Contribution of Machine Learning for the Determination of 3D Models of Porous Soil

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Abstract

This study explores the application of advanced machine learning techniques, particularly the U-Net architecture, for the extraction and analysis of porous soil structures from grayscale images. Originally developed for biomedical image segmentation, the U-Net model is adapted also for materials science due to its ability to effectively capture both local and global context.

Pore extraction involves identifying and isolating the pore regions within soil structures to enable detailed quantitative analysis of their size, distribution, and volume. Beyond pore extraction, this study focuses on two critical tasks: skeleton extraction and pore image generation. Skeleton detection builds upon this by identifying the connectivity of the pore network, providing insights into the structural integrity and mechanical properties of the material. The goal of Pore Image Generation is to demonstrate the application of Generative Adversarial Networks (GANs) for synthesizing realistic 3D representations of porous structures. These processes are crucial for understanding the permeability and functionality of porous soils in applications ranging from agriculture to construction.

The results demonstrate that the U-Net model excels in accurately extracting pore regions and detecting pore skeletons, achieving high performance across all evaluation metrics. The proposed approach automates the traditionally labor-intensive process of pore analysis, offering a powerful tool for materials scientists seeking to advance their understanding of porous soil systems. This work paves the way for more efficient and detailed studies of material properties, facilitating innovations in soil science and related fields.

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1 Introduction

Porous soils play a pivotal role in numerous scientific and industrial applications, including agriculture, water filtration, construction, and materials science. The intricate structure of pores within these materials governs their mechanical strength, permeability, and overall functionality. Accurately characterizing and analyzing these porous structures is essential for understanding their behavior and optimizing their use in practical applications. Traditionally, this analysis has relied on manual inspection and classical image processing techniques, which are often time-consuming, prone to human error, and limited in their ability to handle complex and diverse datasets.

In recent years, machine learning, particularly deep learning, has emerged as a transformative tool for automating and enhancing image analysis tasks. Among the various architectures available, the U-Net model has gained prominence for its exceptional performance in semantic segmentation tasks. Originally developed for biomedical image segmentation, the U-Net's encoder-decoder structure with skip connections enables it to capture both local and global features effectively, making it highly adaptable to other domains.

This study leverages the U-Net architecture to address the challenge of pore extraction from grayscale images of porous soil. The objective is to develop a robust and automated pipeline that accurately segments pore regions, facilitating further analysis such as pore connectivity and skeletonization. The dataset used comprises grayscale images of porous materials with corresponding binary masks indicating pore regions. By training the U-Net model on this dataset, the aim is to create a system capable of achieving high segmentation accuracy, thereby reducing reliance on manual analysis and paving the way for more comprehensive studies of porous soil properties.

The significance of this work lies in its ability to bridge the gap between traditional materials science methodologies and modern computational approaches. By automating pore extraction, this study not only accelerates the analysis process but also ensures reproducibility and scalability. Furthermore, this work lays the groundwork for subsequent tasks such as skeleton detection and 3D modeling, which are critical for a deeper understanding and modeling of the structural and functional characteristics of porous soils.

2 Related Work

The field of porous media analysis has witnessed significant advancements with the advent of machine learning techniques, particularly in tasks such as segmentation, skeletonization, and network modeling. Traditional approaches often relied on manual or classical methods, including medial axis transformations and morphological thinning, which are prone to user bias and struggle with maintaining topology and medial alignment in complex porous structures.

The U-Net architecture, initially developed for biomedical image segmentation tasks [1], has become one of the most widely used models for image segmentation due to its ability to work with limited data and produce accurate pixel-wise predictions. U-Net is characterized by its encoder-decoder structure, which captures both global and local features through downsampling and upsampling layers, respectively, with skip connections to preserve spatial resolution.

Recent studies have explored the use of deep learning for automating these tasks. For instance, PoreSkel et al. (2023) [2] employed deep learning to directly extract skeletons and distance maps from 2D grayscale images, bypassing the need for segmentation. PoreSkel demonstrated robustness across diverse porous media, achieving high accuracy in skeletonization and preserving critical structural features, even in challenging scenarios such as pore boundary perturbations and the presence of mineral disruptions.

