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Understanding the Role of Neural Network Complexity and Receptive Field in Identifying Nanoparticles in TEM Images

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Trained neural networks are promising tools to analyze the ever-increasing amount of scientific image data, but it is unclear how to best customize these networks for the unique features in transmission electron microscopy (TEM) data. While there are many established architectures from the computer vision community, smaller scientific datasets make large networks infeasible, while smaller networks are harder to improve because it is not clear how architectural constraints affect network performance on TEM images. Architectural constraints include how deep or complex a network is, as well as a network's receptive field, which is the area of the input image that influences a network's final decision. Prior research, in particular, has suggested that networks need to adapt the receptive field to account for the larger feature sizes in TEM images [1].

Here, we systematically examine how neural network architecture choices affect how the networks segment, or pixel-wise separate, crystalline nanoparticles from amorphous background in TEM images. Our base neural network architecture is a UNet structure consisting of residual blocks, which allows for modular changes in network complexity. By comparing performance as we vary the max pooling filter size or the number of trainable parameters, we decouple the effects of receptive field and network complexity [2]. Segmentation performance is evaluated using the dice score which quantifies similarity to the ground truth label between 0 and 1. We focus on two TEM imaging regimes: standard imaging which relies on contrast to distinguish nanoparticle from background (Figure 2a), and high-resolution imaging which depends on both contrast and lattice-fringe texture to identify nanoparticles (Figure 2c).

Receptive field does not majorly impact segmentation performance in standard TEM images, but is a key parameter that limits performance in high-resolution TEM images. Using a dataset of 20nm Au nanoparticles, we find that segmentation performance remains relatively constant as receptive field increases and only slightly improves with greater network complexity (Figure 2b). On the other hand, when networks are trained on a dataset of 5nm Au nanoparticles, segmentation performance instead improves with larger receptive fields before plateauing (Figure 2d). From qualitative analysis of the segmentation results, the smaller receptive field networks struggle with nanoparticle areas with fainter or no visible lattice fringes, suggesting that they have learned a function similar to Fourier filtering. By comparing trends across multiple datasets with differing nanoparticle sizes, we also hypothesize that the larger receptive field is necessary to capture larger-scale changes in contrast, especially for small, low-contrast nanoparticles. Our results provide guidance as how to adapt neural networks for TEM datasets, particularly for small datasets with unknown amounts of phase and/or amplitude contrast.

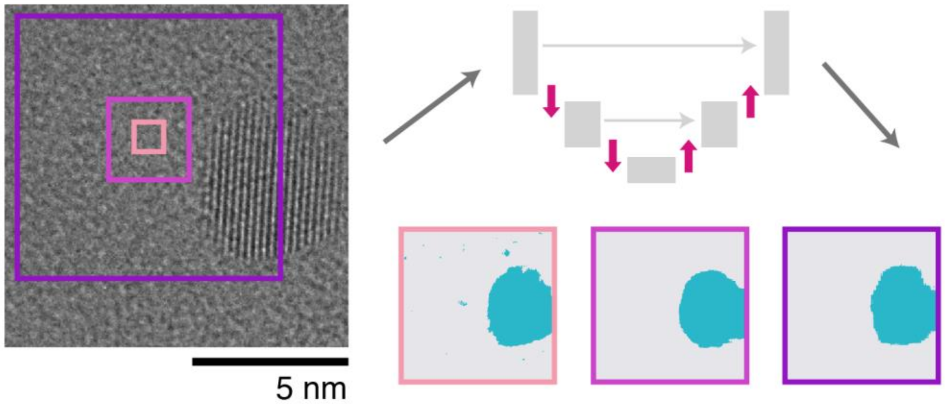

Figure 1. Schematic of the computational setup. Multiple neural networks with a UNet architecture are trained to segment nanoparticles in TEM images. The networks vary in their receptive fields (peach, pink, purple boxes superimposed on the TEM image), and segmentation performance is then compared.

