2024 EAGE ANNUAL 85TH CONFERENCE & EXHIBITION OSLO | NORWAY

Automated grain segmentation and mineral classification in rock thin sections

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Summary

Traditional petrographic analysis of rock thin sections is time consuming, it is potentially subjective, may suffer from operator bias, and the results are not necessarily representative of the bulk rock sample. The challenge to automation of petrographic description is the complexity that is inherent to geology; sedimentary rocks often contain many types of grains, cements, and pores. Here, we present a machine learning solution to automatically characterize minerals and grains in rock thin sections on a whole slide basis. The machine learning-based image analysis approaches outlined in this paper are designed for extraction of first-order rock properties at scale, unlocking latent data from 100s-1000s thin sections per project, including new or legacy slides. This is made possible in part by leveraging large pretrained vision models that can perform segmentation tasks on unseen images without additional training. The presented method also capably predicts most major minerals on a whole slide basis, although some limitations exist. Thin section screening through machine learning enables (1) more informed, data-driven, faster decisions, and (2) allocation of time and resources for specific, targeted microscale sample challenges which are best addressed using advanced imaging techniques such as QEMSCAN, and/or through inspection by a subject matter expert.

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Introduction

Thin section petrography is a classic rock sample preparation and analysis method that enables identification of minerals, organic matter, pores, grains and cements in rocks. It is an important, routine, and popular discipline used to understand key rock properties at the microscale, relevant for a vast range of applications in oil and gas exploration, geothermal energy, carbon capture and storage, minerals and mining, engineering, and environmental applications. Thin sections are rock wafers (typically 30 µm thick), usually impregnated with blue dye-stained epoxy resin, mounted on glass slides. Thin sections are typically analysed using a combination of brightfield (transmitted light), plane-polarised (PPL), cross-polarised (XPL) and incident light microscopy imaging methods, at a range of magnifications. Point counting is traditionally employed to quantify petrographic observations in thin sections. Point counting involves grid-based classification of a number of representative coordinates (e.g., 250) distributed across the slide, where each phase beneath the microscope eyepiece cross-hairs at each coordinate is manually classified in turn. Point counting and classification is usually hierarchical, for example, tier 1 = 'grain', tier 2 = 'sedimentary lithic', tier 3 = 'chert'. Since point counting is a manual process, it is time consuming, it is potentially subjective and suffers from operator bias, and the results are not necessarily representative of the bulk rock sample. The challenge to automation of petrographic description is the complexity that is inherent to geology; sedimentary rocks contain a range of nuanced types of grains, cements, and pores. The expression of each of these classes in thin sections is a function of real geological homogeneity and processes, but is also dependent on sample contamination and preparation effects (e.g., non-uniform thin section thickness, dye concentration, etc).