Many other studies have applied U-Net to various segmentation tasks. For instance, it has been successfully used for segmenting cells in microscopy images [3]. Furthermore, recent studies have adapted U-Net for material science applications, such as the segmentation of microstructures in metals and the analysis of porous materials [4].

In addition to segmentation, skeleton detection and pore network modeling have benefited from the integration of machine learning. These methods emphasize the extraction of accurate and representative skeletons that retain the geometric and topological properties of the original images. By doing so, they address critical challenges in characterizing connectivity, coordination numbers, and permeability within porous media. This study builds upon these works, adapting the U-Net model for pore segmentation in materials science images, where the pore sizes and shapes exhibit significant variability.

3 Methods

3.1 Dataset

- **Pore Extraction**

  The dataset used in this study consists of grayscale images of materials with their corresponding binary masks that delineate the pore regions. Each image has a resolution of 480x480 pixels, and the dataset includes a total of 480 images split into training, validation, and test sets (64% for training, 16% for validation, and 20% for testing). The images were collected using X-ray microtomograph, which provides high-resolution imaging of the material surface.

- **Skeleton Detection**

  The skeleton detection task required preprocessing and structuring a dataset that aligned skeleton images with their corresponding original images. Binary skeleton masks were further processed with **tresholding**, **dilation**, and **resizing** to enhance their representation, The processed dataset was loaded using a custom PyTorch dataset class. To ensure balanced representation and computational feasibility, a subset of 2,000 aligned image-skeleton pairs was randomly sampled. This subset was then split into training, validation, and test sets with ratios of 64%, 16%, and 20%, respectively. Data sampling was implemented with a fixed random seed to maintain reproducibility.

- **Pore Image Generation**

  The dataset consisted of 48 preprocessed 3D image volumes stored in a NumPy array, each volumes contains 64 images. The dataset was normalized to the range [0,1] for stable model convergence. A custom PyTorch dataset class, PoreVolumeDataset, was created to handle the 3D data, which was then wrapped into a DataLoader for efficient batch processing.

3.2 U-Net Architecture

- **Pore and Skeleton extraction**

  The U-Net model consists of two main parts: the encoder and the decoder. The encoder extracts features from the input image using a series of convolutional layers followed by max-pooling operations. This downsampling process reduces the spatial resolution of the feature maps while increasing the number of channels. The decoder consists of upsampling operations that restore the spatial resolution of the feature maps, combined with skip connections from the encoder to preserve important spatial details. The final layer of the decoder outputs a pixel-wise prediction, where each pixel represents the probability of belonging to the pore region.

  The skeleton detection model utilized the same U-Net architecture as for pore extraction, with input and output channels adjusted to align with grayscale images and binary skeleton masks.

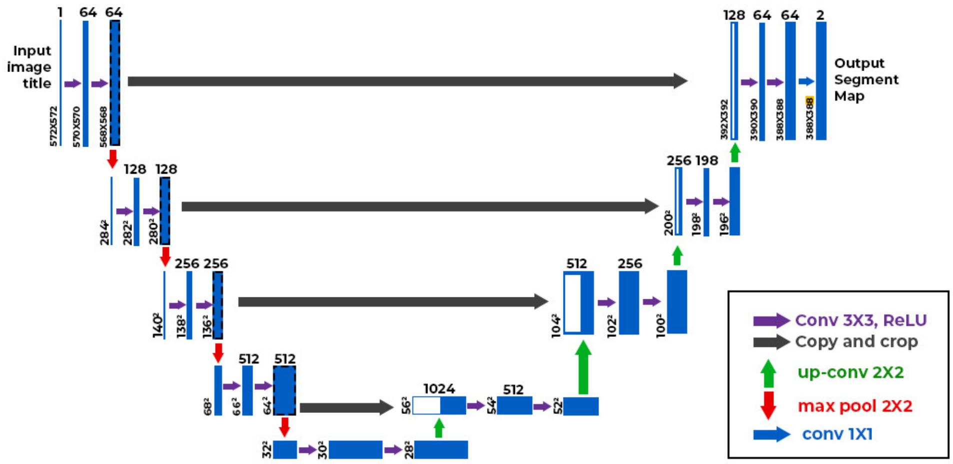

Figure 1: U-Net architecture for pore segmentation.

