doi:10.1017/S1431927622011667
Microsc. Microanal. 28 (Suppl 1), 2022

Gated Dense Convolutional Neural Networks for Unbalanced Representations in STEM Tomography

Arda Genc [1]*, Libor Kovarik [2], Hamish L. Fraser [1]

[1.] Center for the Accelerated Maturation of Materials, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA
[2.] Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, USA
* Corresponding author: genc.2@osu.edu

It is well-known that manual image segmentation of vast 3D data sets is a challenging task in computed electron tomography and has been one of the most significant hurdles in comprehensive 3D analysis. A volume rendering approach has often been preferred for 3D visualization owing to its simplicity and speed, even though a detailed representation of the features in 3D is compromised, leading to the loss of critical morphological and quantitative information. To address this problem, we have investigated deep learning architectures of U-Net with specific decoder units' variants using the 3D analysis of a γ-Alumina (Al_2O_3)/ Pt catalytic material in a class imbalance situation [1,2,3]. In heterogeneous catalysts, complex surface structure, relatively poor intrinsic contrast of the oxide support material, and sparse distribution of the catalytic nanoparticles over the background of TEM images present a significant challenge for pixel-wise image classification, including the current state-of-the-art deep learning-based modalities.

We compared the results obtained from the U-Net architectures in the form of a standard U-Net, U-Net with the additive attention gates, and U-Net with the attention gates and residual connections, as shown in Figure 1. Self-attention gates have been introduced in Natural Language Processing (NLP), aiming to enrich the contextual information and improve the robustness of the recurrent neural networks [2]. Recently, it has been adapted in convolutional networks to mainly suppress the irrelevant feature mapping through the skip connections and thus, enhance the performance of the classification models [4]. We discuss the accuracy of our segmentation results by assessing the commonly used semantic segmentation metrics on the overall overlap between the ground-truth and predicted segmentations, as shown in Table.1. Preliminary results on the validation data sets have demonstrated comparable effects on the segmentation performance of the U-Net models for the γ-Alumina segmentation task and relatively higher performance for Pt nanoparticle segmentation with attention units. Figure 2. visualizes exemplar segmentation results from γ-Alumina and Pt nanoparticles, respectively. For each patch of the validation data, ground-truth and predicted segmentations of γ-Alumina and Pt nanoparticles are compared separately in the binary images. An example of differences in the segmentations of the standard U-Net model is shown explicitly in the false negative and false positive maps highlighting the discrepancies in the overlap of each class. Nevertheless, the deep learning-assisted automated semantic segmentation of the HAADF STEM tomography reconstructions unlocked the comprehensive 3D visualization of the catalytic material and a clearer insight into the long-standing debate on the characteristics of γ-Alumina surfaces and their relationship with the catalytic Pt nanoparticles [3], as shown in Figure 3.

This work fully exploits open-source resources in deep learning and computed electron tomography analyses. The electron tomography study was conducted using a Python programming script based on the tomviz software for the image shift and tilt alignments and TomoPy and ASTRA Toolbox for the maximum likelihood expectation maximization (MLEM) reconstructions. Paraview software was employed to generate 3D visualizations from the fully segmented reconstructions.

References:
[1] O. Ronneberger, P. Fischer, T. Brox, U-Net: Convolutional Networks for Biomedical Image Segmentation, In International Conference on Medical Image Computing and Computer-Assisted Intervention, 9351 (2015) 234-241.
[2] A. Vaswani, et al., Attention is All You Need, arXiv 1706.03762v5 (2017).
[3] A. Genc, L. Kovarik, H.L. Fraser, arXiv 2201.07342v1 (2021).
[4] O. Oktay et al., Attention U-Net: Learning Where to Look for the Pancreas, arXiv 1804.03999v3 (2018).

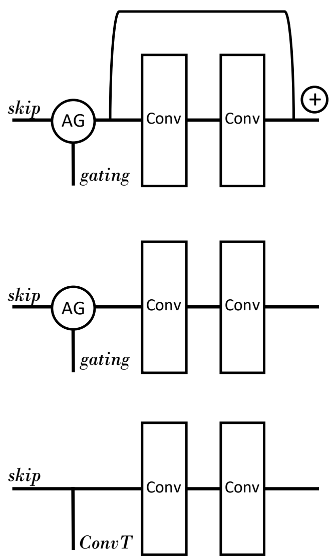

Figure 1. Variants of the decoder units.

Table 1. Evaluation performance of the U-Net architectures.

	γ-Alumina	Pt NPs	Bckgrnd/Pores
Method	Dice Similarity Coefficient		
U-Net	0.963	0.844	0.992
Attention U-Net	0.963	0.864	0.992
Attention Res-U-Net	0.963	0.872	0.992

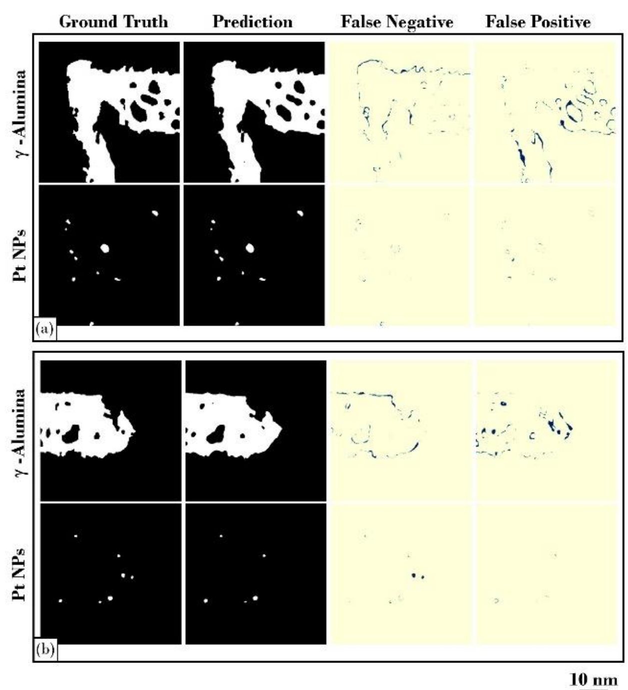

Figure 2. Ground-truth and predicted segmentations, and false negative and false positive maps.

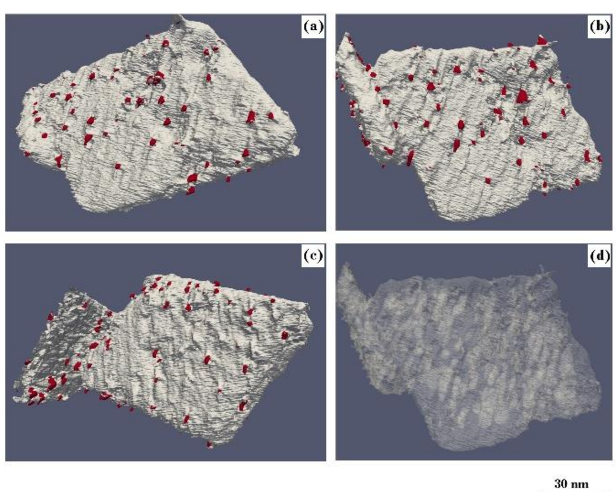

Figure 3. 3D visualizations of the γ-Alumina catalytic particle and Pt nanoparticles.

https://doi.org/10.1017/S1431927622011667 Published online by Cambridge University Press