



BAUXITE RESIDUES AS A SOURCE OF SPECTRAL SIGNATURES FOR FE AND AL EXPLORATION USING MACHINE LEARNING AND SENTINEL-2 DATA

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DOI: 10.2478/minrv-2026-0042

received – 09.03.2026 / revised – 13.03.2026

accepted – 07.05.2026 / published – 22.09.2026

Abstract: The Dom Bosco Syncline (DBS), located in the southern portion of the Quadrilátero Ferrífero, Brazil, contains significant Fe and Al deposits. However, dense vegetation cover and geological heterogeneity impose substantial limitations on mineral prospecting using orbital remote sensing. In this context, the machine learning model MinMap-S2 (Mineral Mapping via Sentinel-2) is proposed to support mineral exploration in the DBS. MinMap-S2 is a hybrid model based on spectral signatures derived from bauxite residues deposited in the Marzagão tailings dam (MTD), located within the DBS, for the detection of Fe- and Al-rich mineralization. The model was developed using Python, and its methodology integrates the algorithms Self-Organizing Maps (SOM) and Extreme Gradient Boosting (XGBoost) to process Sentinel-2 multispectral data. SOM is employed to generate a spectral library from bauxite residues and surrounding surface materials, which is subsequently used by XGBoost for supervised classification and spatial prediction. The model was applied to a region located in the eastern portion of DBS, characterized by detrital-lateritic covers and metasedimentary rocks, including itabirites, phyllites, schists, quartzites, and sericitic metarenites. Validation of the results was conducted through geological mapping, field sampling, and petrographic analyses. The results demonstrate that MinMap-S2 effectively identifies areas with spectral responses associated with Fe- and Al-rich mineralization, supporting the discrimination of mineralized zones in heterogeneous terrains and under dense vegetation cover. Overall, the proposed methodology demonstrates potential as a supporting tool for mineral exploration using Sentinel-2 multispectral data.

Keywords: Bauxite residues, Machine learning, Remote sensing, Mineral exploration, Sentinel-2 image, Quadrilátero Ferrífero

1. Introduction

The Quadrilátero Ferrífero (QF), located in Minas Gerais, Brazil, covers an area of approximately 7,000 km² and is recognized as one of the world's most important mineral provinces. Within this geological setting, the Dom Bosco Syncline (DBS), situated in the southern portion of the QF, contains significant deposits of gold, iron, manganese, topaz, and aluminum [1, 2].

Despite the region's pronounced geodiversity, dense vegetation cover imposes substantial limitations on mineral prospecting using orbital remote sensing. Under such conditions, the detection of mineralogical targets is restricted to exposed surfaces, including rock outcrops, mining fronts, road cuts, and bare soil areas. In this context, machine learning techniques have emerged as valuable tools for mineral prospectivity mapping using Sentinel-2 satellite imagery across the DBS.

Satellite imagery, such as that provided by the Sentinel program of the European Space Agency, enables the extraction of information on mineral occurrence through advanced multispectral indices derived from

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Sentinel-2 data [3]. This approach is cost-effective, provides broad spatial coverage, and enables the integration of remote sensing data with field observations.

In addition, the integration of remote sensing and machine learning has emerged as a promising approach for the characterization and mapping of spectral and temporal signatures associated with minerals in bauxite residues [4]. The spectral signature of such residues arises from the combined optical responses of their constituent minerals, particularly iron oxides (hematite, goethite, and magnetite) and aluminum oxide-rich phases (gibbsite, boehmite, and diaspore) [3].

In this context, this study proposes the development and validation of MinMap-S2, a hybrid machine learning model designed for mineral prospectivity mapping using Sentinel-2 multispectral data. The model integrates Self-Organizing Maps (SOM) and Extreme Gradient Boosting (XGBoost) with spectral signatures derived from bauxite residues, enabling improved identification of Fe- and Al-rich occurrences and providing a decision-support tool for mineral exploration.

MinMap-S2 was developed using spectral signatures derived from bauxite residues and adjacent soils at the Marzagão Tailings Dam (MTD). Tailings dams such as the MTD may represent important secondary mineral resources, as they preserve the mineralogical history of their host regions. This cumulative characteristic transforms these deposits into valuable spectral databases, providing a reliable foundation for training and validating machine learning models integrated with remote sensing techniques for mineral exploration.

The following sections present the architecture of MinMap-S2 and examine the strategic role of the MTD and its surroundings as a source for spectral library construction. A case study is subsequently conducted to evaluate the performance of the proposed model, followed by a discussion on its scalability and potential applications.

2. Algorithmic background

The process of labeling remote sensing images based on their spectral characteristics is a fundamental task and often requires significant time and effort. In recent years, this process has been increasingly enhanced by machine learning algorithms capable of capturing complex nonlinear relationships within multispectral and hyperspectral datasets [5]. In the MinMap-S2 model, image classification is implemented through a hybrid architecture that integrates unsupervised and supervised learning methods.