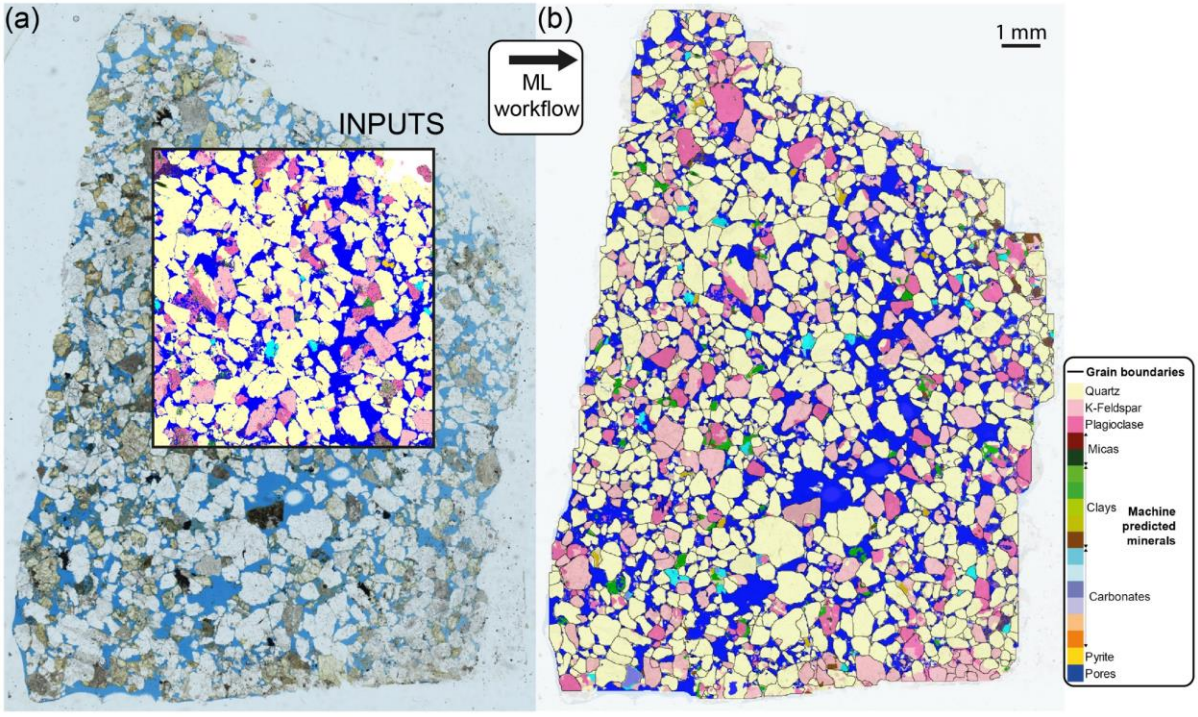

Figure 1. *(a) An example of a whole slide scan of a geological thin section in brightfield imaging. This is overlaid with corresponding QEMSCAN mineral map, which is available only for a small region of interest. (b) The results of the machine learning workflow for grain boundary and mineral prediction.*

More advanced imaging techniques are helping to solve the automation challenge in petrography. Here, we focus on QEMSCAN® (Quantitative Evaluation of Materials by Scanning Electron Microscopy), a technique which automatically delineates minerals via Scanning Electron Microscopy (SEM) coupled to energy-dispersive X-ray spectroscopy (EDS). The QEMSCAN technique yields a discrete quantized colour map corresponding to the observed mineralogy in rock samples (Fig. 1a). However, as with all techniques, QEMSCAN has weaknesses. Firstly, QEMSCAN is primarily sensitive to elemental

composition, which may preclude the precise delineation of adjacent grains and cements with the same composition (e.g., quartz). QEMSCAN is also operationally more expensive and time consuming in comparison to optical microscopy. To reduce costs and increase efficiency, QEMSCAN is often applied to a small region of interest rather than the entire thin section. Finally, all SEM techniques require an exposed sample surface and are thus unable to image legacy thin sections, which are covered by glass slips (cover-slipped thin sections). As a result, QEMSCAN and optical techniques are usually employed in tandem and in a complementary manner, and in many cases, petrographers still rely on optical images to accurately determine grain-based statistics such as texture, microporosity, and lithic rock fragments.

With the advance of machine learning (ML), it is now possible to improve the efficiency of identifying individual grains in a thin section for further analysis (replicating point counting), whilst potentially simultaneously delineating mineralogy. For example, Das et al. (2021) applied a deep neural network to perform semantic segmentation of sand grains in thin sections. Rubo et al. (2019) used multilayer perceptron and random forests for a pixel-by-pixel mineral classification of certain minerals and pores, with training labels generated from SEM. Izadi et al. (2020) developed a method to include both segmentation of grains and mineral classification. Nonetheless, these existing approaches have some challenges, especially the robustness and reproducibility of the machine learning result and a lack of reliable and diverse training datasets.

In this work, we present a refined ML workflow for dual grain and mineral detection in thin sections, using the latest advancement in deep learning for vision tasks, including pretrained foundation models for grain detection. We leverage QEMSCAN mineral maps in order to develop a model for prediction of major minerals in thin sections. Finally, we combine the grain segmentation and mineral classification outputs in order to improve the overall accuracy of the machine predictions.

Methodology

We use a suite of thin sections including cored late Jurassic sandstones located on the Frøya High, North Sea. Our method comprises three steps:

1. Data preparation: The QEMSCAN mineral maps are used as a training label for automatic mineral classification using the brightfield optical images. The QEMSCAN region of interest typically occupies only a small portion of the whole slide (Fig. 1a) and is often associated with a different pixel resolution compared to the optical images. To address this challenge, we employ cross-correlation algorithms to automatically align and scale the two image sets.

2. Multi-scale Grain Segmentation: Next, we perform grain segmentation with ML on the optical transmitted light images. We employ the Segment Anything Model (SAM), a state-of-the-art image segmentation foundation model (Kirillov et al., 2023) across multiple scales, optimising it for the detection of grains of various sizes. We integrate these multi-scale outputs based on an overlap threshold. By leveraging foundation models such as SAM, this helps to circumvent manual labelling of discrete grains, which is time consuming, subjective, and prone to error.

3. Mineral Classification: Finally, we train a UNET using optical images as inputs and QEMSCAN mineral maps as the target. Label cleaning is performed on QEMSCAN mineral maps using grain masks from Step 2, thereby reducing noise in the labels. This is achieved by assigning to each grain the majority mineral present. Augmentation (e.g., rotation, flip) was applied to help generalize the model.