- **Pore Image Generation**

  The **generator** takes a latent vector of size 1000 and transforms it into a realistic 3D pore structure. It uses fully connected layers and transposed convolutions to upsample the latent vector into a 64×256×256 3D volume. Activation functions include ReLU for intermediate layers and Tanh for the output layer.

  The **discriminator** is a convolutional network designed to classify input 3D volumes as real or fake. It uses leaky ReLU activations and progressively reduces spatial dimensions through 3D convolutions. A final fully connected layer outputs the probability of the input being real.

3.3 Evaluation Metrics

The performance of the model is evaluated using several standard metrics for segmentation tasks:

- **Dice Coefficient (Dice Score)**: A measure of overlap between the predicted and ground truth masks, ranging from 0 (no overlap) to 1 (perfect overlap).
- **Intersection over Union (IoU)**: The ratio of the intersection to the union of the predicted and ground truth masks, indicating the quality of the segmentation.
- **Precision**: The proportion of correctly predicted pore pixels out of all predicted pore pixels.
- **Recall**: The proportion of correctly predicted pore pixels out of all ground truth pore pixels.
- **F1 Score**: The harmonic mean of precision and recall, providing a balanced measure of performance.

3.4 Training Procedure

The model is trained using the Adam optimizer with a learning rate of 0.001. The training procedure involves minimizing a combination of the Dice loss and binary cross-entropy loss. The Dice loss is particularly useful in segmentation tasks where class imbalance exists, as it focuses on the overlap between predicted and ground truth regions. Binary cross-entropy loss is also used to ensure that the model learns to classify each pixel correctly.

The input images are normalized to have pixel values between 0 and 1, and data augmentation techniques, such as random rotations and flips, are applied during training to improve the model's generalization. The model is trained for 100 epochs with early stopping to prevent overfitting.

For **Image generation**, Binary cross-entropy **(BCE)** loss was used for both the generator and discriminator. The models were trained for up to 30 epochs, with checkpointing implemented to save the best generator, with Early Stopping to prevent overfitting.

4 Results

4.1 Pore Extraction

The model's performance on the test set is shown in Table 1, which reports the Dice coefficient, IoU, precision, recall, and F1 score.

Metric	Value
Dice Coefficient	97.39%
IoU	94.92%
Precision	97.10%
Recall	97.70%
F1 Score	97.39%

Table 1: Segmentation performance on the test set. The U-Net model achieves high accuracy in segmenting pore regions.

Figure 7 shows sample segmentation results for an input image, the predicted mask, and the ground truth mask. As seen in the figure, the U-Net model is able to accurately segment the pore regions, even in the presence of noise and variations in pore size and shape.

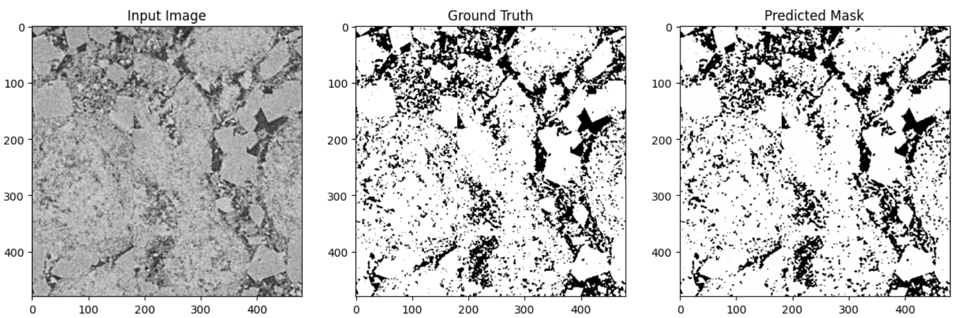

Figure 2: Sample segmentation results: input image, predicted mask, and ground truth.

