Machine Learning Approaches to Predict Properties from Microstructure Images in Ceramic-Metal Composites

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Objective:

Predict electrical conductivities of composites of $Li_4Ti_5O_{12}$ anode and Ni current collector particles from SEM microstructure images and identify which microstructural features contribute the most to conductivity for different samples.

Motivation:

Samples of composite oxide batteries were processed to design structural batteries for aerospace applications. These solid batteries have high energy densities and increase safety while not requiring the parasitic waste of casings because there are no liquid electrolytes [1]. Specific electrical conductivities are achieved through the microstructure, and this project identifies which microstructural features lead to certain conductivity ranges.

Data & Processing:

- 58 samples, each with 1 average conductivity measurement and 3 SEM images (10,000x)
- Conductivities evenly distributed 10^{-2}-10^{4} S/cm.
- All images have the same dimensions and pixel count.
- Image processing in Python with OpenCV package normalizes for inconsistencies in sample preparation and imaging so human factors do not influence future modeling.
- Transform images using flipping and rotation while preventing redundancy or warping.
  - Microstructural features preserved but reoriented.
  - Isotropic properties ensure physical systems are not misrepresented.
  - Turn one image into six all using the same conductivity value.
  - Compensates for original sparsity of data.

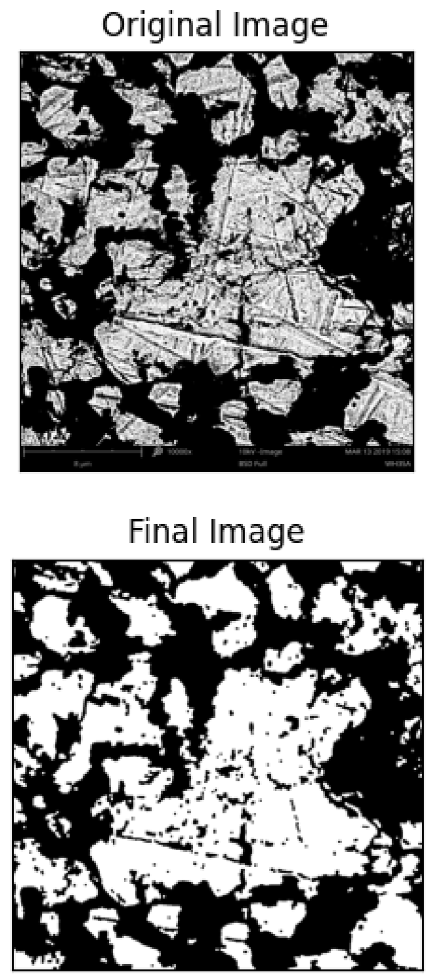
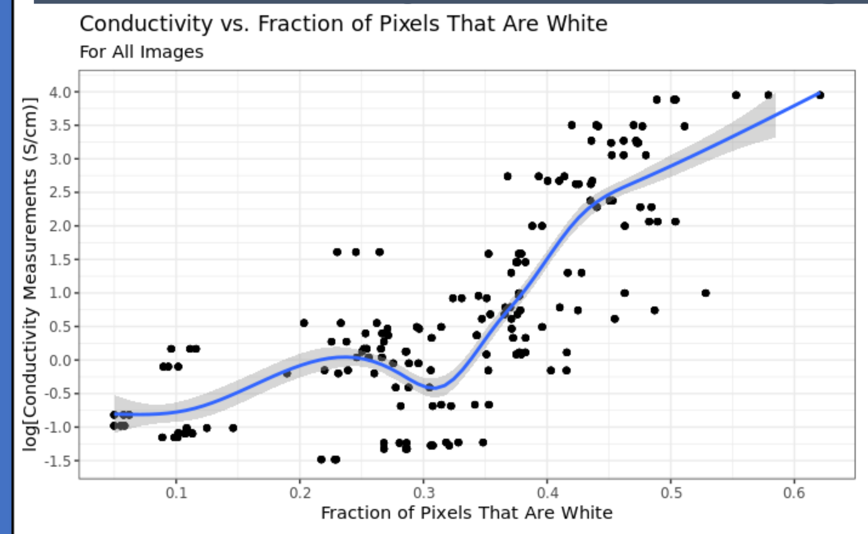


Figure 1. Example of image before and after processing.