The SOM, proposed by [6], is an unsupervised artificial neural network designed for dimensionality reduction and data clustering. The algorithm projects high-dimensional data onto a lower-dimensional space while preserving topological relationships, ensuring that similar data points remain close in the resulting map.

In multispectral remote sensing applications, SOM facilitates the identification of spectral similarities among pixels by grouping them into clusters with comparable reflectance patterns. This capability is particularly relevant for mineral mapping, as it enables the detection of subtle mineralogical variations that may not be evident through conventional analysis [7].

Complementing this approach, XGBoost is employed as the supervised classification method. XGBoost is a gradient boosting algorithm based on decision trees, designed for high-performance classification tasks. The method constructs an ensemble of weak learners in a sequential manner, where each iteration minimizes the residual errors of the previous model.

Its regularization mechanisms improve generalization and reduce overfitting, making it well-suited for complex remote sensing datasets. Within the MinMap-S2 model, XGBoost uses labeled spectral data derived from the SOM stage to perform classification and generate spatial predictions of mineral prospectivity.

3. Marzagão tailings dam

The MTD, UTM Zone 23K (652,200.77 m E, 7,743,627.90 m S, WGS 84 datum), illustrated in Fig. 1, is situated in the southern portion of the DBS, in the municipality of Ouro Preto. For more than five decades, the structure served as a terminal storage facility for bauxite residues. Currently, the dam is undergoing a decommissioning process and contains an estimated volume of 3.8×10^6 m³ of suspended and consolidated material. [8].



Fig. 1. Overview of the MTD: True color composite (RGB) illustrating the spatial distribution of the tailings and the surrounding geological landscape

The chemical composition of the bauxite residue (Tab. 1) indicates that Fe and Al oxides account for approximately 77% of the total, accompanied by oxides of Si, Na, Ca, and Ti. From a mineralogical perspective, iron is predominantly present as hematite and goethite, whereas aluminum occurs mainly in the form of gibbsite.

Table 1. Chemical composition of the bauxite residue from the MTD [9, 10]

Bauxite residues(%) by weight		
Elements	Barros (2017)	Santana (2020)
Fe ₂ O ₃	50.2	52.8
Al ₂ O ₃	25.9	24.6
SiO ₂	6.7	7.77
Na ₂ O	5.7	7.1
TiO ₂	3.7	3.7
CaO	1.9	1.9

The geology surrounding the MTD is characterized by schists, carbonaceous phyllites, sericitic and hematitic phyllites, and fine-grained quartzites. Latosols derived from the weathering of these lithologies constitute the predominant soil type in the region [8].

Analysis of Fig. 1 reveals that the central portion of the residue beach is characterized by the presence of sodium hydroxide crystals, formed during the bauxite digestion process and evidenced by an intense whitish coloration. This sector corresponds to the dry zone of the dam, where evaporation promotes crystal efflorescence. Adjacent to this area, supernatant water is observed, along with an intermediate zone displaying variable moisture conditions, whose reddish hue is indicative of high concentrations of Fe oxides.

Analysis of the supernatant water conducted during this study indicates slightly alkaline conditions (pH = 8.4), accompanied by high turbidity (41.9 NTU), color (453 uC), and an average electrical conductivity of 403 $\mu\text{S}/\text{cm}$, indicating a substantial load of suspended and dissolved constituents typical of bauxite residue.

Although moisture variations influence the visual response, Fe- and Al-rich oxides are distributed throughout the tailings deposit and exhibit limited spectral separability in Sentinel-2 data. In the surrounding areas, a pronounced contrast exists between dense vegetation cover, the dam's engineered structures, and exposed soil surfaces, contributing to the spectral complexity of the study area.

These characteristics make the MTD and its surroundings a suitable environment for the acquisition and analysis of spectral data related to local geology and mineral composition, particularly when integrated with remote sensing and machine learning techniques.

4. Methodology

The MinMap-S2 model is developed based on an integrated workflow that transforms multispectral data into validated mineralogical mappings. The main steps of this methodology are described below.

4.1 Processing and target enhancement

Sentinel-2 multispectral images comprise 13 spectral bands with spatial resolutions ranging from 10 m to 60 m. For consistency, all bands were resampled to a spatial resolution of 10 m before analysis. The initial stage involved the acquisition and selection of cloud-free scenes over the MTD. The selected scene corresponds to September 2022, representing dry-season conditions in the region, during which the relative proportions of water and bauxite residue within the dam were approximately balanced.

