameters in their pursuit of the best machine learning model for segmentation. To ensure the best possible performance that meets their unique needs, this procedure is essential. The training duration for the Quadratic Discriminant model was approximately 5 seconds. However, it's interesting to note that other models were also being trained at the same time as this one. Figure 7 presents the results of the test conducted using the MATLAB Classification Learner. Given that the test dataset is derived from the same source as the training dataset, the data exhibits greater consistency, which in turn leads to enhanced model accuracy. Furthermore, the similarity of the data distribution to the training data set contributes to the high performance of the model. It should be noted that the test data is not used for any training purposes and is not referenced as training data. The results of using the Quadratic Discriminant model to evaluate test data that had not been utilized before are displayed in Figure 8. The pseudo-
RGB picture obtained from the hyperspectral image is shown in the upper left figure; the segmentation result is shown in the upper right figure; the Ground Truth is shown in the bottom left figure; and the absolute difference between the segmentation result and the Ground Truth is shown in the lower right figure. It can be seen that the hues magenta or green visibly depict the amount of difference between the two photos in Figure 8's lower right panel. The

findings show that plastic containers have a lower discrimination performance because of their transparency, which causes them to blend in with the backdrop color. For albite and anorthite, on the other hand, the model shows accurate categorization skills. The hue of the difference in magnitude is either green or magenta. Figure 9 shows a histogram of the number of pixels in each class. In addition, Table 7 presents the segmentation results evaluation, indicating an 85% accuracy rate per pixel. When plastic container and background misclassifications are taken out of the equation, this accuracy supports the tool's effectiveness in mineral detection. These results highlight the model's potential for categorizing samples that are difficult for humans to visually identify. The idea of augmenting training data to improve segmentation accuracy points to potential directions for future improvements in the classification problem.

Table 6 Machine learning models accuracy for validation data.

Model Type	Accuracy %	Model Type	Accuracy %
CNN	98.3	Medium KNN	99.0
Fine Tree	97.3	Coarse KNN	92.9
Medium Tree	94.1	Cosine KNN	99.3
Coarse Tree	76.5	Cubic KNN	99.2
Linear Discriminant	100.0	Weighted KNN	99.3
Quadratic Discriminant	100.0	Boosted Trees	97.6
Efficient Logistic Regression	53.4	Bagged Trees	98.6
Efficient Linear SVM	79.9	Subspace Discriminant	99.9
Gaussian Naïve Bayes	65.7	Subspace KNN	99.7
Kernel Naïve Bayes	66.6	RUSBoosted Trees	95.8
Linear SVM	99.9	Narrow Neural Network	100.0
Quadratic SVM	100.0	Medium Neural Network	99.8
Cubic SVM	100.0	Wide Neural Network	99.8
Fine Gaussian SVM	99.7	Bilayered Neural Network	99.9
Medium Gaussian SVM	99.3	Trilayered Neural Network	99.9
Coarse Gaussian SVM	94.8	SVM Kernel	99.8
Fine KNN	99.7	Logistic Regression Kernel	98.7