References:

[1] W. Huddleston, F. Dynys, and A. Sehirlioglu, Nickel percolation and coarsening in sintered Li4Ti5O12 anode composite, Journal of the American Ceramic Society, vol. 103, no. 8, pp. 4178-4188, 2020, doi: https://doi.org/10.1111/jace.17159.

EDA & Simple Modeling:



- Relationship between fraction of picture that is associated with Ni (white) and conductivity.

Figure 2. Conductivity as a function of fraction of pixels that are white in SEM images.

- Modeling this relationship with no regard for spatial distribution serves as a baseline.
- Generalized linear models (GLM) fit on training data with a degree of 4 performing the best on the testing data.
  - Mean absolute error (MAE) = 0.7246, r^2 = 0.6302

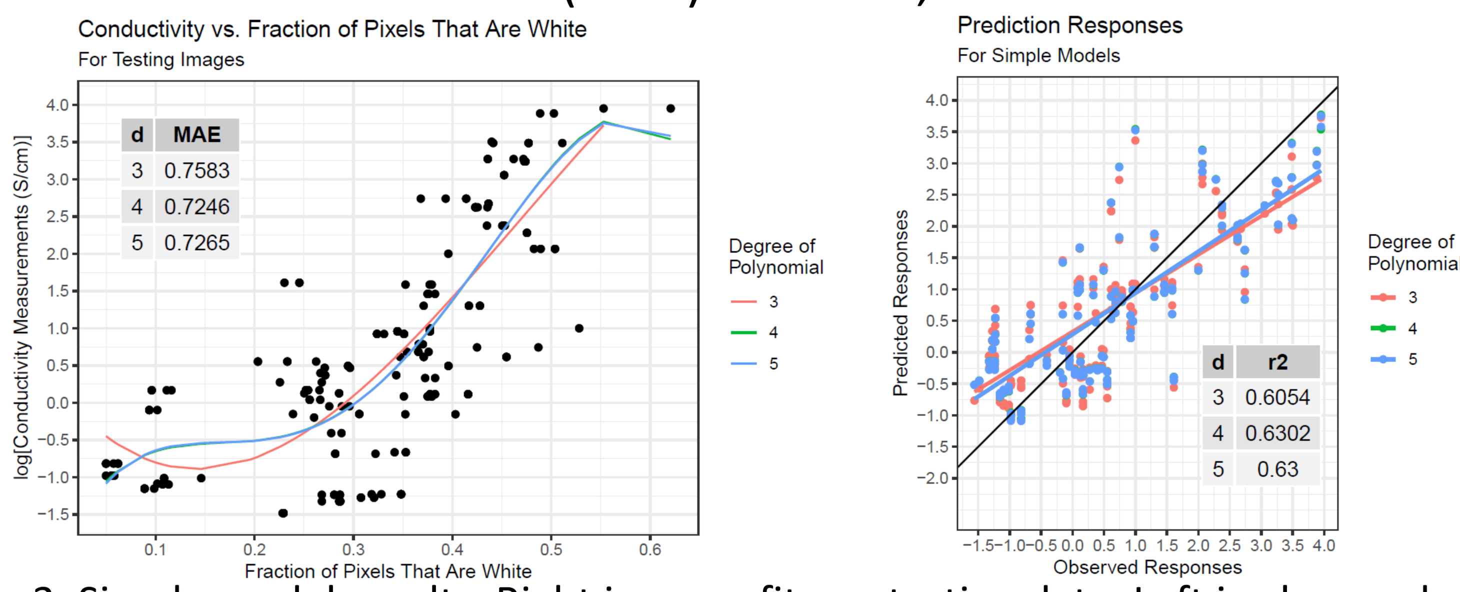


Figure 3. Simple model results. Right is curve fits on testing data. Left is observed and predicted responses for the different curve fits.

