

New tools for Automated Particle Deagglomeration: Machine-Learning from Mineralogy Data

Bilal Hasan Aslan

aslbil001@myuct.ac.za

Department of Computer Science
University of Cape Town
Cape Town, South Africa

Geoff Nitschke

gnitschke@cs.uct.ac.za

Department of Computer Science
University of Cape Town
Cape Town, South Africa

Chi Ly

Chi.Ly@bruker.com

Bruker Nano Analytics
Houston, Texas, USA

Jonathan Knapp

jonathan.knapp@hitachi-hightech.com

Hitachi High-Tech America, Inc.
Chicago, Illinois, USA

Abstract

Rock classification depends on mineral composition and morphology, such as size, angularity, or mineral associations. Traditionally, optical petrography by skilled and experienced professionals was used for this purpose. Many tools have been developed to provide data on bulk mineralogy, such as *X-Ray Fluorescence* (XRF), *Short-Wave Infrared* (SWIR), and *Fourier Transform InfraRed* (FTIR). However, automated mineralogy provides insightful mineralogy and textural information, but is limited in its ability to recognize individual particles in a granular specimen, as it relies on programmatic and rules-based methods to deagglomerate particles, defined as a mineral area surrounded by background phases. This is especially noticeable for fine particle-size specimens, where traditional deagglomeration techniques are limited in recognizing an irregularly shaped particle compared to multiple touching particles, which a trained analyst could recognize. We describe a new automated mineralogy computational tool for particle classification and analysis, leveraging the general classification capacity of large neural networks (deep-learning), multi-label classification, and established computer-vision (machine-learning) techniques to improve particle deagglomeration across various granular specimens.

1 Introduction

Automated mineralogy has undergone significant advancements since its inception in the 1970s at the CSIRO laboratories in Australia (Pirrie & Rollinson, 2011). Initially an X-ray-driven process, it now integrates detailed morphological data using *Scanning Electron Microscopy* (SEM) imaging techniques. These advancements, exemplified in tools like MLA (Sylvester, 2012) and AMICS (AMICS, 2024), have revolutionized mineralogical analysis by enhancing image resolution and providing robust segmentation capabilities to classify various mineral assemblages. The addition of high-resolution images has simplified the extraction of detailed mineralogical information, which aids in decision-making for mineral processing. Also, higher quality images facilitate the development of more efficient measurement routines that can distinguish mineral particles and assemblages. However, this push for greater precision also presents new challenges: the demand for more refined extraction of mineralogical information requires continual improvements in image processing algorithms, including particle and grain segmentation, as well as enhanced image stitching techniques to handle complex mineral associations.

Traditionally, automated mineralogy has made use of many image-processing techniques developed for biological sciences, particularly in the segmentation of cells and other biological structures (Meijering, 2012). While useful, these techniques present limitations when applied to geological materials. Biological samples tend to feature smooth, rounded edges, while geological materials often exhibit sharp,

angular features, which result from crystallographic growth patterns. This fundamental difference reduces the effectiveness of traditional segmentation methods in geological contexts, often necessitating manual intervention. Mineralogists frequently have to segment grains and particles manually based on their visual interpretation of the image, an approach that, while accurate, is time-consuming and inefficient as the analytical throughput of modern automated mineralogy instruments continues to improve.

In this study, we explore alternative segmentation methods that bypass the limitations of traditional image processing techniques. Specifically, we investigate approaches leveraging surface shape factors and grey-level shifts to distinguish particles and grains, alongside the integration of advanced ML algorithms. A primary goal of our research is to replicate the manual segmentation process—where mineralogists use their expertise to visually identify and separate particles—by training an ML model to learn and replicate this process autonomously. We focus on using computer vision techniques to achieve particle deagglomeration in crushed rock samples, which are representative of common specimens encountered in mineral processing and mining applications.

