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Daniel C. Elton, Ph.D.

Skills

- Machine learning, natural language processing, scientific writing and presentation
- Programming languages: Python, Matlab, Fortran
- Python libraries: *numpy*, *matplotlib*, *scikit-learn*, *pandas*, *keras*
- limited experience: C++, Mathematica, openMP/openMPI, HTML
- git, LaTeX, GNU/Linux, MacOS, MS Windows, MS Office

Experience

2018- **Assistant Research Scientist**, *University of Maryland, College Park*

Supervised by Prof. Peter W. Chung and Prof. Mark D. Fuge.

- Demonstrated for the first time that machine learning models can predict the properties of explosive materials with high accuracy and low computational cost. (neural networks, ridge and LASSO regression, kernel ridge regression, random forest models, dimensionality reduction)
- Developed methods for using machine learning to discover molecular structure-property relationships. (model sensitivity analysis, feature importance ranking)
- Explained the utility of machine learning methods to program managers and chemists in the Navy Research Office and Army Research Laboratory.
- Wrote a review article on deep learning architectures for molecular generation and demonstrated how a generative adversarial network can be used to generate sets of potentially useful molecules.
- Supervised a masters student and four undergraduate students on a natural language processing project to extract chemical names, properties, and functionalities from large corpora of text extracted from pdfs and patent applications. Wrote code to calculate word2vec and GloVe embeddings and studied the clustering of chemical names in the word embedding space.

2017-2018 **Postdoctoral Associate**, *University of Maryland, College Park*, Same as above.

2018- **Talent**, *Mindfire Global*, Davos, Switzerland

- I was chosen as one of 36 "talents" out of hundreds of applicants to participate in the Mindfire program. Mindfire (www.mindfire.global) is a new initiative which brings together top talents in artificial intelligence, neuroscience, and other fields to help develop novel biologically inspired approaches to AI.

2012-2016 **Graduate Research Assistant**, *Stony Brook University*

Ph.D. adviser: Prof. Marivi Fernández-Serra

- Wrote a Fortran code (*PIMD-F90*) for quantum molecular dynamics simulation and a Python package (*spectrumfitter*) for fitting dielectric spectra. Parallelized code with MPI and ran large scale molecular dynamics simulations on HPC clusters.
- Planned and executed a detailed study of the dielectric properties of water which led to the discovery of optical phonon-like modes in liquid water.

Education

Dec. 2016 **Ph.D. Physics**, *Stony Brook University*, Stony Brook, NY

Aug. 2009 **B.S., Physics**, *Rensselaer Polytechnic Institute* , Troy, NY

Select Publications

2018 Z. Boukouvalas, **D. C. Elton**, M. D. Fuge, and P. W. Chung. "Independent Vector Analysis for Data Fusion Prior to Molecular Property Prediction with Machine Learning" To be submitted to 2018 Neural Information Processing Systems (NIPS) workshop on Machine Learning for Molecules and Materials.

2018 B. C. Barnes, **D. C. Elton**, Z. Boukouvalas, D. E. Taylor, W. D. Mattson, M. D. Fuge, and P. W. Chung, "Machine Learning of Energetic Material Properties", 16th International Detonation Symposium, Cambridge MD (arXiv:1807.06156)

2018 **D. C. Elton**, Z. Boukouvalas, M. S. Butrico, M. D. Fuge, and P. W. Chung, "Applying machine learning techniques to predict the properties of energetic materials", *Scientific Reports* **8**, 9059

2016 **D. C. Elton** and M.-V. Fernández-Serra, "The hydrogen-bond network of water supports propagating optical phonon-like modes", *Nature Communications*, **7**, 10193