Automatic Detection of Fractures in X-ray Material Tomography using Unsupervised Machine Learning

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Abstract: Automatic fractures detection in X-ray material tomography using machine learning will significantly benefit material monitoring in an efficient way. This problem can be treated as Salient object detection (SOD) to identify the most interesting regions within a 2D image. Weakly-supervised annotations like scribble are explored recently due to their flexibility to label winding objects and low-cost compared to annotating per-pixel saliency masks. However, using scribble labels to learn salient object detection in X-ray material tomography has not been explored. In this paper, we explore unsupervised outlier detection with 3D structural information to solve the fracture detection in X-ray material tomography, which is under limited exploration in literature. We evaluate on 3D x-ray material tomography at different time stamps and show the experimental results.

Keywords: X-ray material tomography, Underperceived Machine Learning

1. Introduction

Fractures are three-dimensional (3D) features that have 3D effects on the flow properties of materials [1]. Considering fractures are characteristically rough and uneven, flow across hem would preserve a meandering trajectory of least resistance defined by local pressure gradients. The fracture topology is heavily determined by them with specific variation in aperture and surface roughness. Therefore, fractures are optimally explored and characterized in three dimensions and in-situ, and accurate depiction of fracture aperture and roughness is important for both intuitive understanding and meaningful numerical modeling. Figure 1 shows one 2D slice sample (x, y direction) from 3D X-ray material tomography (x, y, z direction). The key barrier to learn an effective machine learning model for fracture detection is the insufficiency of fracture annotation. From Figure 1, we can observe that it will be very time-consuming and expensive to annotate fracture for every pixel in an image, while scribble annotations are easier to provide as shown in the sample.



Figure 1: Multiple 2-D slice samples with fractures annotated by scribbles in 3D X-ray material tomography.

Automatic fracture detection using machine learning is an important tool as it has the potential to identify the fracture region and the changing fracture behavior quickly and accurately. In the LAMDA project, automatic fracture detection is especially important in the workflow between the new X-ray tomography instrument and the

ThermoFisher PFIB. This pair of instruments will use stepwise in-situ loading and X-ray imaging at $1 \sim \mu m$ resolution to create cracks and defects in the sample. Then, the damaged sample will be removed and transferred to the ThermoFisher plasma focused ion beam scanning electron microscope (PFIB) for ion milling and SEM with nanometer resolution. The coupling between the two instruments depends on identification of the region on interest in the tomography dataset. Consider the respective volumes: The tomography sample volume is $(1 \sim mm)^3$ and the PFIB sample volume is $(1000 \sim nm)^3$; the volume ratio is on the order of 10^9 , making selection of the optimal PFIB sampling volume a 1 in a billion problem. In other tomography-PFIB labs, the workflow from beginning to end can be a single week; the 1 in a billion problem needs to be solved rapidly and automatically.

In this paper, we explore unsupervised deep outlier detection techniques [2] to solve fracture detection in X-ray material tomography, which is under limited exploration in literature. Existing works focus on traditional images like scene/objects, which are very different from X-ray material tomography. Anomaly detection is a binary classification between normal and abnormal patterns. However, it is impossible to train a fully supervised model for this task, because we often lack unusual samples, and anomalies may have unexpected patterns. Therefore, anomaly detection models are often estimated in a class of learning settings, i.e., when the training data set contains only images from the normal class and the anomaly sample is not available during training. At the time of the test, examples that differed from normal training data sets were classified as anomalies.

To address this, we first focus on 2D-slice fracture detection, and then extend the focus to 3D segmentation by exploring the structure information between any two continuous 2D slices. Specifically, we propose a 3D segmentation model based on Patch Distribution Modeling (PaDiM) [2] and Convolutional LSTM Network [3] by capturing the spatial and temporal information along 3 directions.

2. Unsupervised Outlier Detection Algorithm

Given the 3D X-ray material tomography $X = \{x_i\} \vdash_{\{i=1\}}^n$, and x_i is a 2D slice, the goal is to detect the fractures in each slice. The general observation is that the fracture regions at continuous slices are consistent with each other. To detect the fractures from normal regions, we follow the 2D anomaly detection and localization approach, i.e., Patch Distribution Modeling (PaDiM) [2], which concurrently detects and localizes anomalies in images in a one-class problem setting.

For each slice, we first deploy a pretrained Convolutional Neural Network (CNN) to extract patch embedding to save the computation costs and mitigate the insufficiency of well-annotated training data. Specifically, we adopt pretrained ResNet-50 [4] network as the backbone to extract the layer-wise 3D feature maps. After that, each patch of the normal images is associated to its spatially corresponding activation scores in the ResNet-50 activation maps. Activation scores from various layers are then concatenated to obtain new embedding features carrying information from diverse semantic levels and resolutions. Hence, a raw input image is able to be patched into a grid of $(i, j) \in [1, W] \times [1, H]$ positions, in which $W \times H$ is the resolution of the largest activation map used to achieve embeddings. To incorporate the temporal information across continuous slices, we adopt Conv-LSTM [3] to refine the 3D features with a new reconstruction output for the next step process.

To learn the normal image characteristics at position (i, j), we assume that each path X_{ij} is generated by a multivariate Gaussian distribution $N(\mu_{ij}, \Sigma_{ij})$. The goal is to calculate the mean and covariance for normal image characteristics. In fact, each possible patch position is associated with a multivariate Gaussian distribution by the matrix of Gaussian parameters. The extracted patch embedding vectors preserve information from various semantic levels. Each estimated multivariate Gaussian distribution can capture the information from different layers as well and the covariance contains the inter-level correlations.

3. Experimental Results

Considering we have no ground-truth pixel-level fracture annotation, we provide the segmentation results by visualizing the fracture masks. Here Stamp t@k denotes the t time stamp and the k-th slice per 450-slice 3D cube at time t. From the experiments, we notice that there is consistent pattern across different time stamps at the same location, also there is a consistent across continuous slices per same time stamp.





4. Conclusion and Future Work

In this paper, we explored the fractures on 2D slice first (x, y direction) and then integrate them together to reach 3D segmentation (x, y, z direction) by exploring the temporal connection between any continuous slices. The output of this project will provide by integrating three directions, which casts a light in 3D anomaly detection. Thus, we plan to continue working on this problem by exploring both spatial and temporal information to help fracture detection by manually annotating scribble labels, making it possible to explore weakly supervised segmentation technique [5]. Secondly, we will combine the explainable AI techniques into the segmentation models, aiming to provide more hints on specific patterns for fractures.

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