Yixuan Sun

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Scientific Machine Learning, Graph Neural Networks, Operator Learning.

Education

Purdue University **West Lafayette, IN**
Doctor of Philosophy *2018 - 2022*
School of Mechanical Engineering

Purdue University **West Lafayette, IN**
Master of Science *2016 - 2018*
School of Mechanical Engineering
Thesis: *Deep Neural Network Regression and Sobol Sensitivity Analysis for Daily Solar Energy Prediction Given Weather Data*

Shandong University **Jinan, China**
Bachelor of Science *2012 - 2016*
Energy and Power Engineering & Financial Mathematics

Working Experiences

Argonne National Laboratory **Lemont, IL**
Postdoctoral Appointee *Oct 2022 - current*
- Developing safety-constrained reinforcement learning approaches for complex system control.
- Investigating surrogate neural networks' abilities to match the adjoints of physical forward solvers for ocean and climate models.
- Contributing to DeepHyper with physics-informed neural network benchmark and development.

Argonne National Laboratory **Lemont, IL**
Givens Associate (*Remote*) *May - July 2021*
Traffic Incident Detection: data-centric weak supervision approach
- Developed data-centric supervised learning pipeline for incident detection on traffic networks with quantified uncertainty.
- Performed efficient neural network training on Argonne's JLSE GPU cluster and hyper-parameter tuning with DeepHyper.

Argonne National Laboratory **Lemont, IL**
Givens Associate (*Remote*) *May - August 2020*
Traffic Incident Detection: Detecting traffic incidents with time-series analysis and deep learning.
- Built a pipeline for processing raw traffic data and matching incidents.
- Implemented matrix profile, dynamic graph diffusion convolutional recurrent neural network (DCRNN), and other elementary anomaly detection methods to detect incidents.

Pacific Northwest National Laboratory **Richland, WA**
Machine Learning Engineering Intern *May - August 2018*

Generation Dispatch Prediction: Predicting generation dispatch for multi-area under contingencies.
- Investigated the sufficiency of local features for generation dispatch prediction in power grids.
- Developed an accurate random forest-based regression model and conducted feature importance and sensitivity analyses.

Hyundai Card **Seoul, South Korea**
Graduate Student Intern *Dec 2017 - Jan 2018*
- Conducted experiments of deploying the Daemo crowdsourcing platform for Hyundai Card.

Projects

Emulating a Target Trial: Deep Learning-based Prognosis in Healthcare
- Modeled the dependency between treatment policies, patient characteristics, and treatment results.
- Quantified the adequate time interval of measurement for effective prediction.
- Established LSTM recurrent neural networks and Gaussian process-based logistic regression models to infer patients' survival.

Convolutional Neural Networks-based Distracted Drivers Detection
- Adopted convolutional neural networks to classify driving behaviors in the given images, where Mask-RCNN was used as a part of feature engineering.
- Visualized network's attention on images via the global average pooling in ResNet, generating Class Activation Maps. Demonstrated the localization ability of global average pooling given image-level labels.
- Gaussian process-based logistic regression models to infer patients' survival.

Permeability Regression of Porous Media
- Proposed a novel descriptor connectedness for permeability prediction with a polynomial regression model.
- Investigated the connection between the Minkowski Functionals and connectedness.

Publications

Chakraborty, S., **Sun**, **Y.**, Lin, G., & Qiao, L. (2022). Vapor–liquid equilibrium estimation of n-alkane/nitrogen mixtures using neural networks. *Journal of Computational and Applied Mathematics*, 114059.

Sun, **Y.**, Mitra, S., Deva, A., Garcia, E., & Lin, G. (2022). Artificial intelligence inferred microstructural properties from voltage-capacity curves. *Scientific reports*.

Han, G., **Sun**, **Y.**, Feng, Y., Lin, G., & Lu, N. (2021). Machine learning regression guided thermoelectric materials discovery–a review. *ES Materials & Manufacturing*, *14*, 20–35.

Sun, **Y.**, Mallick, T., Balaprakash, P., & Macfarlane, J. (2021). A data-centric weak supervised learning for highway traffic incident detection. *arXiv preprint arXiv:2112.09792*.

Sun, **Y.**, Hanhan, I., Sangid, M. D., & Lin, G. (2020). Predicting mechanical properties from microstructure images in fiber-reinforced polymers using convolutional neural networks. *arXiv preprint arXiv:2010.03675*.

Yang, J., Li, Q., & **Sun**, **Y.** (2020). A wavelet-cnn-lstm model for tailings pond risk prediction. *arXiv preprint arXiv:2010.00518*.

Yang, J., Sun, Y., Li, Q., & **Sun**, **Y.** (2020). Effective risk prediction of tailings ponds using machine learning. *2020 3rd International Conference on Advanced Electronic Materials, Computers and Software Engineering (AEMCSE)*, 234–238.

Huang, Y., Xu, Q., Hu, C., **Sun**, **Y.**, & Lin, G. (2019). Probabilistic state estimation approach for ac/mtdc distribution system using deep belief network with non-gaussian uncertainties. *IEEE Sensors Journal*, *19*(20), 9422–9430.

Keller, N., Vacca, A., **Sun**, **Y.**, Zhou, Y., & Lin, G. (2019). Classification of machine functions: A case study. *the 16th Scandinavian International Conference on Fluid Power*.

Sun, **Y.**, Lin, G., Han, Q., Vian, C., & Yang, D. (2019). Exploratory data analysis for achieving optimal environmental and operational parameter settings for making quality crossmember castings. *Die Casting Congress Exposition 1*.

Yang, J., Wang, W., Lin, G., Li, Q., **Sun**, **Y.**, & Sun, Y. (2019). Infrared thermal imaging-based crack detection using deep learning. *IEEE Access*, *7*, 182060–182077.

Sun, **Y.** (2018). *Deep neural network regression and sobol sensitivity analysis for daily solar energy prediction given weather data* (Doctoral dissertation). Purdue University.

Sun, **Y.**, Fan, X., Huang, Q., Li, X., Huang, R., Yin, T., & Lin, G. (2018). Local feature sufficiency exploration for predicting security-constrained generation dispatch in multi-area power systems. *2018 17th IEEE International Conference on Machine Learning and Applications (ICMLA)*, 1283–1289.

Skills

Programming Languages: Python, R, C++, Matlab, SAS

Libraries: PyTorch, JAX, PyG, TensorFlow, Keras, Scikit-Learn, Numpy, Pandas, Jupyter, OpenCV, PIL, CUDA

Presentations

MCS seminar, Argonne National Laboratory **Lemont, IL**
Seminar Talk *2022*
DeepGraphONet: A Deep Graph Operator Network for Learning the Dynamics of Networked Systems.

The "Celebrating Discovery Park District" Event **West Lafayette, IN**
Poster presentation *2022*
DeepGraphONet: A Deep Graph Operator Network for Learning the Dynamics of Networked Systems.

Teaching

Teaching Assistant **West Lafayette, IN**
Intermediate Heat Transfer *Spring 2019*
- Held office hours to answer students' questions.
- Graded and desgined homework problems/exams.

Teaching Assistant **West Lafayette, IN**
Fluid Mechanics *Fall 2018*
- Held office hours to answer students' questions.
- Graded homework problems and laboratory reports.
- Guided students through laboratory sessions.

Services

Reviewer

- Accident Analysis & Prevention.
- The Transportation Research Board (TRB) 102nd Annual Meeting.

Volunteer **West Lafayette, IN**
2016-2017
- Helped local high schools, shelters, and government organize, distribute, and manage event items.

Languages

English: Proficient.
Mandarin: Native.

References

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