PNNL-34713

Multimodal Few-Shot Segmentation of Electron Micrographs

August 2023

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U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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operated by
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for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC05-76RL01830

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Abstract

Scanning transmission electron microscopy (STEM) is one of the most used methods of analyzing the chemistry and composition of materials. By analyzing microstructures, these microscopes can help scientists better understand the molecular underpinnings of microelectronics, batteries, and more. However, STEM data can be difficult to interpret, so recent developments have been made in applications of machine learning to analyze these images. The PNNL-developed pyCHIP Classifier has achieved results in segmenting STEM these images via few-shot learning, a method which requires little data and human input, perfect for quickly analysis. In my internship I (Eli Meyers) investigated a multimodal improvement of this classifier by incorporating energy dispersive x-ray spectroscopy (EDS) data into the classification process for a more accurate segmentation. Furthermore, I encoded the spectral data by training a mass spectrometry encoder on the EDS data to extract a more meaningful representation of the data.

Acknowledgments

Thank you so much to Steven Spurgeon, Jenna Pope, Sarah Akers, Arman Ter-Petrosian, Bethany Matthews, and Sarah Akers at PNNL. Steven made time in his busy schedule to mentor me through my internship. Sarah helped me understand the multimodal classifier and introduced me to spec2vec. Jenna introduced me to skimage and atomap, helped me set up spec2vec, and helped me work through the many technical problems with my environments. Arman helped me use Atomap, and Bethany provided spectral data and helped me understand it. Some of the microscope data was collected in the Radiological Microscopy Suite (RMS), located in the Radiochemical Processing Laboratory (RPL) at PNNL.

This work was supported by the Chemical Dynamics Initiative / Investment (CDi) Laboratory Directed Research and Development (LDRD) program at Pacific Northwest National Laboratory (PNNL). PNNL is a multiprogram national laboratory operated for the U.S. Department of Energy (DOE) by Battelle Memorial Institute under Contract No. DE-AC05-76RL0-1830. STEM was conducted in the Radiological Microscopy Suite (RMS), located in the Radiochemical Processing Laboratory (RPL) at PNNL. Some sample preparation was performed at the Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research and located at PNNL.

Contents

1.0 Introduction

Material science is on the cusp of a data revolution. The current state of materials science has unprecedented control over the structure of materials. With this ability, the focus of material sciences is shifting to analyzing the properties and structure of materials at a large scale to use data to improve our understanding of process-structure-property (PSP) linkages.

Recent efforts have been made to implement machine learning algorithms to improve our (analytical) understanding of materials by analyzing electron micrographs. Electron microscopy allows an unparalleled level of vision into the molecular structure of a material. By improving our methods of analyzing these images, we can further grasp how the structure of the material influences its properties.

To this end, our team has developed the pyCHIP classifier, a machine learning model which can segment electron micrographs (Akers 2021). Unfortunately, electron microscopy lacks big data with regards to analyzing these images, so the few-shot uses minimal human supervision and extraneous/other data. In this internship, I improved on this few-shot learning model by incorporating other modes of data, particularly energy dispersive x-ray spectra (EDS) data. Transmission electron microscopes (TEM) provide two forms of images with each (micrograph), so by incorporating both modalities of data, we can to better segment the micrographs.

2.0 Results and Discussion

Few-shot learning is a supervised machine learning algorithm which classifies vectors using minimal human input (Snell 2017, Pahde 2020). To perform few-shot segmentation on an image, the image is ‘chipped’ into a grid, and then those chips are clustered in the following way. First, a few representative samples, or ‘supports’, are chosen from each intended class. Then, the support chips are encoded using an image encoder. For each class, the support chip embeddings are averaged into a single prototypical member of the class, and each chip is classified with the closest prototype to its embedding under the Euclidean metric (Akers 2021).

The benefits of few-shot analysis come from the human supervision and that it only requires the image needed for segmentation and no other data. The pyCHIP classifier using only image data proved useful, but with the addition of spectra data, we can greatly improve the accuracy of the model. We will segment the image using spectral data alone, with and without an encoder, and finally we will incorporate the spectral data and the image data together to create the multi-modal pyCHIP classifier.

2.1 Few-Shot Spectral Classification

Few-shot segmentation has been successful using microscope image data, but we can also use the spectral EDS data generated by the (TEM microscope). To implement few-shot classification from the spectral data, we create the chips by summing the spectrum at each pixel of the image to create a detailed spectrum representing the entire chip as in Figure 1. First, we preform few-shot without a spectral encoder. The structure of the spectra data lends nicely to the Euclidean distance metric. The peaks in spectra indicate different concentrations of elements in that specific chip, so close together spectra under the Euclidean metric will have similar atomic breakdowns.