Results and Discussion

Figure 1b shows an example of the results from the ML workflow: a combined grain segmentation output (grain boundaries in black) and mineral classification on a whole slide basis. Thus, we show it is possible to generate upscaled pseudo-QEMSCAN mineral maps with precise delineation of grain boundaries using optical images as inputs. Figure 2 shows examples at each stage of the workflow within an example QEMSCAN region of interest. We evaluated a confusion matrix to quantitatively assess the accuracy of the mineral classification using optical images (Fig. 3a). The confusion matrix is a pixel level comparison of QEMSCAN mineral labels and the corresponding UNET predictions. The

weighted F1 score for the validation data is 85.2%, and the confusion matrix shows the UNET performs well for most mineral classes. However, the clay mineral group is poorly classified, because clay is often a by-product of breakdown of other minerals, which cannot be consistently distinguished from the optical images in this dataset. As a result, ML prediction for clay minerals using optical images alone is challenging and is unreliable using the present workflow. The bulk mineral metric is often used by geologists for quantifying mineral composition of rocks, calculated as percentage of each mineral in the sample. The bulk abundance of major minerals in the machine learning output compares favourably to the QEMSCAN ground-truth in this dataset (Fig. 3b).

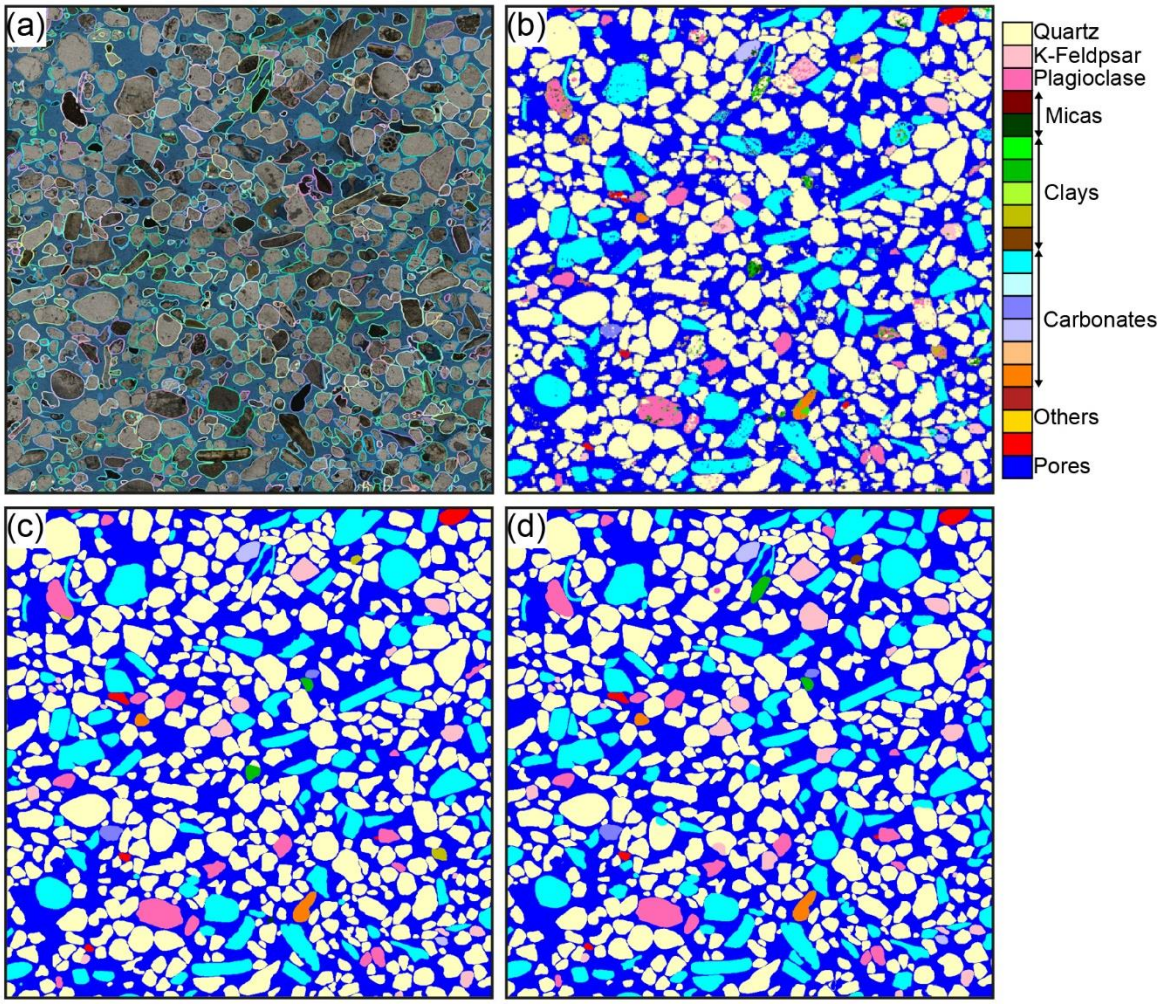

***Figure 2**. (a) Optical thin section image with instance segmentation of grain boundaries, where the coloured lines correspond to the detected grain boundaries; (b) QEMSCAN mineral map (ground-truth); (c) Simplified mineral map using the most common mineral on a grain-by-grain basis from (a); (d) Machine learning mineral classification.*