4.2 Skeleton Extraction

For skeleton extraction, The model's performance on the test set is shown in figure 3 and 4, which show the progress of loss and IoU over epochs.

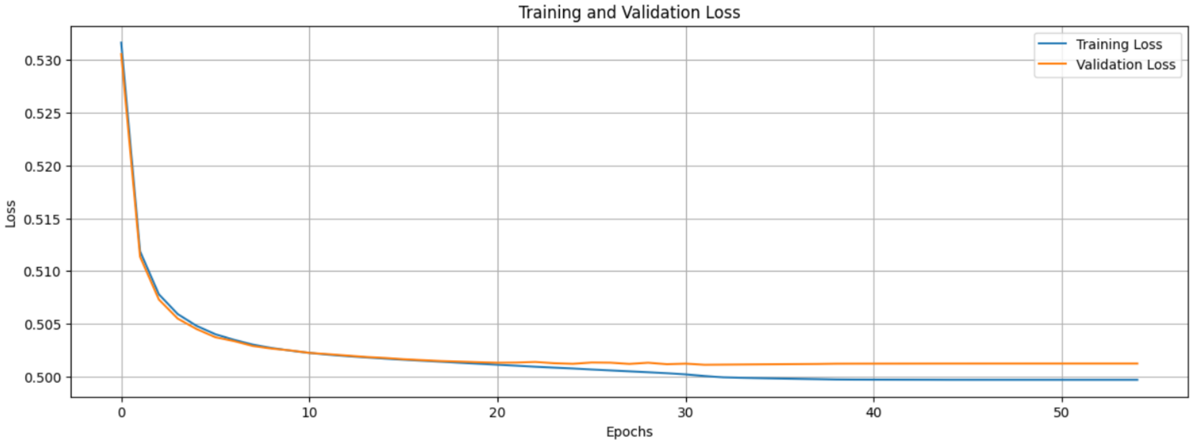

Figure 3: Training and validation loss

The losses plateau around epoch 20, showing that the model has likely converged. The early stopping mechanism appears to have been triggered around epoch 50, as there is minimal further improvement in validation loss. This prevents overfitting and saves computational resources.

Figure 5 shows sample skeleton extraction results for an input image, the predicted skeleton, and the ground truth mask. As seen in the figure, the U-Net model is able to accurately segment the pore regions, even in the presence of noise and variations in pore size and shape.