Spec2Vec has been a very successful in encoding mass spectra (Huber 2021). Because it uses unsupervised learning and trains on a database of spectra, we can train it on EDS spectra instead. the spectral chips as the training data. We lack a large versatile dataset as in Huber 2021, but training a spec2vec model on the spectral chips still showed accurate results.

Figure 1 shows a comparison of the spectral classification on samples. It seems very effective at picking out the difference of atomic structure, but less effective at picking of properties of the atoms. The first two rows have samples which are different materials in each segment, whereas the bottom row shows an experiment where sections of the image are irradiated.

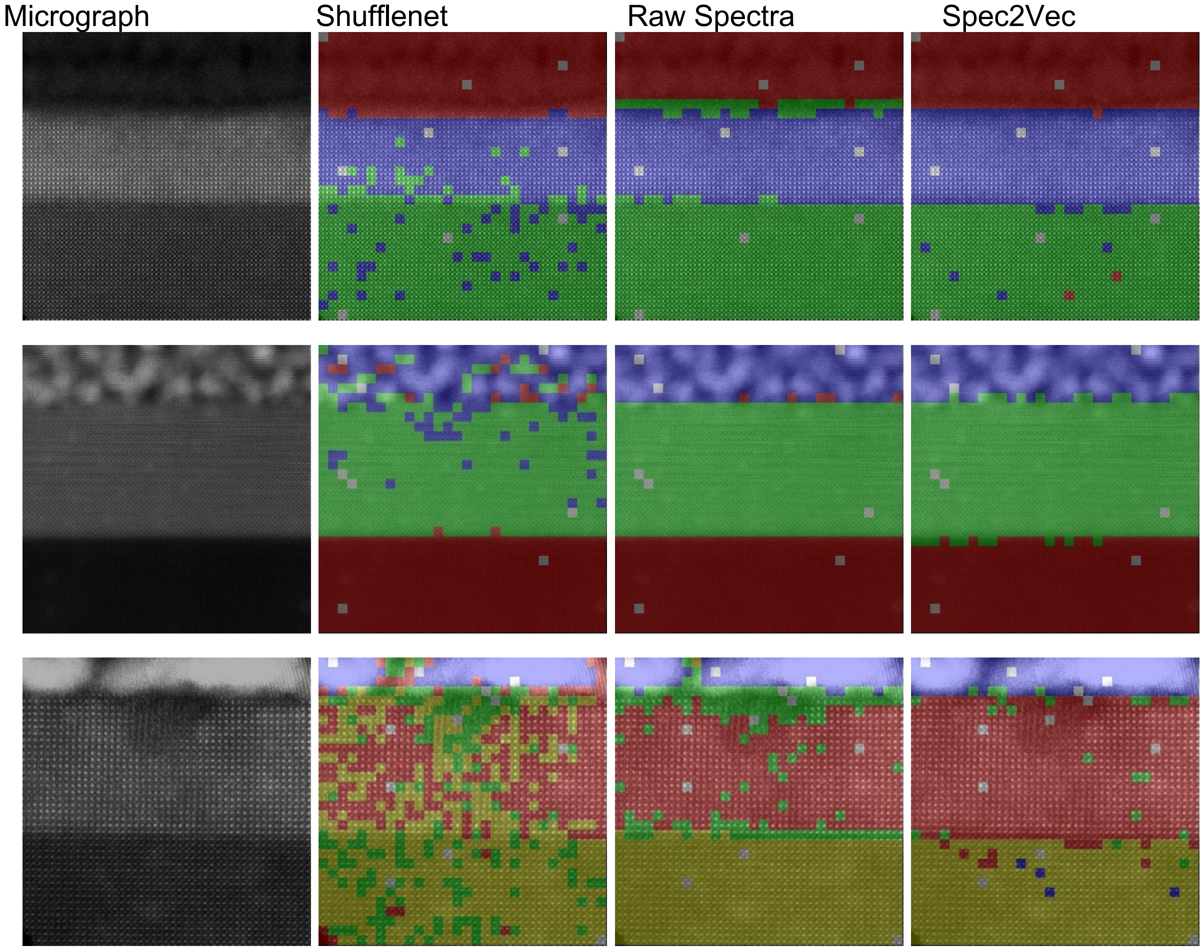

Figure 1. This figure compares image classification to raw EDS spectral classification to spec2vec classification. Each row is a different sample. The left column is the image classification result, the middle is raw spectra, and the right is spec2vec. The grey squares are the chosen supports for each class.

