Ryan Henderson, Ph.D.

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RECENT EXPERIENCE

Exogene Ltd., Oxford, UK (remote) — *Senior machine learning scientist*

November 2021 - present

- Architected, trained, and benchmarked state-of-the-art TCR-peptide enrichment model (publication forthcoming)
- Developed appropriate training targets with external team of biologists
- Built training and hyperparameter tuning pipeline on AWS Sagemaker and GCP Vertex AI

Bayer AG, Berlin, DE — *Machine learning scientist*

April 2020 - October 2021

- Paper accepted to top machine learning conference (ICML): Improving Molecular Graph Neural Network Explainability with Orthonormalization and Induced Sparsity
- Improved internal Graph Convolutional NN models for ADMET property predictions by ~10%
- Co-developed ChemInformatics Model Explorer (CIME): exploratory analysis of chemical model explanations
- Open source contributions to pytorch-geometric

corrux, Munich, DE — *CTO/Co-founder*

August 2018 - December 2019

- Raised $3.1 million seed round together with cofounder
- Hired and grew technical team to 12 engineers covering frontend, backend, analytics, and hardware (IoT)
- Drove early sales through analytics on construction asset data
- Developed techniques for failure detection using variational autoencoders
- Implemented cross-team Agile development

Merantix, Berlin, DE — *Machine Learning Engineer*

February 2017 - July 2018

- Major contributor to FRCNN project for automatic mammogram screening: preprocessing, model architecture and scaling
- Picasso, a CNN visualizer
- Added multithreaded execution to LSTM-based trading algorithm
- Added test coverage and CI across code base, and drove standardization and containerization of developer and model training environments

Ascribe/BigchainDB, Berlin, DE — *Sen. Software Engineer*

November 2014 - December 2016

- Core contributor to BigchainDB, a scalable blockchain database
- Principal author of image searching library scalable up to billions of images
- Graphs and some backend for https://www.whereonthe.net/ (no longer

SKILLS

Programming: Python (incl. Tensorflow, Numpy, Pandas, etc.), RDKit, pytorch (incl. Torch-geometric, pytorch lightning). *Some exp. in*: Javascript (React, d3), C++, C, Java, AWS, Google Cloud Platform, Azure

Databases: PostgreSQL, Elasticsearch, RethinkDB, MongoDB

Scientific: X-Ray crystallography, structure refinement, solid-state synthesis, automated manufacturing, wafer scan/review, Mathematica

AWARDS, TALKS, WORKSHOPS

ICML 2021 Spotlight Talk

PyData Berlin 2016 Speaker on image-match library

Bayer Teaching Excellence Award *May 2009* awarded to top teaching assistants annually

online)

Intel, Portland, OR — *Defect Metrology Engineer*

January 2013 - May 2014

- Isolated defect sources in chip manufacturing process using data from hundreds of wafers/day over dozens of instruments
- Broad familiarity with most semiconductor fab techniques

EDUCATION

Cornell University, Ithaca, NY — *Ph.D.*

Fall 2007 - Spring 2013

- Ph.D. Theoretical Chemistry GPA: 3.20/4.00
- DAAD German Academic Exchange Service Fellow 2009

Bowling Green State, Bowling Green, OH — *B.S.*

Fall 2003 - Spring 2007

- B.S. Physics & Applied Mathematics - Magna Cum Laude
- GPA: 3.92/4.00 - Presidential Scholarship (full tuition, 4 years)

SELECTED PUBLICATIONS

- R. Henderson, D. Clevert, F. Montanari. “Improving Molecular Graph Neural Network Explainability with Orthonormalization and Induced Sparsity.” *ICML 2021.* https://arxiv.org/abs/2105.04854
- R. Henderson, D. Clevert, F. Montanari. “Gini in a Bottleneck: Sparse Molecular Representations for Graph Convolutional Neural Networks.” *Machine Learning for Molecules Workshop @ NeurIPS 2020.* https://arxiv.org/abs/2010.04535
- R. Henderson and R. Rothe. "Picasso: A Modular Framework for Visualizing the Learning Process of Neural Network Image Classifiers." *Journal of Open Research Software* 5.1 (2017). DOI: http://doi.org/10.5334/jors.178
- S. Lee, R. Henderson, et al. “Pseudo-five-fold diffraction symmetries in tetrahedral packing” *Chem. Eur. J.*, July 2013 DOI: 10.1002/chem.201203758
- P. Jana, R. Henderson, et al. “Site Preference in Cmplx Au-Cr-Zn phases.” *Inorg. Chem.,* Apr. 2013 DOI: 10.1021/ic302244