Machine Learning Tracking and Detection for Nanoparticle Feature Analysis

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Summary

Taking measurements for the size and shape of particulate matter in (Scanning) Transmission Electron Microscopy (S)TEM is a difficult task, and is limited by the acquisition method and analysis software. In-situ experimentation is slowed down by this additional analysis stage, calling for a fully automated approach to the measurement of the morphology of nanoparticles. Recent strides in deep learning present improved potential for efficient prediction for particle tracking and morphology analysis. This project presents an approach for the segmentation of particles from the background, calculation of their morphology and analysis of their topology inspired by MASK-RCNN.

Background

Quantification and mapping of and shape (morphology) of nanoparticles and their special arrangements (dispersion) within the reactive medium are a key analytical measure for understanding the chemical processes behind dynamic chemical observations. Extracting quantitative information from nanoscale images is a repetitive and costly process, often made more difficult by the low-signal/noise ratio in the images resulting in many images incomplete or rapidly varying from frame to frame.

In-situ STEM experiments are bottlenecked in part by the manual/semi-automated processing of particle morphology calculations on existing software. Particles are often difficult to discern with constraints of large disparities in their noise patterns, spatial/temporal resolution, magnification or low signal-to-noise ratio.

Convolutional Neural Network(s) (CNNs) are an established architecture for real-time object detection and segmentation. R-CNN introduced a region proposal mechanism using a CNN and a linear search algorithm. Multiple advancements were subsequently made in terms of speed and efficiency

Aims and Objectives

The aims and objectives for this project are as follows:

- Compare state of the art machine learning models such as Mask-RCNN, Mask-RPN, Mask-FPN and U-Net for the feature recognition and morphology tracking of nanoscopic particles.
- Develop a performant CNN model for the tracking and analysis of Nanoparticles with high levels of noise in STEM microscopy images.
- Integrate an efficient and performant CNN model for use with subsampled images.

Results

A comparison of existing network architectures need to be evaluated for their accuracy and efficiency to aid analysis in chemical microscopy. In Figure 2, recent results have been a transfer learning approach was applied to the MASK-FPN/RPN network using Coco weights at the inception of training. The nucleus dataset [4] was leveraged due to the similarity of the available data.

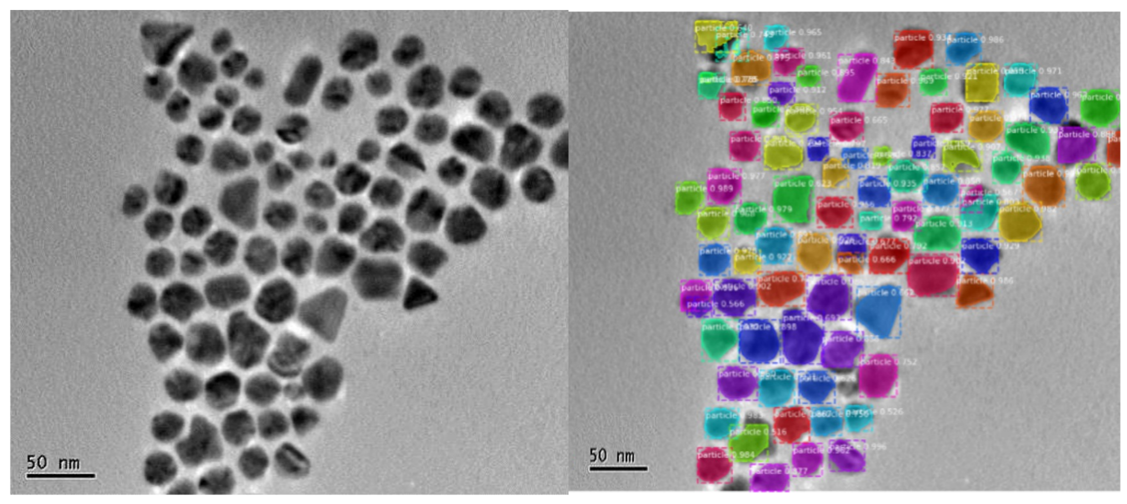

Figure 2: Transfer Learning MASK-FPN/RPN results for particle prediction from our training and network reshaping [2]. Strong preliminary results from transferring learning from Coco [4] network weights, freezing all expect the final three layers and training with more suitable data.

Proposed model

Our work extends upon work such as this by developing a suitable convolutional neural network architecture for multi-target tracking and segmentation of nanoparticles (Figure 1).

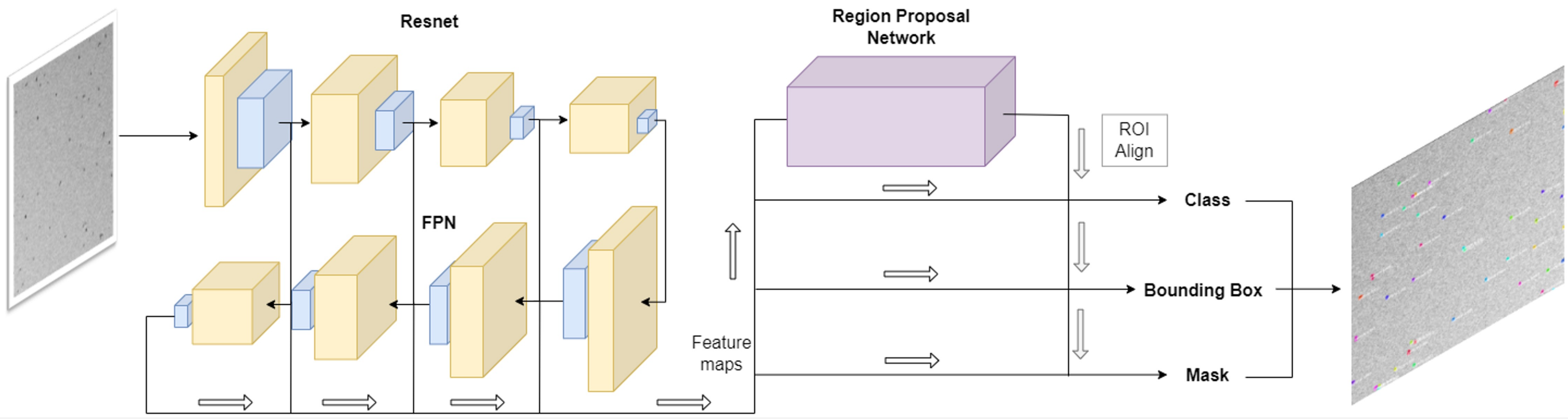

Figure 1: Network architecture for Deep Learning implementation of segmentation and region proposal network inspired my MASK-RCNN, FPN and Faster R-CNN.

Future Work

This work aims to contribute towards further machine learning based automation in the SEM/(S)TEM experimentation pipeline. Future aims include:

- Developing noise-imperviousness. Accommodating for high amounts of noise and varying degrees of contrast in image data.
- Developing a temporal tracking mechanism for video data (tracking and calculation of morphology and dispersion in real-time).
- Apply model to sub-sampled data. Overcome challenges posed in sub sampled scanned SEM images with a compressed-sensing input and input mapping.

References

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