2.2 Multimodal Classification

Improving the signal-to-noise ratio (SNR) is an important concept in data processing. By incorporating both forms of data, we effectively increase the SNR. To combine both the spectra data and the image data for multi-modal few-shot classification, we have two new considerations: (a1) how we encode the spectra data, and (a2) how we recombine the spectra and image data to ultimately classify the chips.

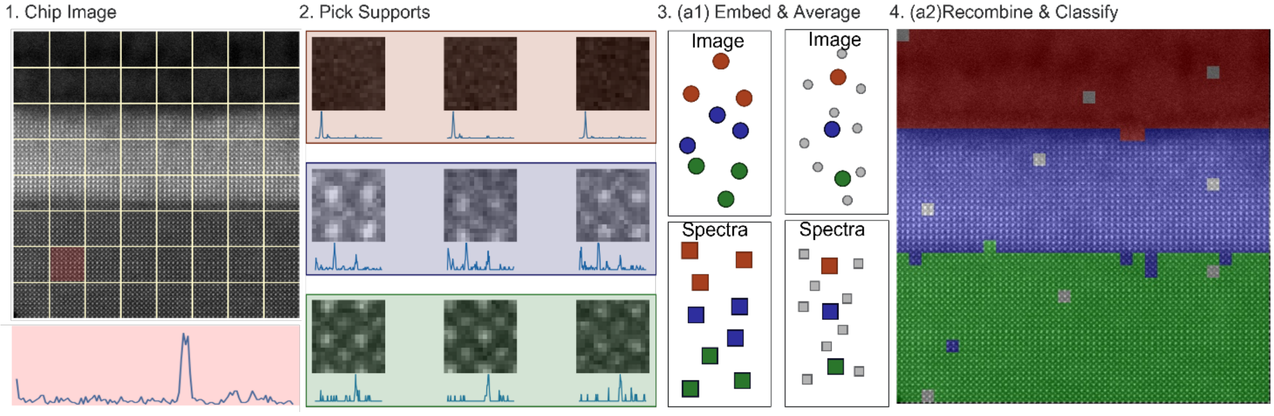

Figure 2. Multimodal few-shot classification diagram. First the image is chipped into small squares. The spectral chips are generated by summing the spectra at each pixel of the image. The chips in this image are larger to show the concept. Second, the supports are hand-picked by the scientist to represent the image. Third, the image and spectra of supports are embedded separately and then averaged to create the prototypes for each support. Finally, the distances are generated according to the protocol selected, and each chip is classified by its closest prototype. In this example we used spec2vec encoding (b2) and computed distances separately and then averaged (c2).

We process the image data as in the pyCHIP implementation, with a Resnet encoder and Euclidean distance. With respect to (a1), we (try) both (b1) raw encoding, where the spectra vectors are used as the embedded vectors, and (b2) spec2vec encoding, and with respect to (a2), we (try) both (c1) concatenating the embedded vectors and then taking the Euclidean distance between the new vectors and (c2) computing the distances separately and then scaling and averaging the distances.

The problem with (c1) concatenating the vectors is that the distance between image embeddings and the image prototype tended to be much smaller than that between spectral embeddings and spectral prototypes. With (c2), we generate the distances between all (embedding, prototype) pairs for spectra and image separately, and then divide all the spectra by the biggest spectral difference and do the same for image distances. Then we average the resulting scaled differences to classify each chip. The result seems to cancel the error in each unimodal model to improve the overall classification.