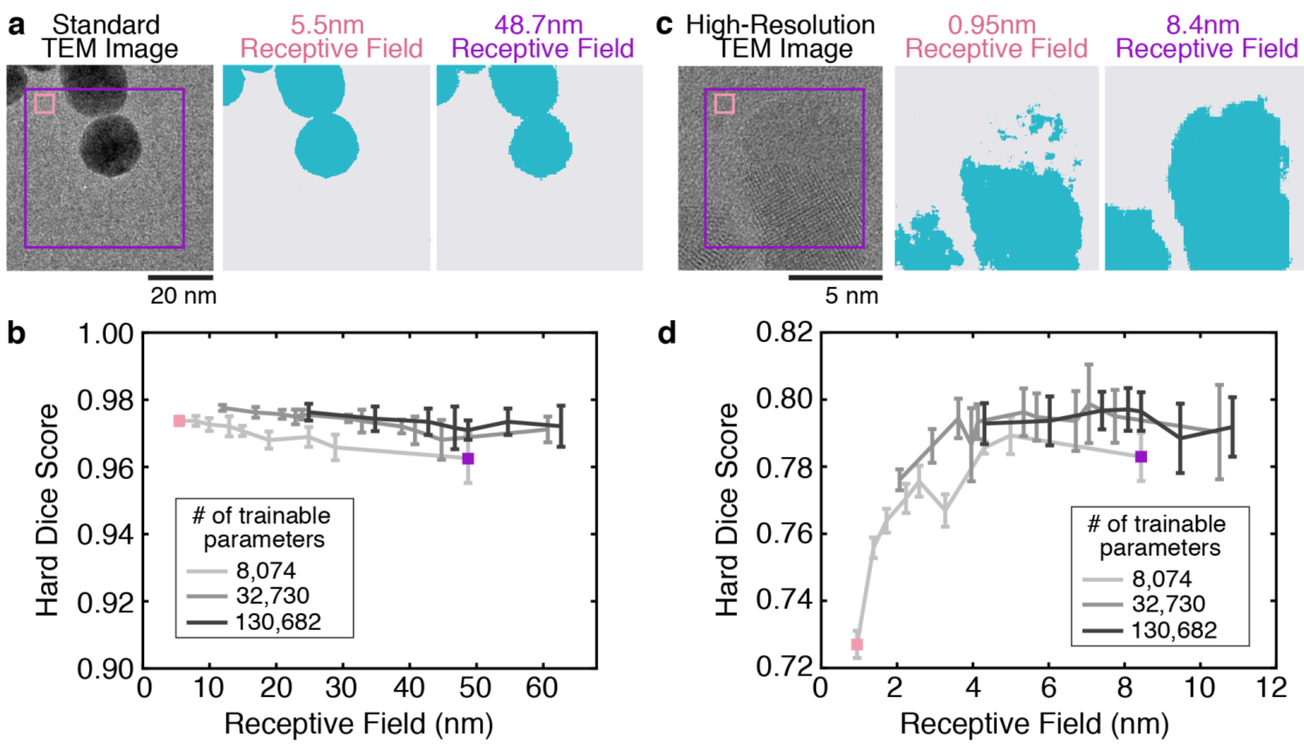

Figure 2. Segmentation performance as a function of receptive field for (a,b) standard TEM images and (c,d) high-resolution TEM images. (a) Example standard TEM image of 20nm Au nanoparticles with superimposed squares denoting the relative sizes of a 5.5nm and 48.7nm receptive field, and segmentation results from networks with the aforementioned receptive fields. (b) Segmentation performance on standard TEM images for three different network complexities. Pink and purple dots highlight the networks that produced the results in (a). (c) Example high-resolution TEM image of 5nm Au nanoparticles with superimposed squares denoting the relative sizes of a 0.95nm and 8.4nm receptive field, and segmentation results from those same networks. (d) Segmentation performance on high-resolution TEM images for three different network complexities. Pink and purple dots highlight the networks that produced the results in (c).

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