The data processing followed the methodological guidelines of [3] and [4], with emphasis on the detection of diagnostic absorption features associated with Fe oxides and hydroxyl-bearing minerals. The prediction bands (B) and the band ratios used (Tab. 2) for mineralogical analysis are as follows:

- B2 (Blue, 490 nm): Sensitive to absorption of iron oxides and useful for enhancing spectral contrast in altered materials.
- B3 (Green, 560 nm): Applied to identify iron oxides and hydroxyl-bearing minerals.
- B4 (Red, 665 nm): Sensitive to the absorption of metallic oxides and the reflectance of iron oxides.
- B8 (NIR, 842 nm): Helps distinguish areas rich in ferruginous minerals.
- B11 and B12 (SWIR, 1610 and 2190 nm): Critical for identifying hydroxyl-bearing minerals, such as gibbsite and phyllosilicates, which exhibit diagnostic absorption features, particularly near 2200 nm (B12). These bands also enable effective discrimination of water bodies due to strong SWIR absorption, as well as differentiation of latosols based on their characteristic spectral response.

Table 2. Band Ratios

Band Ratios	Sentinel-2A Bands
All iron oxides	$\frac{4}{2}$
Ferric Oxides	$\frac{11}{8}$
Ferric Iron	$\frac{4}{3}$
Laterite Index	$\frac{11}{12}$

Vegetation masking was performed using the Normalized Difference Vegetation Index (NDVI), excluding pixels with NDVI values greater than 0.2. This step reduced the influence of vegetated areas and minimized spectral interference from soil-background mixtures, while also decreasing model training time. Additionally, it improved class balance, reducing bias in the classification model toward dominant surface types such as soil.

4.2 Hybrid model architecture

The architecture of MinMap-S2 is organized into two sequential stages. First, the SOM algorithm is applied to generate a spectral library and identify targets such as bauxite residue, water, and soil. Subsequently, the spectral library generated by the SOM is used to train and validate the XGBoost-based MinMap-S2 model, which performs the final classification and spatial prediction of new areas of interest.

The predictive performance of MinMap-S2 was evaluated using the accuracy metric. The model achieved an accuracy of 96.44%, demonstrating its capability to discriminate and classify spectral responses associated with the target classes identified in the MTD.

Fig. 2(a) displays the MTD area in an RGB color composite, while Fig. 2(b) presents the four clusters identified by the SOM. Fig. 2(c) shows the median spectral signatures associated with each cluster.

As shown in Fig. 2(c), the spectral response of Cluster 0 (red) is associated with the occurrence of iron oxides, characterized by absorption features near B2 (490 nm) and in the NIR region (B8 and B8A), within the range of 783–842 nm [11]. Similar patterns have been reported by [12] in the spectral discrimination of laterite and bauxite outcrops.