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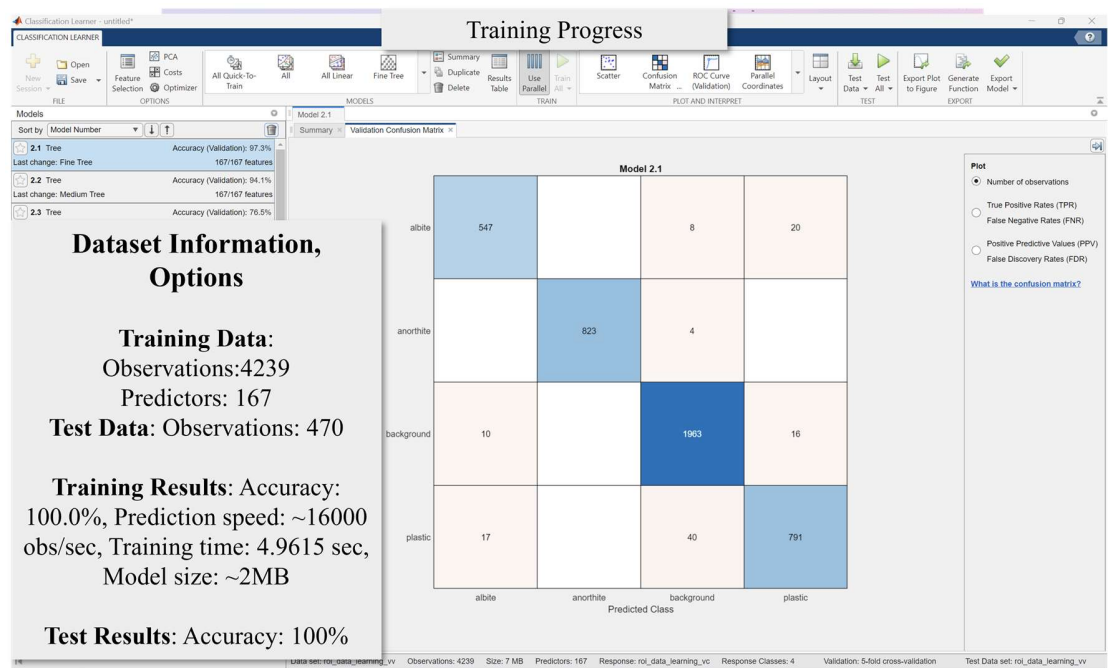


Figure 7 Training progress of machine learnings for classification analysis.

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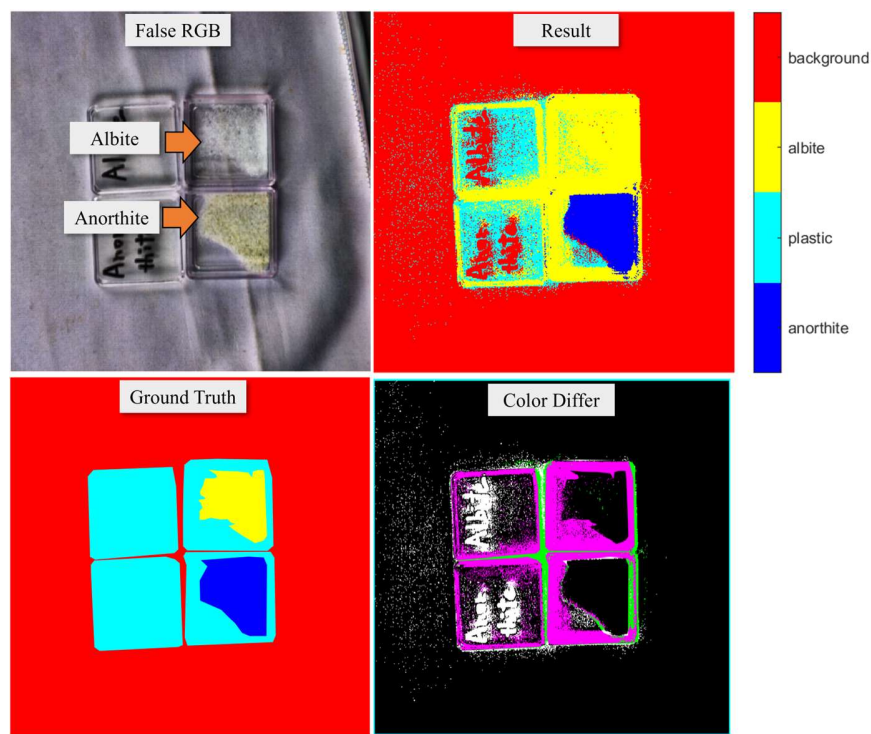


Figure 8 Segmentation result using “Quadratic Discriminant” from Machine Learning App.