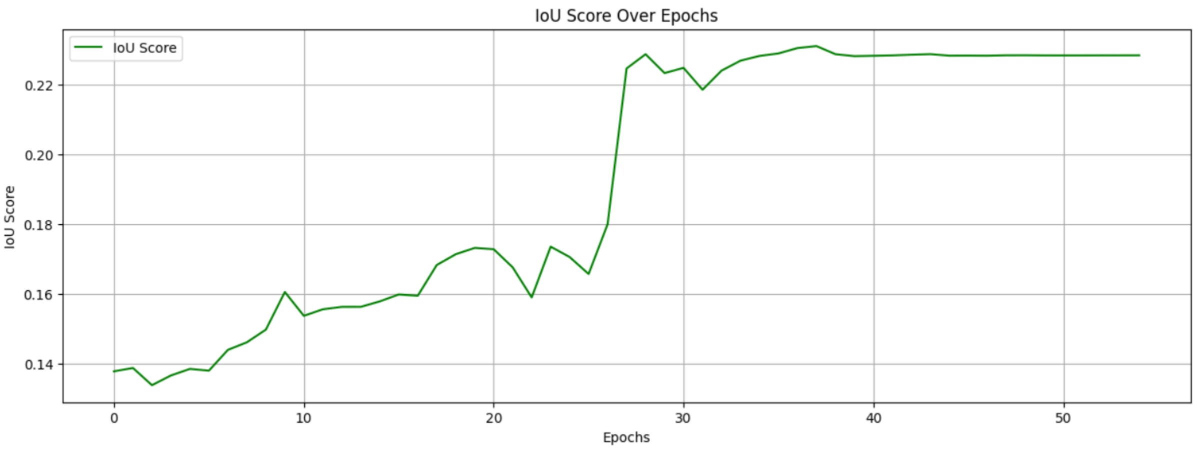

Figure 4: IoU over epochs

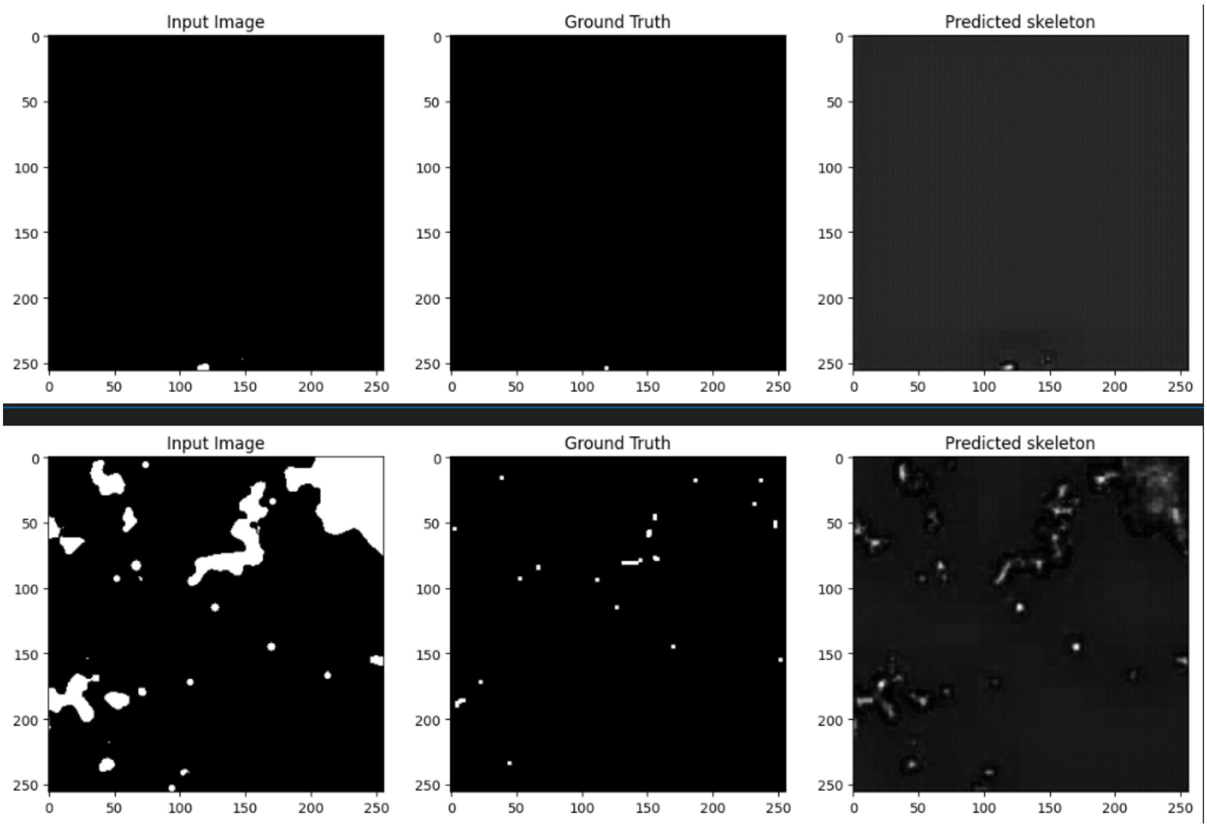

Figure 5: Sample skeleton extraction results: input image, predicted mask, and ground truth.

While the model achieves moderate accuracy on the training dataset, its predictions deviate from the ground truth on the validation set. For example, the IoU metric is only 0.22, indicating poor alignment between the predicted and actual masks. Additionally, visual inspection shows that the model struggles to identify smaller objects and misses finer details in segmentation. These issues suggest that the model is underperforming and requires further tuning or a more robust architecture.

4.3 Pore Image Generation

During training, the generator loss decreased steadily, indicating its ability to produce increasingly realistic pore structures. The discriminator's loss oscillated, as expected in adversarial training. The early stopping mechanism ensured computational efficiency by halting training once the generator reached optimal performance.