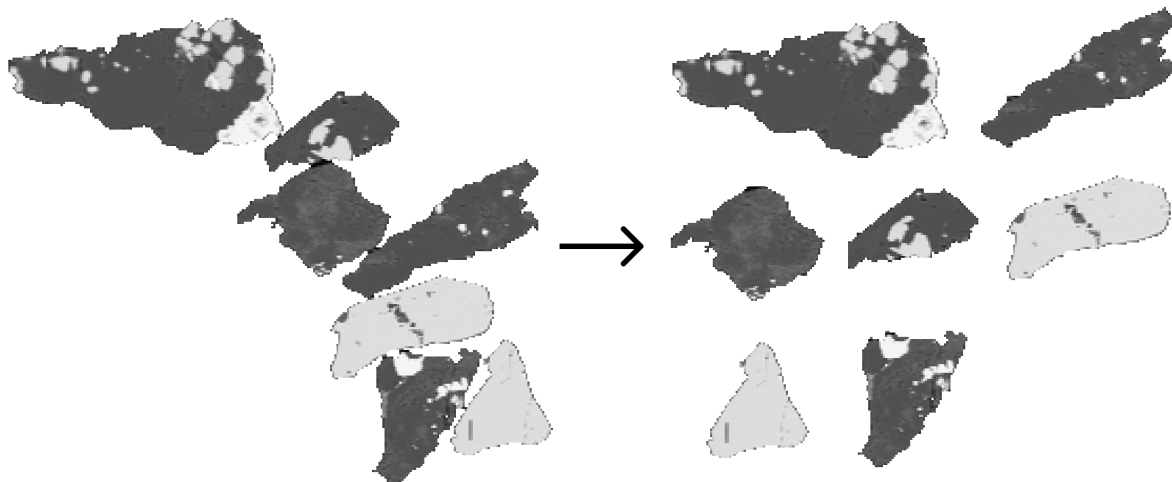


Figure 1: (a) Shows the original images of particles before manual deagglomerate and (b) shows the same set of particles that have been manually processed.

2 Methods

The primary challenge in developing such an ML-based system is the creation of a high-quality training dataset. As with any supervised learning approach, the accuracy of the model is contingent on the quality of its training data. To maximize performance, we curated a training dataset through manual processing by experienced mineralogists, ensuring that the algorithm learns to recognize complex agglomerated particle structures. Figure 1 is an example of the original data set and the processed data used as the training data set to teach the ML algorithm to recognize “touching” particles.

We have chosen to investigate the U-Net neural network (Siddique et al., 2021), a model originally designed for biomedical image segmentation. U-Net’s adaptability to context-based segmentation, rather than pixel-based, makes it particularly suited for separating touching particles (Figure 1), as it captures broader structural information in the image. The model’s relatively small size also offers computational efficiency, which is essential when dealing with the large datasets typical of mineralogical scans. U-Net is inherently generalizable, allowing it to perform well even with relatively limited training data, though carefully curated training sets remain crucial for handling the complexities of mineralogy.

The U-Net architecture (Figure 2) consists of two main paths: a contracting path and an expansive path. The contracting path follows a conventional convolutional neural network (CNN) structure, employing repeated 3x3 convolutions with ReLU activations and max-pooling layers. In contrast, the expansive path involves up-sampling feature maps and concatenating them with corresponding feature maps from the contracting path. The architecture’s U-shape facilitates the transfer of contextual information across the network, enabling precise segmentation.

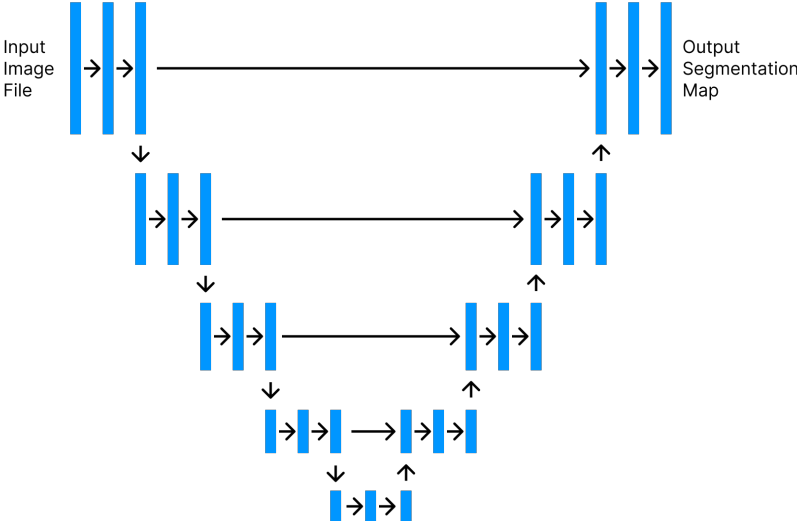


Figure 2: U-Net model architecture: Arrows indicate various operations within the network, while the blue boxes represent the feature maps at each layer. The input image is introduced on the left, and after being processed through the network, a segmentation map is produced as the output on the right.