Discussion and Challenges

A key finding from this work is the use of robust grain masks for subsequent label refinement ahead of UNET training, which produces significant improvements in the model accuracy. By performing multi-scale grain segmentation using SAM, it is possible to improve the detection of very fine grains at the scale of single microns, which are otherwise challenging to identify. This approach yielded a robust grain detection irrespective of shape, size, or mineralogy, and improves the quality of grain size and shape statistics. Despite this, in some rare cases, a multi-scale grain segmentation approach results in over-segmentation of grains, particularly where fine fractures in grains can be recognised as boundaries.

A petrographer requires approximately 1 day to manually analyse 8-10 thin sections, assuming manual counting of 300 points of pores and minerals per thin section. The ML workflow presented is at least

an order of magnitude faster than point counting, and it is an approach which considers all grains and phases in the slide (i.e., it is fully representative.). In terms of accuracy, the grain segmentation model presented is not currently able to detect or classify grains to the same level of detail as an experienced petrographer, but ML has immediate value for the purposes of high throughput screening and the technology is still in its infancy. The acquisition time for QEMSCAN analysis varies depending on a variety of factors, but in general terms, optical imaging coupled to ML is an order of magnitude faster than QEMSCAN on a whole slide basis. However, QEMSCAN is a direct measurement: it is data-rich, precise, and sensitive to small phases such as clay minerals and microporosity; it can detect virtually all rock-forming minerals and phases and can be coupled with auxiliary detectors (e.g., SEM-CL).

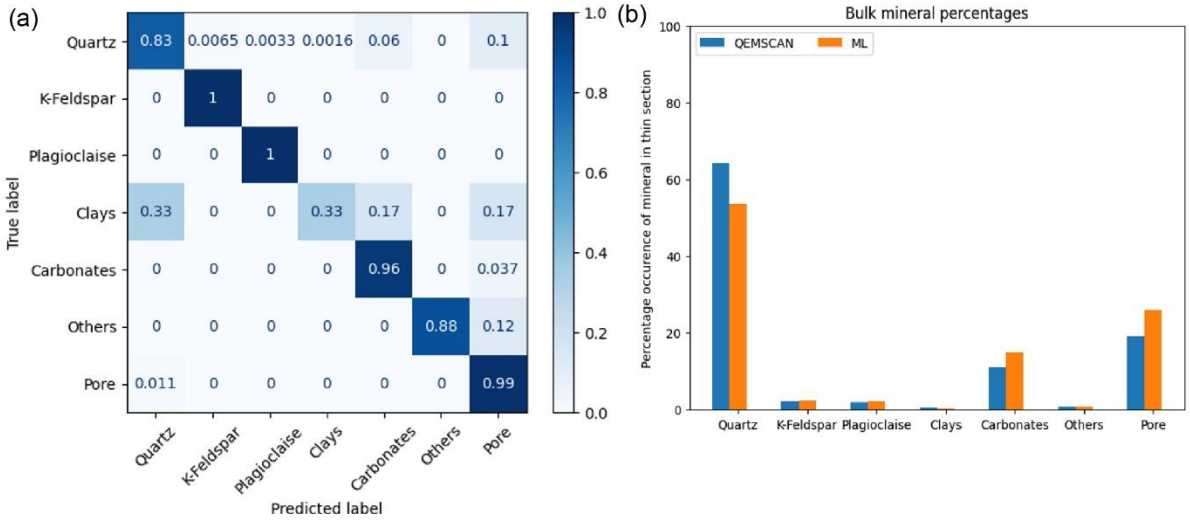

Figure 3*. Comparison of the QEMSCAN (ground-truth) and the machine learning mineral predictions: (a) Confusion matrix for major mineral groups; (b) Bulk mineralogy comparison.*

Conclusions

The machine learning based image analysis approaches outlined in this paper are designed for extraction of first-order rock properties at scale, unlocking latent data from 100s-1000s thin sections per project, including new or legacy slides. This is made possible by leveraging large pretrained vision models that can perform segmentation tasks on unseen images without additional training. The presented mineral classification method capably predicts most major minerals on a whole slide basis, but several limitations exist. At present, a dual grain and mineral prediction approach is well suited to high throughput screening of thin sections, which helps to make more informed, data-driven, faster decisions. Additionally, thin section screening through machine learning can be used to guide the allocation of time and resources for specific, targeted microscale sample challenges, which are best addressed using advanced imaging techniques such as QEMSCAN and/or through inspection by a subject matter expert.

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