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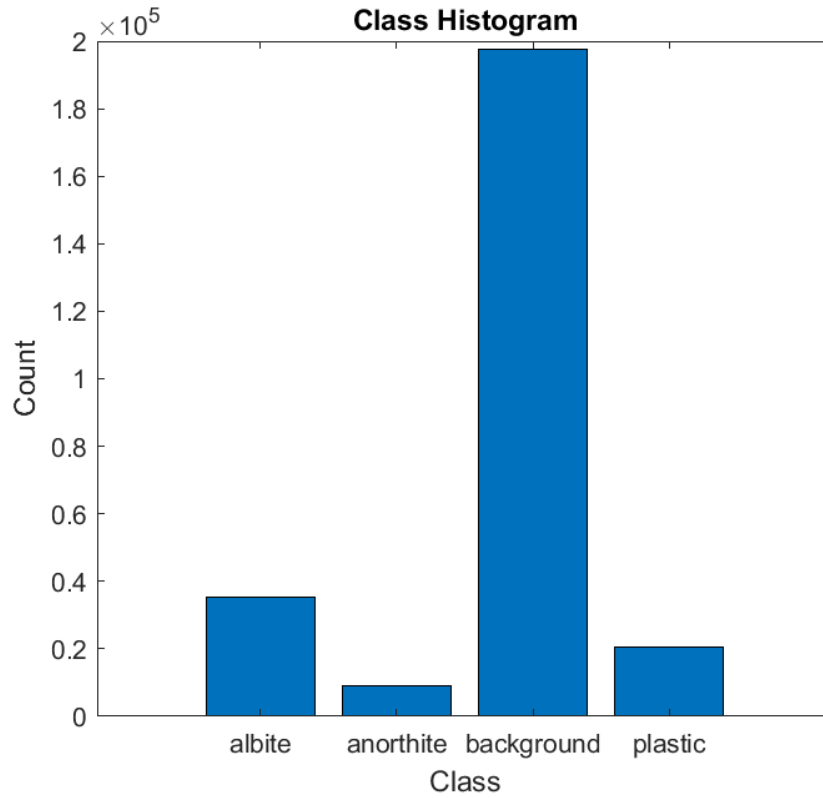


Figure 9 Histogram for machine learning results.

Table 7 Evaluation results.

Evaluation method	Value
Average difference	30.616
Total difference	26486154
Per-pixel accuracy rate	85.0185 %
Average absolute error	30.616
Structural Similarity Index (SSIM)	0.75694

Depending on the characteristics of the data to be load, overlearning may occur, and these must be addressed. In the case of this experiment, 100% classification accuracy was obtained for some of the models. It is thought that the accuracy was high because the learning data and test data originated from the same data, but the possibility of overlearning is also possible. Therefore, for the Quadratic Discriminant (QDA) method, which showed the highest performance, a scatter plot for each band is shown to estimate the degree of difficulty of classification. We used

Minimum Redundancy Maximum Relevance (MRMR) to extract the 5 most informative combinations and visualize their scatter plots. The MRMR allows us to extract feature sets that are maximally dissimilar to each other [27] and showed in Figure 10. The horizontal axis shows the Importance score and the vertical axis shows the Features. The top five bands with the highest information content (bands 1, 144, 10, 3, and 51) were extracted. For each of the five extracted bands, a scatter plot was created with each band on the vertical and horizontal axes. As shown in Figure 11, the bands are classified as clusters even if only two axes are taken, and the high performance values exhibited by QDA in the experiment using this sample can be attributed to the interpretability of this data.

