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Machine Learning Enabled Reproducible Data Analysis for Electron Microscopy

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Advances in hardware and computation technologies are enabling large Electron Microscopy (EM) datasets to be produced at rapidly increasing spatial and temporal resolutions. This presents exciting opportunities for microstructure characterization but also poses great challenges in data analysis. We propose to address such challenges by applying machine learning (ML) techniques to improve the efficiency and accuracy of EM image data analysis.

Specifically, we trained ML models from the region-based convolutional neural network (R-CNN) family [1, 2] to detect and segment microstructure features in EM images. The R-CNN models show remarkable performance in processing natural images for use cases like autonomous driving and are recently being used for microstructure image analysis tasks [3]. The R-CNN models have only been applied to analyze a few specific kinds of microstructures until now. However, they are highly generalizable and can potentially handle EM images of very different microstructures. We show this point by training R-CNN models to solve two challenging microstructure analysis tasks. Both tasks are difficult to complete with traditional image processing algorithms.

In the first task, we trained a mask-RCNN [2] model to detect and segment vesicles and holes in a biological image dataset. The vesicle images were taken using the TEM bright field mode. An example image is shown on the right side of Figure 1. There are three major classes of objects in this image: big vesicles (large light regions), small vesicles (dark small regions), and small holes (bright small circles). Note that traditional image processing algorithms (e.g., watershed) do not perform well here because the microstructure features (especially the large vesicles) have low contrast. The dataset contains 14 training images and two validation images. Each image contains approximately 30 large vesicles, 120 small vesicles, and 30 holes. These microstructure features (i.e., vesicles and holes) were annotated by hand and prepared in the Microsoft COCO [5] format for model training. The R-CNN models were first pretrained on the ImageNet dataset to overcome the small size of our image dataset. One mask-RCNNs was trained independently for each detection task using the detectron2 library [4] and model hyperparameters were tuned via random search. The model performed well in detecting the big vesicles and small vesicles. To give some intuitions about the model performance, the segmentation result on one validation image is illustrated in Figure 1. Mean average precision (mAP), one of the most popular segmentation performance metrics from the computer vision community, is used to evaluate the overall model performance [2]. Our model achieved a 95.86 % training mAP and an 86.64 % validation mAP for the large vesicle segmentation task, and a 54.58 % training mAP and a 63.71 % validation mAP for the small vesicle segmentation task.

In the second task, we trained a faster-RCNN [1] to detect overlapping nanorods in a High Angle Annular Dark Field STEM image dataset. An example image is shown on the left side of Figure 2. Note that the nanorods are highly overlapped, which makes traditional contrast-based object detection

algorithms fail on this task. The dataset contains 19 training images and two validation images, covering a total of 1300 nanorods. The nanorods were annotated using a modified version of LabelImg [6] and were converted to the COCO format for model training. Note that segmentation is not needed in this task since the nanorods have relatively regular shapes. Rotated bounding boxes are needed but are not available in the detectron2 library. We developed in-house code to support the rotated bounding box function. We then tuned model hyperparameters via random search and achieved a training mAP of 91.36 % and a validation mAP of 50.51 %. The model performance is illustrated in Figure 2. Note that the training performance is much better than the validation performance (91.36 % mAP and 50.51 % mAP), suggesting that our model is overfitting. This overfitting is probably related to the small size of our dataset (19 training images) and can probably be improved by increasing the number of training images. Nevertheless, note that our current model can successfully detect most nanorods in the validation images (Figure 2c).

With the two microstructure analysis tasks, we show the R-CNN models can be used to detect (and segment) different kinds of complicated microstructure features with a small number (< 20) of training images for each task. Note that once the detection/segmentation is done, microstructure statistics (e.g., size distribution, number counts, shape analysis) can be easily computed from the ML annotated images. Though the image annotation and the ML model training process take some time, a well-trained ML model can analyze many new images with fast speed. This provides exciting opportunities for automated reproducible EM image analysis [7].

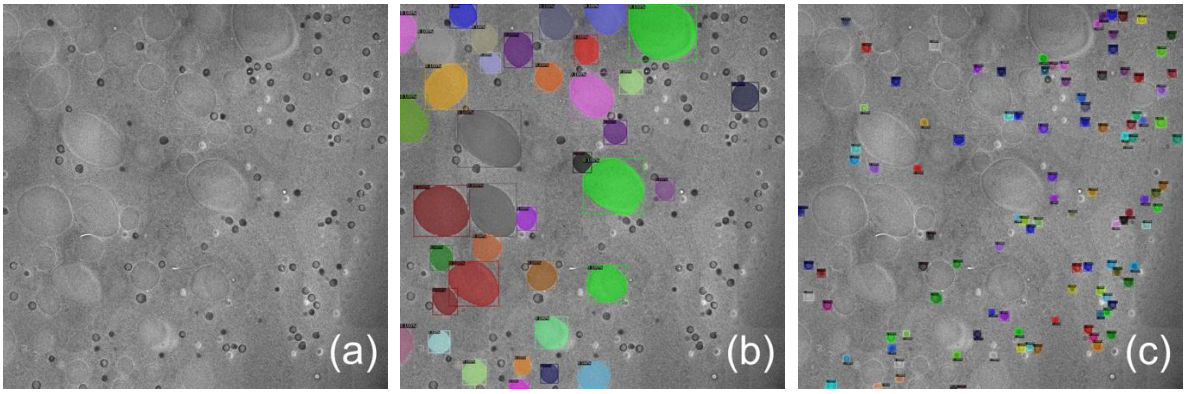

Figure 1. Illustration of the ML model performance on the vesicle segmentation task. (a) An example TEM image from the validation data set. (b) Segmentation performance of the large vesicles. (c) Segmentation performance of the small vesicles.

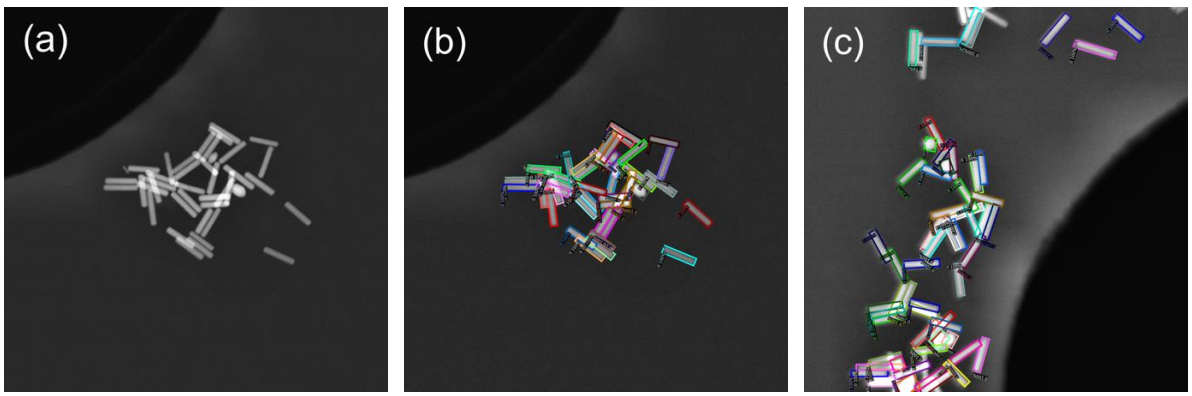

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Figure 2. Illustration of the ML model performance on the nano-rod detection task. (a) An example TEM image from the training data set. (b) Detection performance on the example training image. (c) Detection performance on a validation image.

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