Columbia, SC
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Daniel A. Gleaves

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https://github.com/dagleaves

Experience

Machine Learning and Evolution Laboratory   Jan 2021 – Mar 2023
Research Assistant   *Columbia, SC*

- Reviewed literature to identify a new method of screening inorganic material structures for stability
- Designed and programmed a novel graph neural network-based semi-supervised machine learning model framework for material synthesizability and formation energy prediction
- Cleaned and utilized large-scale datasets containing millions of material structures
- Validated model performance using hold-out and k-fold cross validation methods
- Co-authored a research paper presenting our state-of-the-art results as the primary author

Education

University of South Carolina - Honors College   May 2024
B.S. in Computer Science, Minor in Mathematics, 4.0 GPA   *Columbia, SC*

- Candidate for Graduation with Leadership Distinction in Research
- Coursework: Intro. to Deep Neural Networks; Linear Algebra; Operating Systems; Data Structures & Algorithms; Programming Language Structures; Foundations of Computing; Software Engineering; Networking

Projects

AutoAssistant

https://github.com/dagleaves/AutoAssistant
- LLM assisted automotive diagnostics using LangChain and FAISS
- Combined nascent vector database technology with large language models (LLMs) effectively
- Gathered thousands of automotive diagnostics through data mining, cleaned the data, and constructed a vector database for similarity search
- Designed a novel LLM agent chain to extract diagnostic keywords from user queries, retrieve relevant information, respond to the specific user issue, and cite the information's source from its metadata

LanguageAssistant

https://github.com/dagleaves/LanguageAssistant
- Integrates ChatGPT, OpenAI Whisper, and Google TTS for seamless multilingual vocal conversation
- Implemented real-time transcription for realistic dialogue
- Fully documented and published as a package on PyPi
- Desiged a teacher agent to create and teach a foreign language lesson plan tailored to a user's goals

Image Classification Toolbox

https://github.com/dagleaves/VisionNETs
- Implemented popular image classification models: GoogLeNet, ResNet50, VGG16 in PyTorch
- Analyzed small-image datasets: MNIST, FashionMNIST, CIFAR-10, and CIFAR-100 for normalization
- Utilized distributed training techniques using the university high performance computing cluster with Slurm
- Evaluated and compared architecture performance differences
- Prepared a survey manuscript detailing key results for small-sized image classification tasks

E_hull Calculator

https://github.com/dagleaves/ehull-calculator
- Implemented a program to calculate the energy above the convex hull for any material given its formula
- Reduced the computation time by several orders of magnitude compared to traditional methods to calculate a valuable property for determining the theoretical stability of experimental materials
- Collaborated with material scientists to properly understand the project requirements and dynamics of the problem

- Utilized a large-scale public database of materials to provide the necessary backbone for the computations and for result validation

Honors & Awards

- South Carolina Palmetto Fellows — Aug 2020
- Carter Bays Computer Science Fellowship — Aug 2021
- Science Undergraduate Research Fellowship - Research Grant — May 2021
- Magellan Scholar Award - Research Grant — May 2021

Publications

- Daniel Gleaves, Nihang Fu, Edirisuriya M. Dilanga Siriwardane, Yong Zhao, and Jianjun Hu. Materials synthesizability and stability prediction using a semi-supervised teacher-student dual neural network. *Digital Discovery*, 2:377–391, 2023

Skills & Interests

- **Programming Languages:** Python, JavaScript, C/C++, Java, MATLAB, Bash, R, Haskell, Prolog
- **Libraries:** PyTorch, PyTorch Lightning, pandas, NumPy, scikit-learn, Matplotlib, TensorFlow, Django, ReactJS, NextJS
- **Tools:** Git, GitHub, GitHub Actions, Linux, Google Cloud Platform, AWS, Docker
- **Research Interests:** Applied machine learning, NLP, LLMs, Recommender Systems, Computer Vision