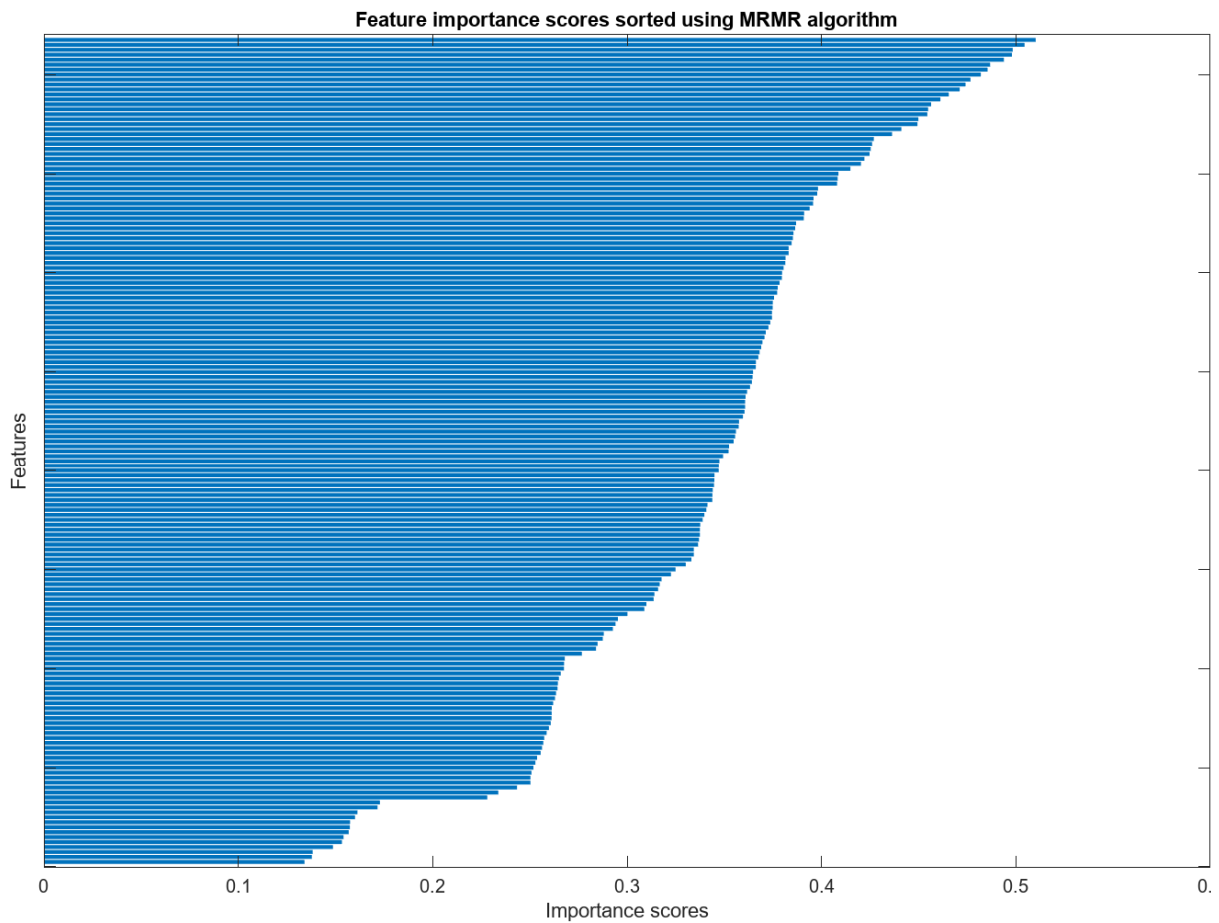


Figure 10 MRMR results.