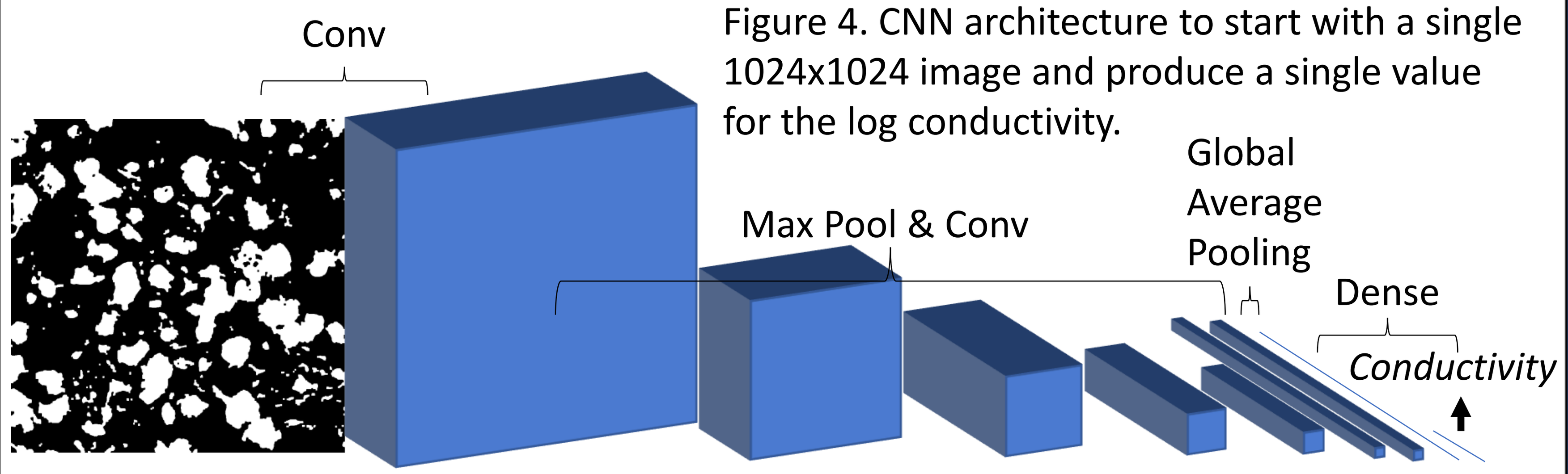


Figure 4. CNN architecture to start with a single 1024x1024 image and produce a single value for the log conductivity.

Deep Learning:

- Convolution neural network (CNN) to determine conductivity directly from images.
- Takes spatial distribution into consideration.
- Alternate between convolution (with padding) and maximum pooling layers then global average pooling and dense layers to produce a single value.

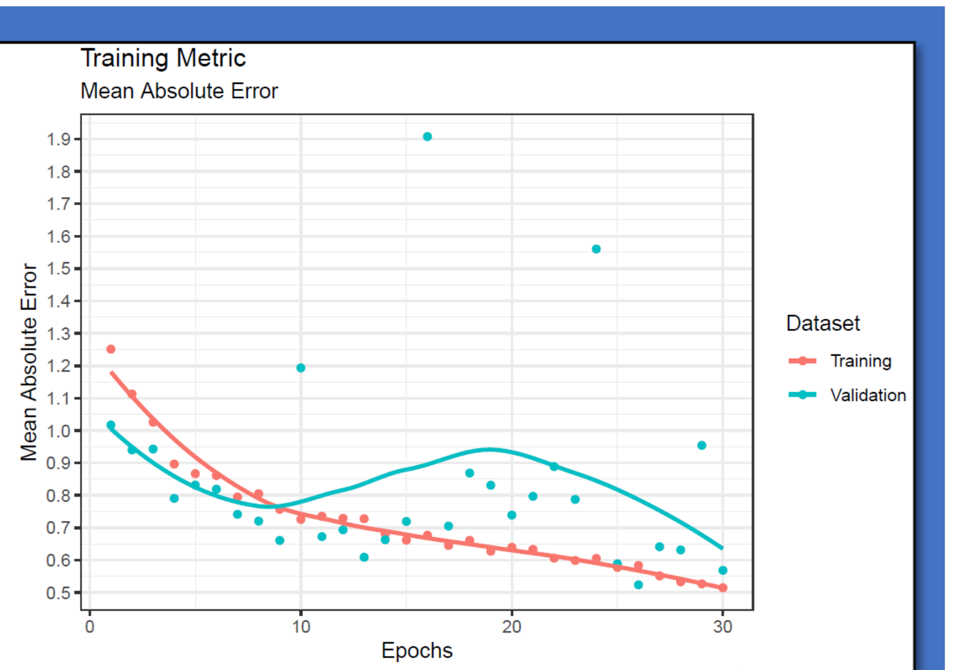
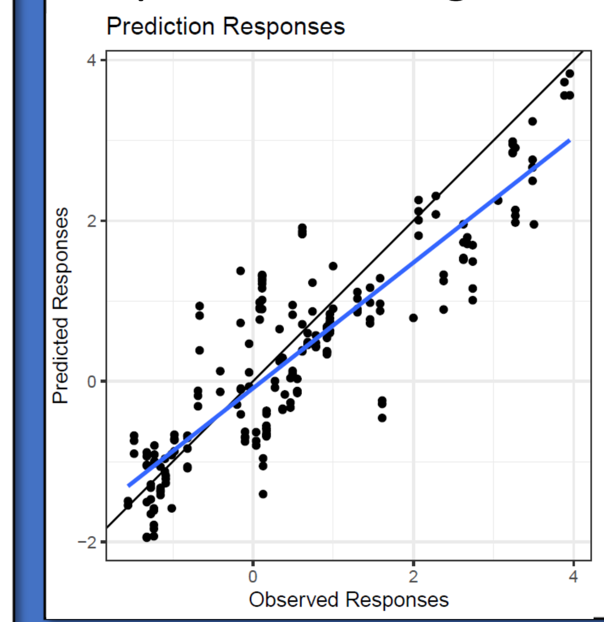