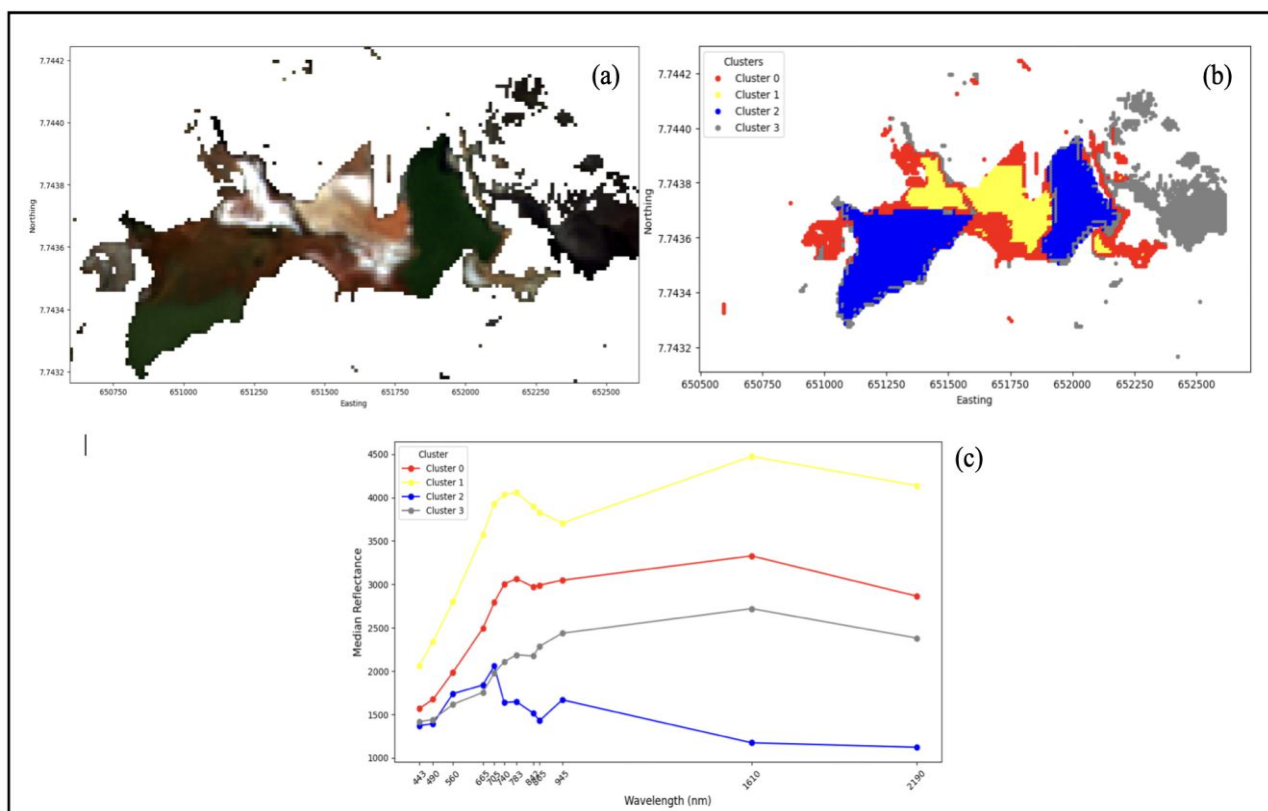


Fig. 2. Characterization of the MTD as a spectral data set for the MinMap-S2 model: (a) True color composite (RGB) with a vegetation mask; (b) Spatial distribution of the four clusters identified by the SOM algorithm; (c) Representative spectral signatures of the identified clusters

Cluster 1 (yellow) is located in the central and driest portion of the MTD, where sodium hydroxide precipitation occurs (Fig. 2a). Studies by [13] indicate that sericitic zones exhibit diagnostic absorption features at B9 (945 nm) and B12 (2200 nm), consistent with the spectral response observed in Cluster 1. This similarity suggests that Cluster 1 can be used to identify phyllosilicates associated with hydrothermal alteration.

Cluster 2 (blue) and 3 (gray) exhibit diagnostic spectral responses for water bodies and bare soil, respectively. The curve for Cluster 2 reflects the low reflectance characteristic of water, with near total absorption in the infrared bands B11 and B12.

Cluster 3 displays the typical ascending spectral behavior of latosols in the region, with a subtle absorption feature at B12 associated with clay minerals [14]. Spatially, this cluster is predominantly distributed along the edges of the dam and in its right sector, delineating transition zones between the tailings deposit and the adjacent natural terrain.

Fig. 3 presents a flowchart illustrating the methodological workflow of the MinMap-S2 model.