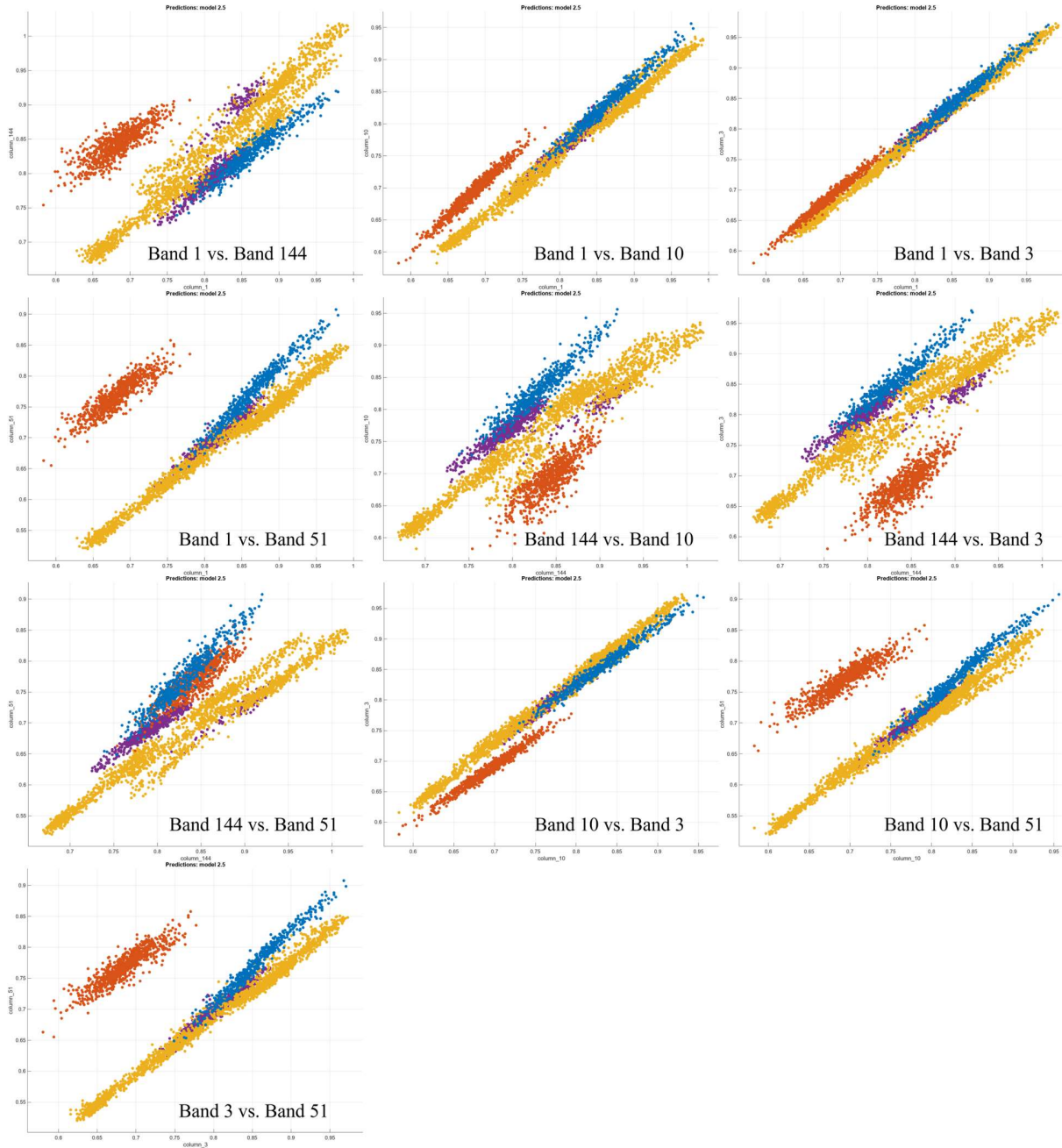


Figure 11 Scatter plots using bands extracted using MRMR analysis.

In addition, the high performance values of machine learning may depend on the parameter values of the network. Therefore, we again trained the network under different conditions and compared the results. Shown in Figure 12 are the values of the delta threshold and Gamma regularization parameters for QDA. Bayesian optimization was used to explore the optimal learning option. Figure 13 shows that while the highest performance is achieved at the 27th trial,

the accuracy is significantly degraded in the case of non-optimized conditions. Therefore, although some classification tasks show significantly higher performance and over-learning is suspected, it is necessary to consider that along with the possibility of over-learning, data interpretability and network parameter values also contribute to classification discrimination performance.