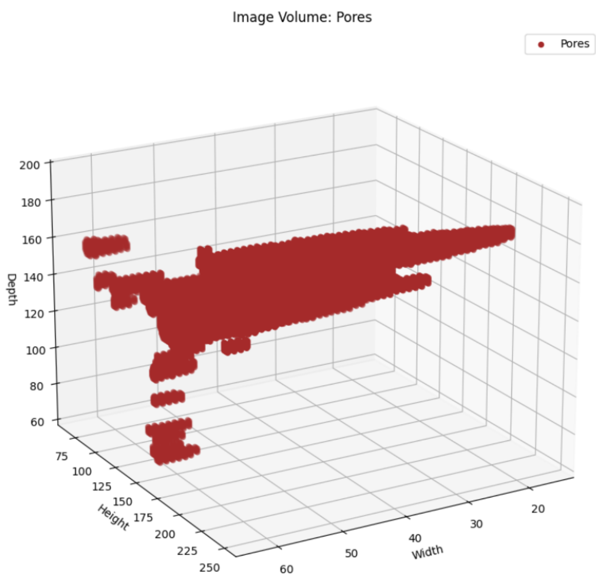

Figure 6: Example of 3D pore

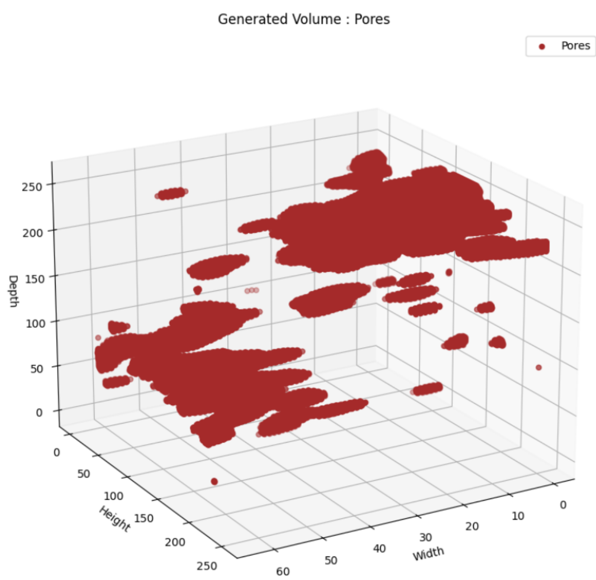

Figure 7: Example of a generated pore

The generated 3D pore images demonstrate the feasibility of using GANs for synthetic pore structure creation

5 Discussion

The results indicate that the U-Net model effectively extracts pore regions in materials science images, achieving high scores across all metrics. The model's ability to capture both local and global context through its encoder-decoder structure is a key factor in its performance. Additionally, the combination of Dice loss and binary cross-entropy loss ensures that the model learns to handle class imbalance, which is common in segmentation tasks with binary masks. However, the model demonstrates poor performance in skeleton extraction tasks, where it struggles to accurately delineate fine structures and connectivity. This limitation suggests the need for specialized approaches or additional post-processing techniques to improve the extraction of skeletonized features.

6 Future Work

Future research will focus on exploring the use of 3D U-Net for handling volumetric images, as pore segmentation in 3D can provide more detailed and accurate information about the material structure. Additionally, ensemble methods could be employed to combine the outputs of multiple models, further improving segmentation accuracy. Finally, the model's application to real-time material analysis could be explored, enabling automated inspection of materials in industrial settings. As well as for Image generation, Future work may include exploring alternative architectures and loss functions to enhance the realism and diversity of generated structures.

7 Conclusion

This study demonstrates the effectiveness of the U-Net architecture in segmenting pore regions in materials science images. The model's high performance, as evidenced by quantitative metrics, suggests that it is a valuable tool for automating pore analysis and improving research workflows. By leveraging deep learning techniques, materials scientists can gain more accurate, automatic, and efficient insights into material properties, leading to advancements in material design and characterization.

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