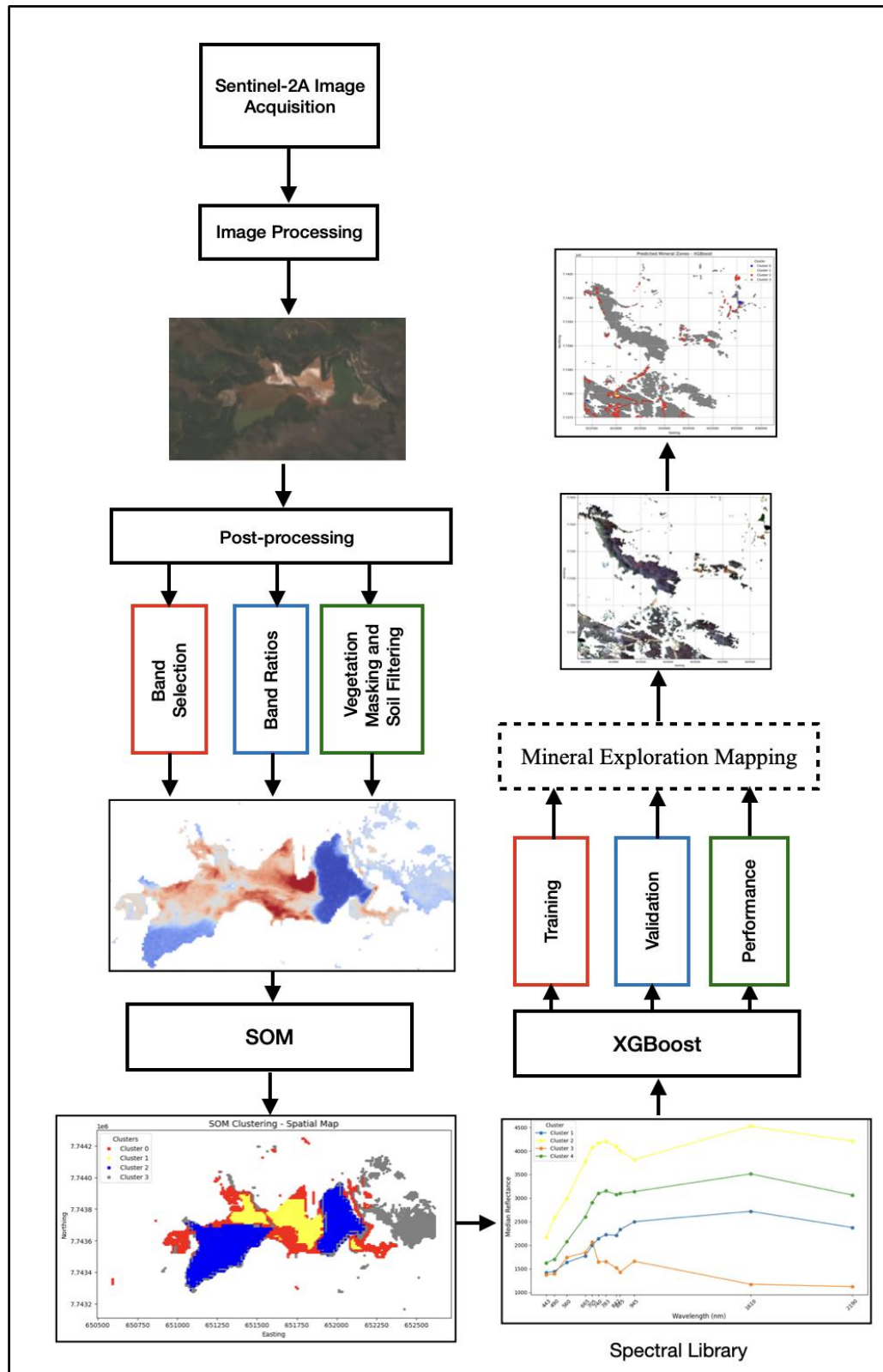
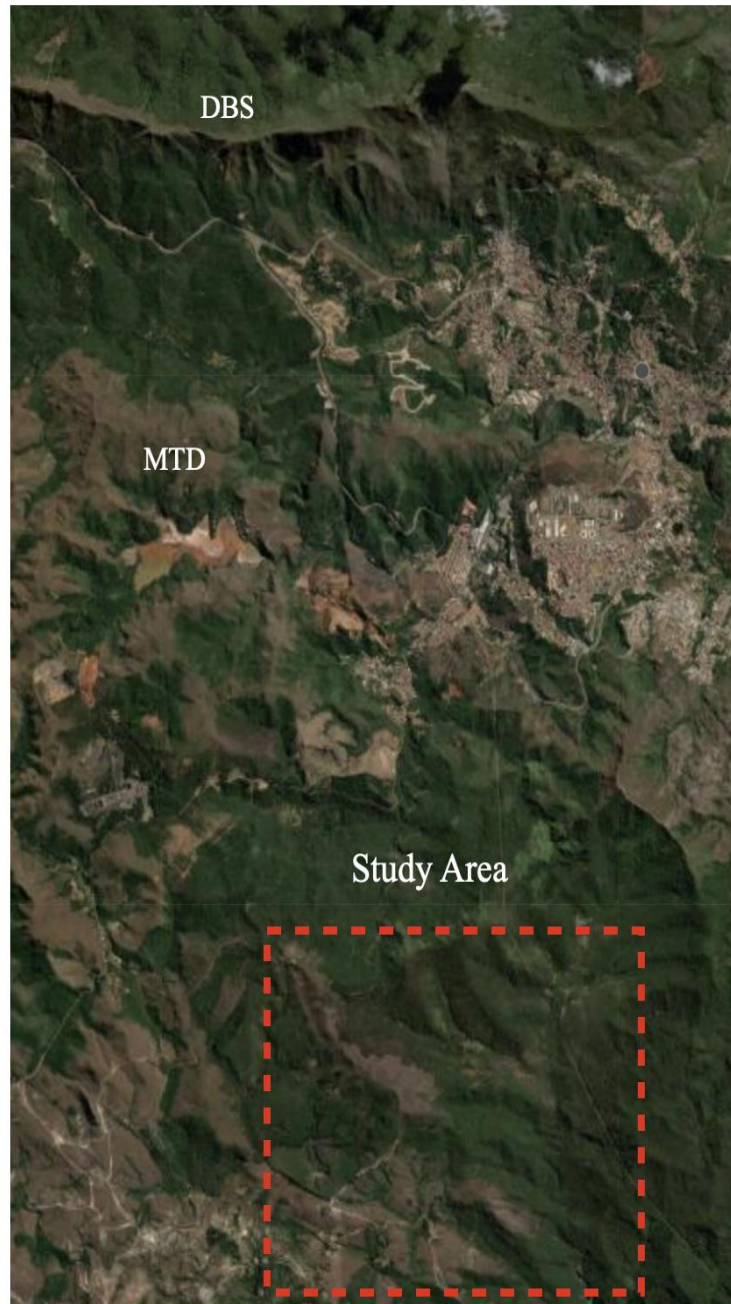


Fig. 3. Methodological flowchart of the MinMap-S2 model

5. Case study

The MinMap-S2 model was applied to a study area of approximately 12.25 km² located in the eastern portion of the DBS, near the MTD. The selection of this area was based on its accessibility for field validation, the availability of consolidated geological mapping, and the presence of mapped outcrops and mineral occurrences available through the GeoSGB portal (Geological Survey of Brazil – CPRM) [15]. Fig.4 highlights the DBS, the MTD, and the spatial extent of the study area.