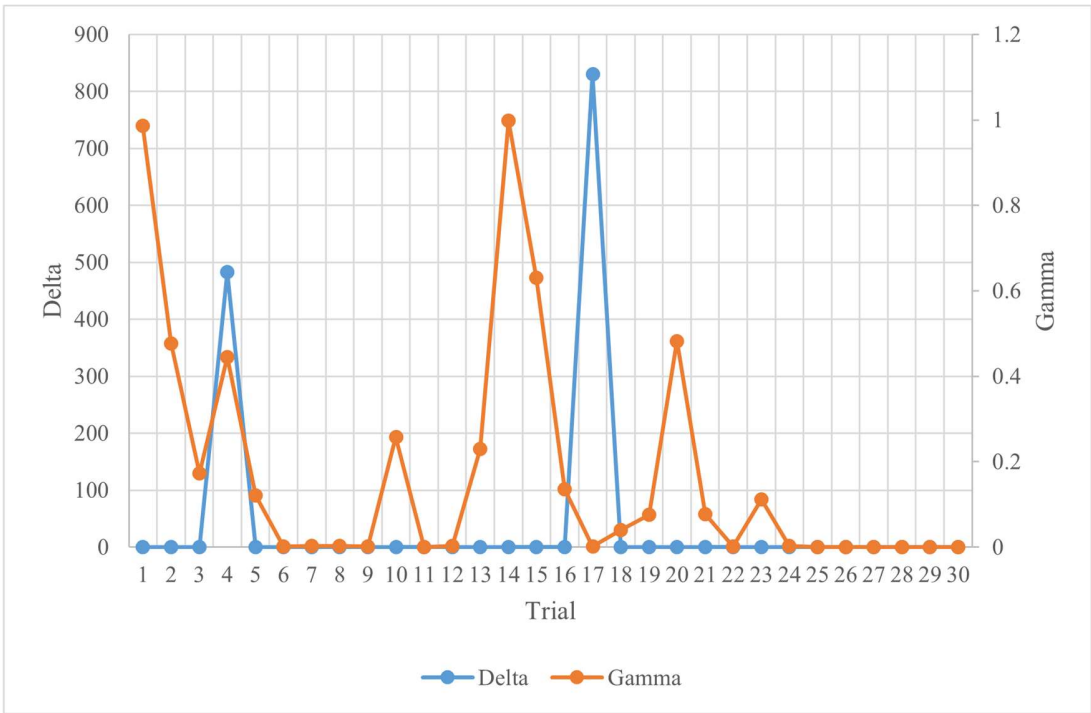


Figure 12 Parameters of QDA, Delta vs Gamma.



Figure 13 Validation accuracy and total cost of trials.

3.5.2. Segmentation results for regression task

ROI selection and numerical labeling were used in the creation of the training dataset for the regression problem, just like in the classification task. For the regression task in this case, the training set was particularly designed to include the concentration of ilmenite in samples that contained both albite and ilmenite. A training model that included the CNN listed in Table 8 was used to carry out regression training. The machine learning training is shown in Figure 14. Training of several machine learning models was performed in parallel. 7,972 training data and 885 validation data were used. Table 8 provides a summary of the training models' performance on the validation data. With a Root Mean Squared Error (RMSE) of 4.5678, post-training results show that Rational Quadratic Gaussian Process Regression (GPR) performs better than other training models. The Rational Quadratic GPR model was used to conduct the segmentation procedure by leveraging these outcomes. Figure 15 provides a visual representation of the segmentation results. The pseudo-RGB image is displayed in the upper left quadrant; the segmentation result is displayed in the upper right quadrant; the Ground Truth is presented in the bottom left quadrant; and the absolute difference between the segmentation result and the Ground Truth is displayed in the

lower right quadrant. It is important to understand that segmentation results are expressed as continuous values in the regression job, not as discrete values. In the regression task, the segmentation results are output as continuous values, not discrete values, so it is necessary to take into account that the color variation is also continuous. The segmentation is carried out with respect to the concentration of ilmenite, as shown by the segmentation result in Figure 15's upper right corner. Interestingly, it is found that the backdrop is almost correctly determined even though it is not explicitly present in the training data. These crucial findings imply that the suggested method has the potential to provide strong support for estimating ore grades. The link that has been seen between color representation and grade percentages suggests that this technique has the ability to offer precise and easily understood visual information about the grade of ilmenite samples. This feature puts the tool in a favorable position to simplify ore grade estimation, making it easier to use, more dependable, and easier to understand. Table 9 shows the evaluation values calculated from the segmentation results and the comparison with Ground Truth. The RMSE value is 58.0126, which is a guarantee of this tool's reliability.