Figure 5. MAE of training and testing (here called validation) data through 30 epochs of training the CNN model.



- Sparse data set for this type of modeling prevents consistent convergence but general outperforms GLM's.
  - MAE ≈ 0.6, r^2 ≈ 0.7

Figure 6. Observed and predicted responses for the testing data from the CNN model with the black line representing perfect prediction and blue line showing the linear regression of actual results.

Regression Activation Map:

- CNN allow creation of activation (heat) maps.
- Use on testing images to determine which microstructural features contribute most to conductivity for each sample.
- Able to engineer desired microstructure and processing conditions to achieve it.

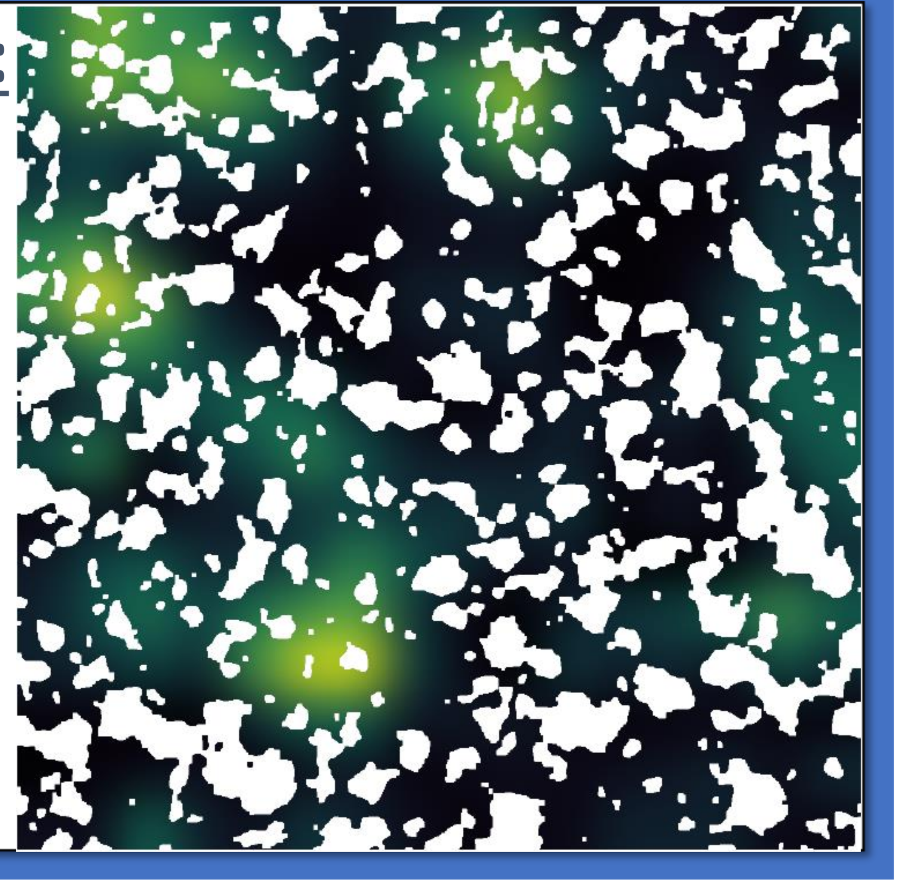


Figure 7. RAM for most accurate testing image prediction for CNN from above.