*Fig. 4. Geographic location of the DBS, the MTD, and the study area selected for the application of MinMap-S2.
Image obtained from GeoSGB [15]*

This area is characterized by significant environmental and geological diversity, including dense vegetation cover and water bodies. Geologically, the region is dominated by Detrital-Lateritic Covers (DLC) (laterites, bauxites, and unconsolidated ferruginous materials), Banded Iron Formations (BIFs), quartzites, phyllites, schists, sericitic metarenites, and ferruginous metarenites (Fig. 5b).

The study area images were processed at a spatial resolution of 10 m and selected from September, corresponding to the dry season in the region. Subsequently, vegetation masking was performed using $NDVI > 0.2$. This procedure reduced the influence of vegetated areas and minimized spectral interference associated with soil-vegetation mixtures. Validation of the results was conducted through the interpretation of geological maps, petrographic analysis of outcrops, and mineralogical characterization of field-collected samples.

Fig. 5(a) presents the study area after vegetation masking, together with the MinMap-S2 predictions superimposed on the geological map of the region (Fig. 5b). The mapped pixels are predominantly associated with outcrops and exposed soil surfaces. Pixels exhibiting spectral signatures compatible with Cluster 0 (red) are mainly concentrated in regions characterized by DLC and BIFs, particularly in the areas represented by points 1 and 2 in Fig. 5(b).

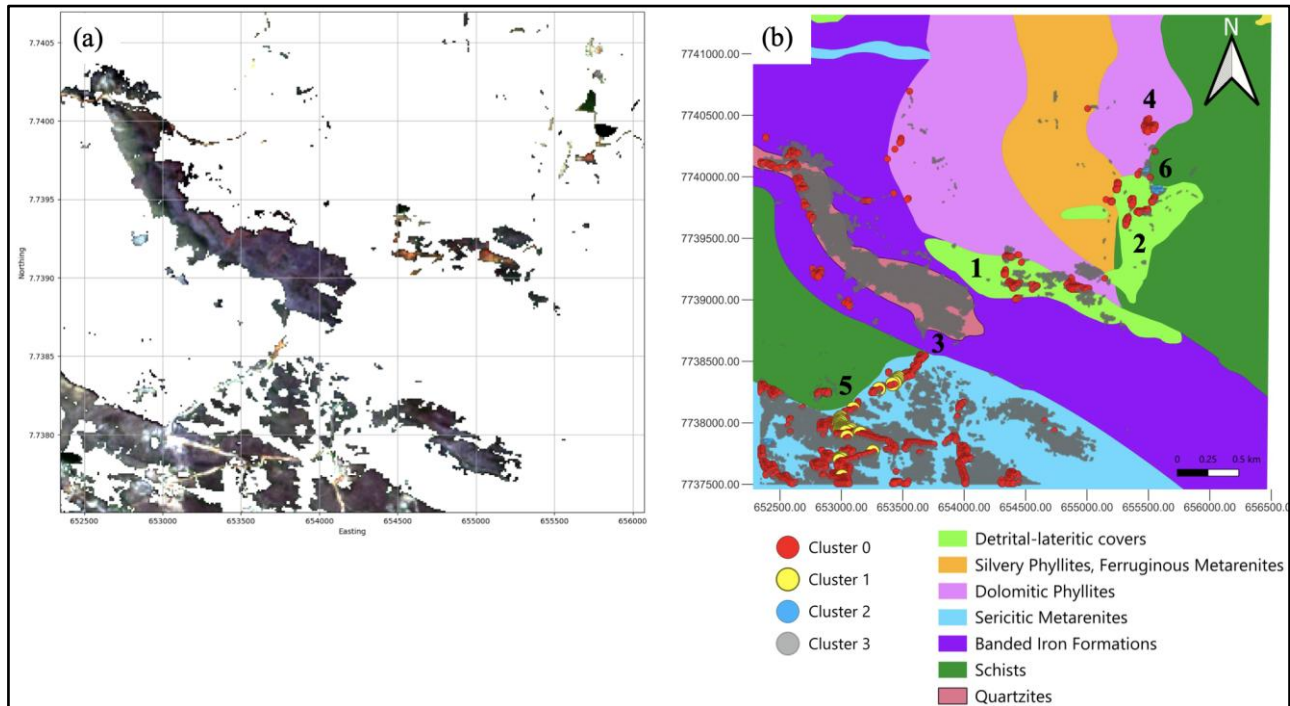


Fig. 5. MinMap-S2 predictions in the study area: (a) vegetation-masked image; and (b) MinMap-S2 cluster predictions superimposed on the geological map

Point 3 corresponds to areas influenced by the leaching and transport of ferruginous materials along unpaved roads, a process controlled by topographic gradients and surface runoff during rainfall events. Point 4 highlights a zone interpreted as the result of lateritic material deposition associated with local topographic variations, probably corresponding to a geological contact between lateritic covers and phyllites.