410

411 **Table 8 Result of regression analysis using machine learning models.**

Model Type	RMSE	Model Type	RMSE
CNN	8.52		
Linear Regression	7.46	Boosted Trees	7.40
Interactions Linear	NaN	Bagged Trees	5.95
Robust Linear	7.48	Squared Exponential GPR	4.74
Stepwise Linear	NaN	Matern 5/2 GPR	4.72
Fine Tree	8.00	Exponential GPR	4.96
Medium Tree	7.34	Rational Quadratic GPR	4.73
Coarse Tree	7.15	Narrow Neural Network	5.48
Linear SVM	12.00	Medium Neural Network	5.38
Quadratic SVM	98.97	Wide Neural Network	5.36
Cubic SVM	51656.60	Bilayered Neural Network	5.21
Fine Gaussian SVM	5.86	Trilayered Neural Network	5.39
Medium Gaussian SVM	6.80	SVM Kernel	11.41
Coarse Gaussian SVM	8.04	Least Squares Regression Kernel	6.90

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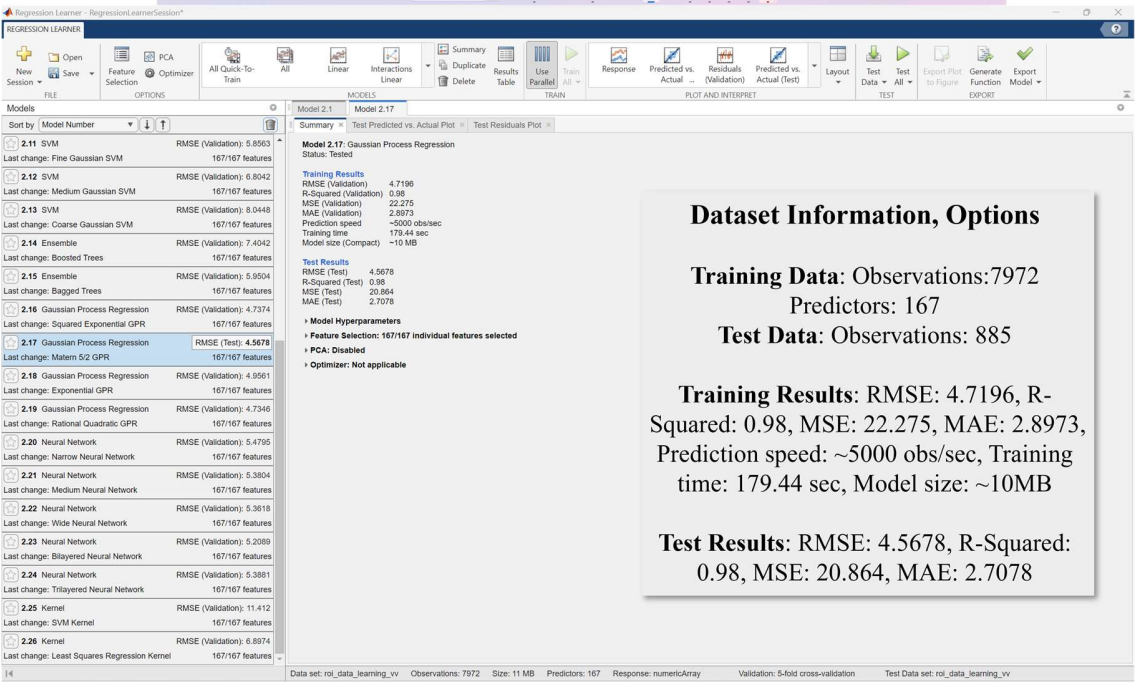


Figure 14 Machine learning process for regression analysis.

