(U) Physics-Informed Deep Learning with Uncertainty Quantification for Weapons Radiography

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Executive Summary

Deep neural network (DNN) models have the potential to provide significant predictive power for a multitude of applications using Nevada National Security Site (NNSS) image data including radiographs, high-speed footage, accelerator data, and aerial monitoring images. However, for these models to be relevant and assimilated within the weapons community, physics-interpretable uncertainty quantification (UQ) of DNN outputs must be provided. This project explores physics-informed DNN models that predict continuous values using image data as inputs, and methods for quantification of the uncertainty associated with the estimates provided by the models.

Description

DNN ensembles, with prediction uncertainties, were developed using a publicly available image dataset comparable to NNSS datasets. The dataset, provided by the Joint Center for Artificial Photosynthesis (JCAP), consists of 179,072 images of metal oxides printed onto glass slides. Each of these images has a corresponding absorption spectrum over the range of visible light frequencies. Ultimately, our objective was to use an ensemble of DNN models to predict a continuous absorption curve corresponding to each of the images in the dataset. Each of the DNN models in an ensemble gives slightly different predictions by randomly dropping out layer nodes, enabling us to calculate an average prediction and corresponding error bars/envelopes.

Prior to developing DNN models, several pre-processing steps were applied to the image data. In particular, we implemented two dimensionality reduction techniques to reduce the data from 64 x 64 x 3 element arrays to 100 x 1 arrays. The two methods implemented were principal component analysis and variational autoencoders. Dimensionality reduction is necessary to ensure that DNN models can effectively learn parameters and provide robust predictions. As a second pre-processing step, we enhanced our image dataset by applying skew, rotation, translation, and noise to individual images, while retaining their corresponding output. This allowed us to considerably increase the number of samples that models can learn from, as well as provide more robust models (i.e., models are able to provide reliable predictions for absorption curves despite significant changes to the images). As a final pre-processing step, we reduced the absorption curves to condensed representations (22 element vectors) using autoencoders (AEs). DNN models, therefore, were specifically trained to use images to predict the AE representations of the spectra, and subsequently the compressed predictions were used to fully reconstruct the spectra. While dimensionality reduction techniques do lead to some information loss, we found that they improve the general performance of models.

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DNN ensemble performance was compared to results published by Stein et al. (2019) using correlation coefficient and absorption error metrics. Our results closely match the trends of the published results (Figure 1), with slight improvements for the R-squared and Pearson coefficient scores. It should be noted that the correlation coefficients drop in value in parallel with the absorption error; while seemingly counterintuitive, this signifies that absorption values at lower energies have much more variability than at higher energy values.

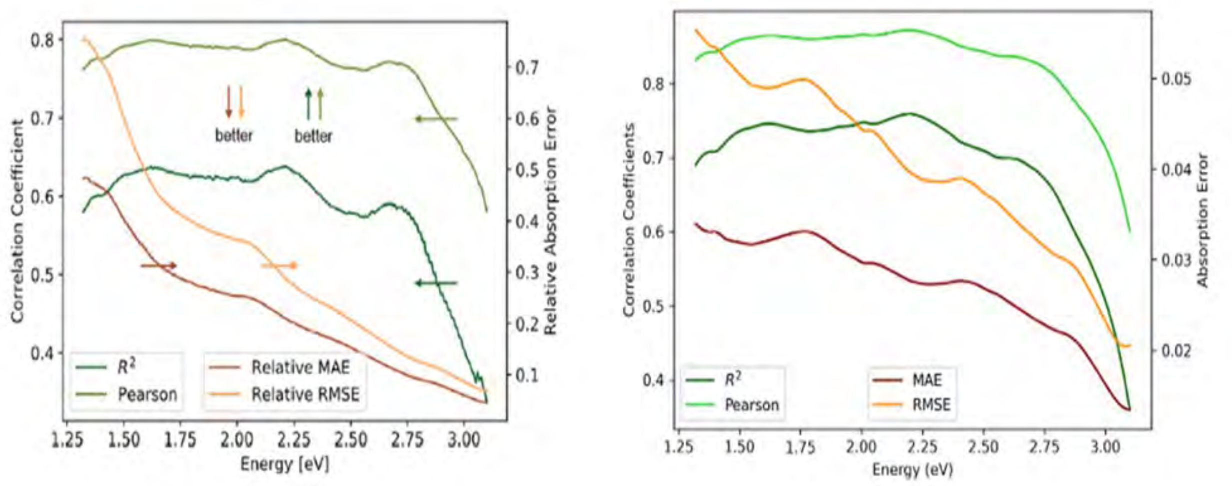

Figure 1. Plot of the R-squared, Pearson, MAE and RMSE for Stein et al. (*left*) and NNSS (*right*) results.

Conclusion

We have demonstrated the capacity to use DNN ensembles to predict continuous value outputs, as well as provide uncertainties associated with each prediction, for image datasets. While this capacity was demonstrated using the publicly available JCAP dataset, matching published results, it will be applied to NNSS image datasets over the course of the 2023 fiscal year. Furthermore, we have established a deep learning (DL) based workflow for image datasets that includes multiple approaches to dimensionality reduction and dataset enhancement. However, predicting continuous values using images, particularly for limited or imbalance datasets, remains an extremely challenging problem with relatively broad ranges of both absolute error and correlation coefficient values. For the JCAP dataset, both our models and the published results produce several predicted spectra with R-squared scores that are approximately zero (indicating that the model prediction is equivalent to the mean of all spectra with respect to error). Such results indicate the need to further explore DNN model architectures, dataset enhancement, ensemble methods, and other DL based methods before applying these models to NNSS data.

Mission Impact/Benefit

The demonstrated capacity to develop DL based models for image datasets that produce physics-interpretable predictions with quantified uncertainties can benefit numerous applications at the NNSS including nuclear event analysis, remote sensing, nonproliferation, and radiography.

As a results of this project, we have established a workflow for applying such DL models, as well as the capacity to run these models on Lawrence Livermore National Laboratory clusters via a virtual environment (without access restrictions on computational tools). Moreover, the UQ methods developed throughout this project will allow NNSS scientists to evaluate the effectiveness of models and explore sources of uncertainty. In total, three scientists and two student-interns have established DL and probabilistic DL expertise in both the underlying mathematical fundamentals and model development using well-established Python platforms. Our team has also retained one of the student-interns, Malcom Hoffman, as a long-term casual employee. As the adaption of DL as a research tool across all sciences continues to grow exponentially, the work done for this project will enable NNSS scientists to both improve current analysis methods as well as continue to effectively collaborate across the DOE complex and other research institutions.

Publications, Technology Abstracts, Presentations/Posters

Lund et al., 2022. “Beginners’ Guide to Livermore Computing for MSTS Staff.”

Gonzalez, 2022. “PyIFRS Image Processing and Automated Trace Reading Modules,” Reaction History Workshop, Nevada National Security Site, North Las Vegas, NV.

Lund, 2022. Emerging Talent Lecture, Association for Women in Mathematics, University of Minnesota, Minneapolis, MN.

References

Stein, H. S., D. Guevarra, P. F. Newhouse, E. Soedarmadji, J. Gregorie. 2019. “Machine Learning of Optical Properties of Materials – Predicting Spectra from Images and Images from Spectra.” *Chem Sci.* **10**: 47-55. Doi: 10.1039/C8SC03077D.