We also explored variants of U-Net, such as Double U-Net (Deb & Jha, 2022) and Dense U-Net (Wang et al., 2019), which improve upon different aspects of the base model’s performance. In terms of data augmentation, our approach is flexible, allowing us to rotate, resize, and alter the contrast of particle images to enrich the dataset. We can also simulate artificial agglomerations by manipulating the spatial relationships between particles.

3 Results and Discussion

The U-Net model demonstrated a high degree of generalizability across various mineralogical scans, successfully segmenting grains that were traditionally difficult to distinguish using conventional methods. In particular, the model excelled in separating attached grains, a known challenge for traditional rule-based deagglomeration techniques. Traditional methods often failed when tasked with segmenting grains that appeared fused or had complex boundary shapes, resulting in either over-segmentation or under-segmentation. However, the U-Net model consistently produced accurate segmentation, capturing the subtle features and boundaries of individual particles, even in cases of agglomeration.

Although our current dataset is limited, the model’s ability to handle diverse mineralogical specimens, varying in texture and size, shows great promise. The U-Net model was applied to scans of varying complexity and resolution, and in all cases, it successfully performed particle deagglomeration without the need for manually tweaking parameters. This represents a significant improvement over traditional methods, which often require manual intervention and parameter adjustments for different specimens or even different regions within the same scan. The ability to automate this process and maintain a high level of segmentation accuracy across varying X-ray scan conditions (for example, resolution, image quality) suggests that the U-Net architecture is well-suited for further applications in mineralogical analysis.

While these preliminary results are promising, further testing is needed to confirm the model’s robustness under more varied conditions. Expanding the dataset to include more complex cases, such as highly dense particle agglomerations and lower-quality scans, will help refine the model’s performance. Current work is focusing on gathering a larger dataset and investigating the use of machine learning not only for segmentation but also for more advanced mineral classification tasks. This will potentially pave the way for a fully automated analysis pipeline, streamlining the labor-intensive process of mineralogical analysis.

4 Conclusion and Future Directions

In this study, we introduced a U-Net-based deep learning approach for automated particle deagglomeration in mineralogical scans, addressing a critical limitation of traditional methods in recognizing and segmenting attached grains. Traditional rule-based deagglomeration techniques often fall short when applied to complex granular structures, particularly when dealing with fine particle sizes or grains that appear fused in the image. By leveraging the powerful segmentation capabilities of U-Net, we successfully demonstrated that our model can handle such challenging cases, achieving accurate segmentation across a variety of scans without requiring manual parameter adjustments.

Our model’s generalizability across different mineralogical specimens shows its potential to streamline and automate key processes in mineral analysis, significantly reducing the time and effort typically spent fine-tuning segmentation parameters for each scan. This represents a promising step towards fully automated mineralogical workflows that minimize human intervention while maintaining high precision and accuracy.

Although the current results are based on a relatively limited dataset, the consistent performance across different scan types suggests that the U-Net model can effectively generalize to more diverse data. However, further work is necessary to fully validate the model’s robustness, including expanding the dataset to incorporate more complex agglomeration cases and testing the model under more varied imaging conditions. We also plan to explore advanced applications, such as grain classification, to develop a comprehensive, fully automated analysis pipeline for mineralogical studies.

In addition to improving particle segmentation, there is potential for deep learning models (LeCun et al., 2015) like U-Net to reduce the manual time spent on parameter optimization. Traditional image processing techniques often require significant fine-tuning of segmentation parameters depending on the scan conditions—resolution, contrast, and the specific type of specimen. In some cases, multiple parameter sets are needed within the same scan, as X-ray images can vary in depth and intensity across the specimen. The generalizability of the U-Net model allows for consistent segmentation without manual intervention, even across scans of varying dimensions and image qualities. In future work, we aim to integrate grain classification techniques into this segmentation workflow, further automating mineralogical analysis and reducing manual labor.

In the future, the integration of deep learning models like U-Net into mineralogy has the potential to not only improve the efficiency of segmentation tasks but also significantly reduce the manual labor required for fine-tuning image processing parameters. This could greatly benefit the mineralogical community by enabling faster, more accurate analysis of mineral samples, ultimately advancing both academic research and industrial applications in mineral processing.

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