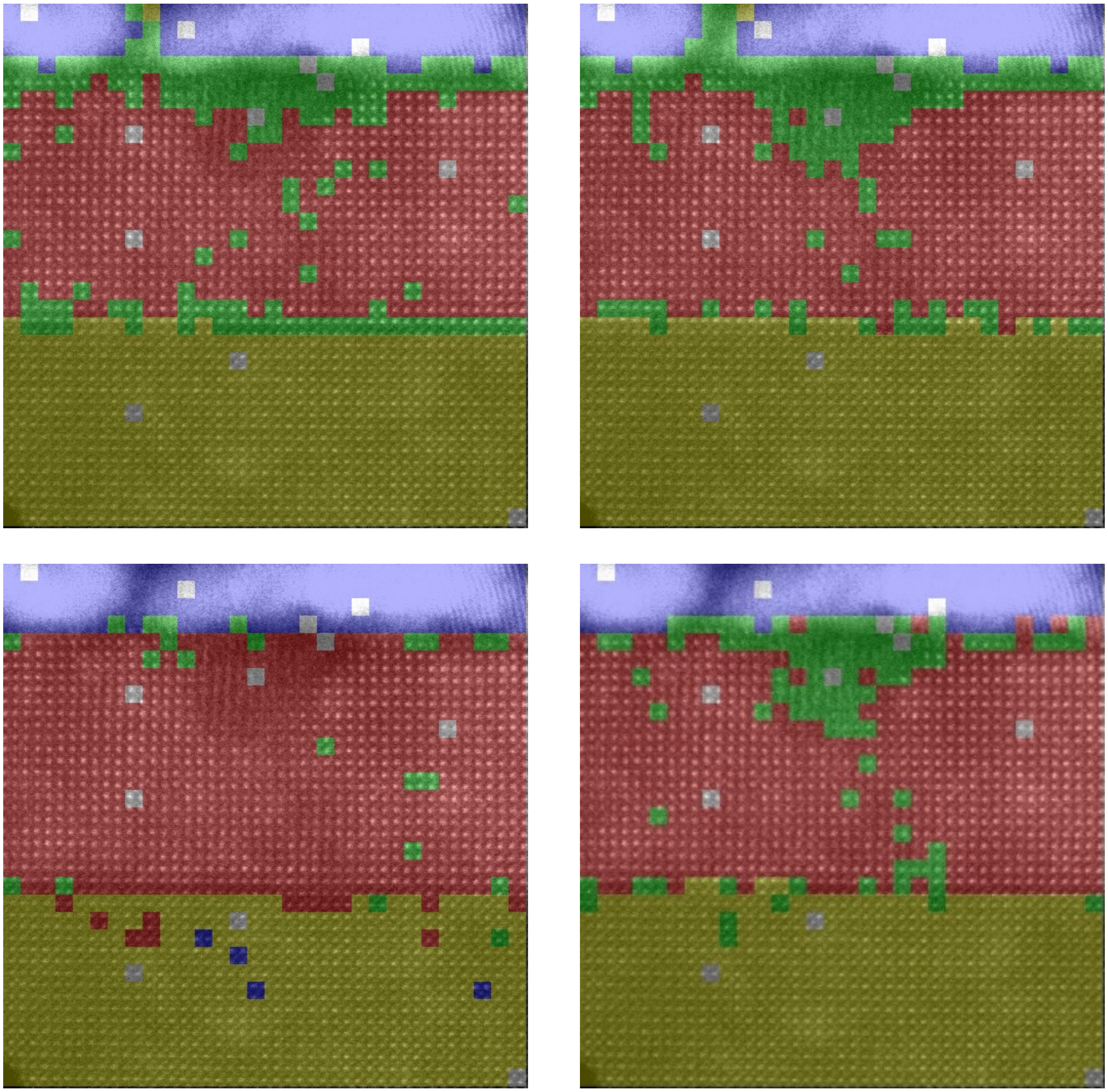

Figure 3. This figure shows all 4 possibilities on a sample image. The left column uses concatenation whereas the right column norms and then averages, and the top row uses raw spectra whereas the bottom uses spec2vec encoding.

2.3 Atom Analysis

With these microscopy images of the atomic structure of materials, looking specifically at the atom positions Another way to mode of data we can use is the atom positions within the micrograph. To identify the atoms, we use the Laplacian of Gaussian method on the entire image, and then we refine the atoms with tools from Atomap (Nord 2017). We do not use Atomap for the entire image because it struggles with sections of differing atomic structure, whereas the Laplacian of Gaussian is more versatile, but ultimately Atomap has useful abilities to solidify the structure. Once the atoms are generated for the full micrograph, we look at the atoms on each chip and compute the pair distribution function for each. We then compare these distributions using Wasserstein distance.

3.0 Conclusions

In this internship, I produced preliminary results for how we can use the spectral data to analyze electron micrographs. Because of its more (detailed) nature, the EDS data proved very useful in few-shot segmentation. Even the raw spectra improved on the image based few-shot segmentation, and the multi-modal model incorporating spec2vec as a spectral encoder seemed much more formidable.

EDS data will prove very useful as machine learning techniques to analyze microstructures. Though some are beginning to be developed, spectral encoders are very much in their infancy. With respect to Spec2vec in particular, EDS spectra do not have the same abundance of data as mass spectrometry, but with a similar dataset to the training data in Huber 2021, the encoder would much more effectively reduce the data to a more meaningful embedding. With more data, we also would be able to better compare segmentation methods. Other algorithms have recently been developed to denoise spectral data (Ozawa 2023), which would be great next steps to incorporate into the few-shot classifier.

Microscopy images can also be better analyzed. By using the atom positions in the images, we can improve the image analysis aspect of the multimodal encoder. There may be more useful ways of comparing the positions beyond just pair distribution functions. EDS data can be used in other forms of analysis. As other forms of machine learning are developed to segment or otherwise analyze electron micrographs, the spectral data can be useful there as well.

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