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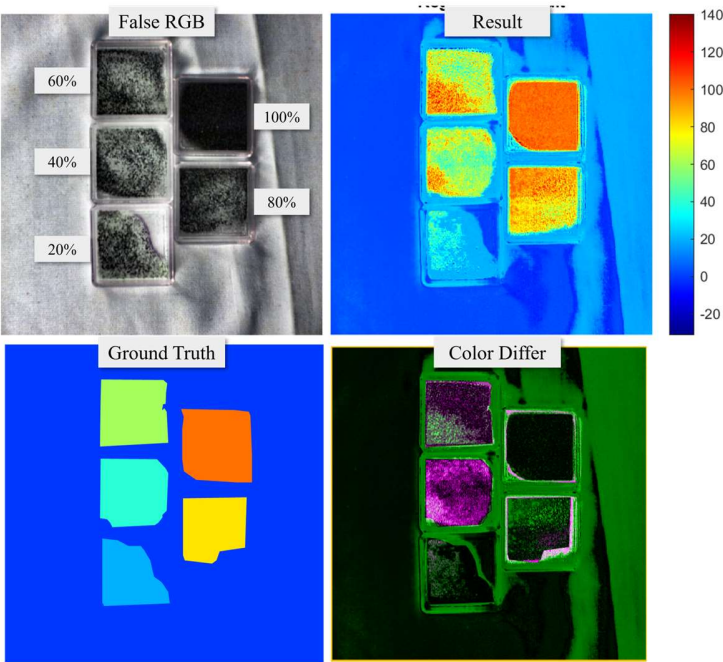


Figure 15 Segmentation result using “Rational Quadratic GPR” from Machine Learning App.

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Table 9 Evaluation results for machine learning.

Evaluation method	Value
Mean absolute error (MAE)	3365.457
Root Mean Square Error (RMSE)	58.0126
Peak signal-to-noise ratio (PSNR)	12.8604
Structural similarity index (SSIM)	0.85677

4. Limitations and future works

Although our proposed system for hyperspectral data analysis has made significant advancements, it currently lacks a satisfactory level of interactivity. Users must manually alternate between script files when using the application, which could hinder the smooth incorporation of the tool into the workflow of researchers and industry professionals. To overcome this constraint and enhance the tool's usefulness, future efforts will primarily concentrate on converting it into a fully operational program with a graphical user interface (GUI). This progression seeks to eliminate the necessity of manual script switching, offering a more intuitive and participatory experience for users. Concurrently, future efforts should prioritize improving the UI of the tool by integrating functions such as drag-and-drop capability, live visualization, and interactive feedback to enhance overall user-friendliness. In addition, the automation of typical workflows in identifying mineral species and estimating their concentrations, with the aim of enhancing the efficiency of the system continues to be a topic of investigation. To remain at the forefront of hyperspectral data analysis, future studies will use sophisticated machine learning algorithms and techniques. Additionally, they will actively solicit user feedback to continuously improve the analysis process based on practical experiences and increasing research needs. Meeting these demands, overcoming the highlighted constraint and ensuring the continued significance and efficiency of our tool in developing mineral-related research and industrial applications within the hyperspectral imaging field will require certain levels of continued development.

5. Conclusion

The MATLAB-based hyperspectral analysis tool proposed in this paper has facilitated the straightforward analysis of hyperspectral data, overcoming the complexities that were previously associated with such tasks. Furthermore, when combined with machine learning tools, this system not only remains user-friendly but also empowers non-experts to perform robust mineral identification without the need for expert intervention. In addition to its capability

for hyperspectral data analysis, the tool accommodates multi-spectral data, suggesting the potential for energy-efficient analysis that eliminates the need for extensive computational resources when coupled with the dimensionality reduction techniques proposed in other studies. The proposed tool stands as an innovative solution that significantly advances the informatization of geological surveys in mining fields, performing resource-efficient analysis and reducing the overall computational footprint.

6. CRediT authorship contribution statement

Natsuo Okada: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Software, Validation, Visualization, Writing – Original Draft.

Brian Bino Sinaice: Conceptualization, Data curation, Formal analysis, Software, Writing – review & editing.

Jaewon Kim: Conceptualization, Data curation, Formal analysis, Software.

Hiromasa Nozaki: Data curation, Formal analysis, Resources, Software, Validation.

Kaito Takizawa: Data curation, Formal analysis.

Narihiro Owada: Conceptualization, Investigation, Methodology, Writing – review & editing.

Yoko Ohtomo: Conceptualization, Resources, Supervision, Writing – Review & Editing.

Youhei Kawamura: Conceptualization, Methodology, Funding acquisition, Project administration, Supervision, Writing – Review & Editing.

7. Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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9. Data availability

Data will be made available on request.

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