Cluster 1 (yellow) identified areas represented by point 5, exhibiting spectral responses associated with sericitic metarenites, reinforcing the spectral affinity between phyllosilicates and the dry sector of the MTD, characterized by sodium hydroxide precipitation. Additionally, Cluster 2 (blue) identified the two lakes in the region (Point 6), whereas Cluster 3 (gray) mapped residual soil areas derived from the different lithologies present in the study area.

6. Discussion

This section discusses the results obtained with MinMap-S2, focusing primarily on Cluster 0, with particular emphasis on Area 1 (Fig. 5b). Cluster 0 identified zones associated with BIFs, represented in the study area by itabirites, as well as lateritic crusts and bauxite occurrences. Field sampling was subsequently conducted to ground-truth and validate these spectral classifications.

Petrographic analyses of samples collected from lateritic crusts and itabirites demonstrated that both lithologies are predominantly composed of iron oxides, reaching approximately 90% in lateritic crusts and 75% in itabirites, with goethite as the dominant mineral phase, followed by hematite. These findings are consistent with the results reported by [16].

Fig. 6 presents photographs acquired during fieldwork. Fig. 6(a) provides an overview of Area 1. In the upper portion of the image, it is possible to identify vegetation cover and lateritic crusts, whereas the lower portion is characterized by ferruginous schists and itabirites. Fig. 6(b) shows the lateritic crust and the residual soil derived from its weathering. Fig. 6(c) illustrates the itabirites, where their characteristic banding can be observed, marked by the alternation of quartz and iron oxide layers. In this area, the itabirites are partially covered by lateritic crusts.

Finally, Fig. 6(d) presents two samples, approximately 3×3 cm in size, consisting of hematite and bauxite collected during field sampling, whereas Fig. 6(e) illustrates the lateritic crust overlying the underlying laterite, with the marked line indicating the contact between the two units.

Overall, the results demonstrate that the spectral signature of bauxite residue represented by Cluster 0 is effective for identifying areas associated with Fe- and Al-rich mineralization. However, an important limitation of MinMap-S2 is the spectral discrimination between BIFs and areas associated with laterites and bauxite occurrences.

This limitation is mainly related to the spectral mixture of iron and aluminum phases present in the bauxite residue, which reduces the model's ability to differentiate these surface materials. In addition, the high Fe content commonly observed in both materials produces similar spectral responses, making their discrimination difficult using Sentinel-2 multispectral imagery [12].

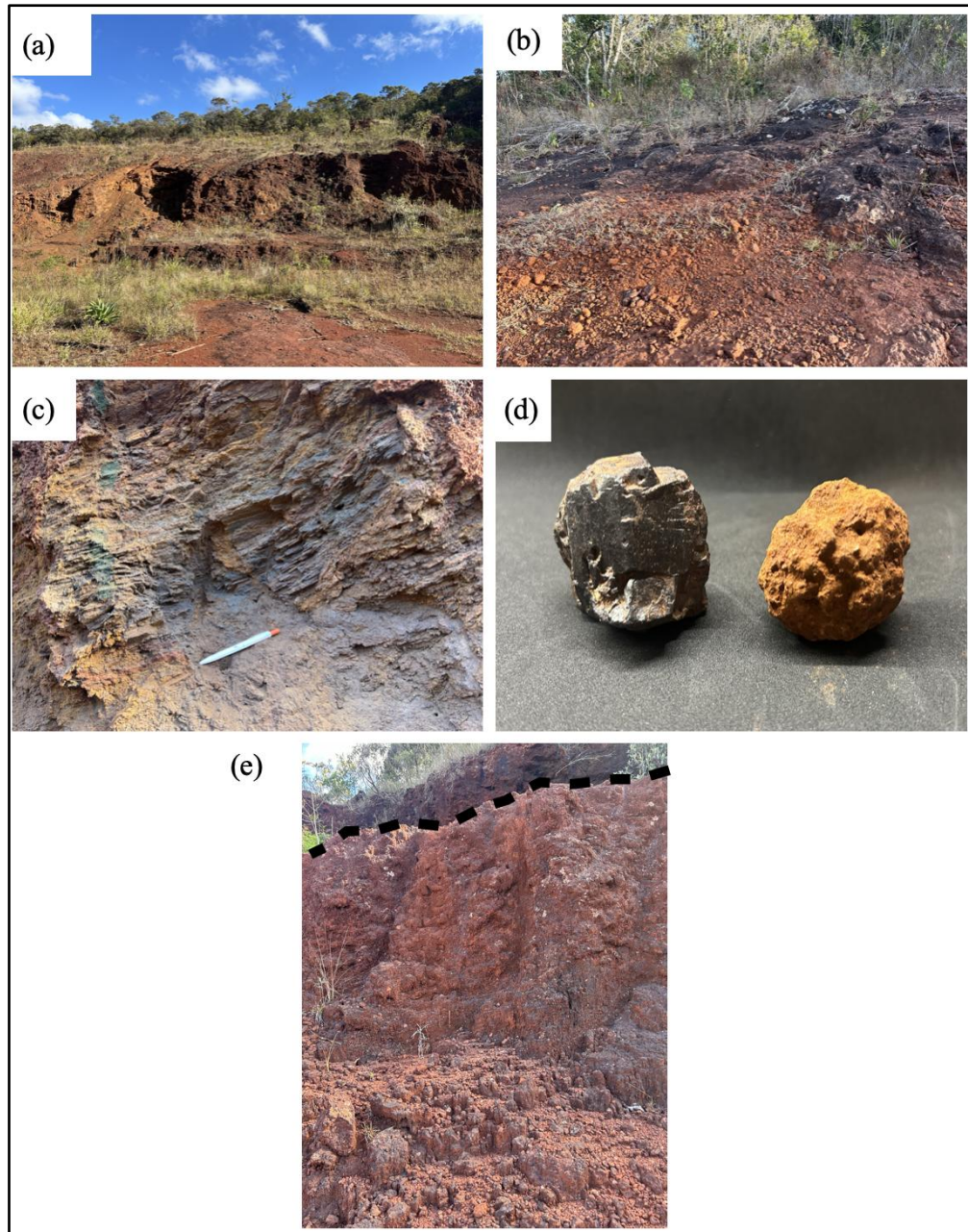


Fig. 6. Field observations and geological validation of MinMap-S2 predictions in Area 1: (a) overview of the study area; (b) lateritic crust and residual soil; (c) BIF outcrop represented by itabirite; (d) hematite and bauxite samples; and (e) lateritic crust overlying the laterite

7. Conclusions

This study proposed and validated MinMap-S2, a hybrid machine learning model integrating SOM and XGBoost algorithms with Sentinel-2 multispectral data for mineral prospectivity mapping in the Dom Bosco Syncline. The methodology demonstrated that spectral signatures derived from bauxite residues deposited in the Marzagão tailings dam can be effectively used to identify areas associated with Fe- and Al-rich mineralization, phyllosilicates related to hydrothermal alteration, water bodies, and residual soils in the region.

The results demonstrated that Cluster 0 is associated with detrital-lateritic covers and banded iron formations. The interpretation of this cluster was validated through field sampling and petrographic analyses of lateritic crusts and itabirites, confirming the predominance of iron oxides, particularly goethite and hematite.

Cluster 1, in turn, identified areas spectrally compatible with sericitic metarenites, whose interpretation was supported by GeoSGB geological data. Collectively, these findings reinforce the reliability and geological coherence of the classifications generated by MinMap-S2.

The integration of remote sensing, machine learning, geological mapping, and field validation demonstrated the potential of MinMap-S2 as a supporting tool for mineral exploration in heterogeneous and densely vegetated terrains such as the DBS. Nevertheless, the spectral discrimination between Fe-rich and Al-rich targets remains challenging in Sentinel-2 data due to the spectral similarity between ferruginous and bauxitic materials.

An important advantage of MinMap-S2 is that its application does not require integration with the SOM algorithm after model training. For application to new areas, it is only necessary to remove vegetation from the input image and use the same spectral bands and band ratios adopted during model training. This characteristic facilitates the application of the model in different geological settings.

The MinMap-S2 model, source code, and associated implementation files are publicly available at: [Link to the source \(drive.google.com\)](https://drive.google.com).

Future investigations should focus on applying MinMap-S2 in different geological settings to further evaluate its applicability for Fe- and Al-rich mineral exploration. Additional applications in regions characterized by distinct lithological, geomorphological, and vegetation conditions may contribute to a broader assessment of the model's performance and generalization capacity for detecting ferruginous and bauxitic mineralization. Overall, the proposed methodology demonstrates strong potential for scalability and application in mineral exploration workflows based on multispectral satellite imagery.

Acknowledgements

The authors acknowledge the Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG) and the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) for the financial support essential to the development of this research.

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