Utkarsh Pratiush

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About me

I am a second year PhD candidate working on Automated materials characterization using machine learning. I believe there is immense potential in integrating **experimental methods**, **theoretical models**, and **data-driven** approaches to discover new materials. Before starting my PhD, I worked in industry for two years as a machine learning researcher. During this time, I developed **advanced skills** in Python programming and efficiently trained deep neural networks on GPUs across various data modalities, including images, text, and tables. I have contributed with publication in peer reviewed journals and Machine learning venue - NeurIPS. I have also volunteered as teaching assistant for python and advanced deep learning courses. I am part of core maintainer team of pycroscopy (link).

Extracurricular stuff I have done and am proud of

- Served as a reviewer for Neurips ML conference 2024
- Participated in LLM hackathon for materials and our team came 1st. link:
- Participated in Bayesian optimization hackathon for materials and our team came 1st. link:
- Did a project with a french finance company for 3 months - Was curious to learn about the data handling - Contributed to feature engineering code on github. link:

Education

- **University of Tennessee** — TN, USA
  Graduate student; Automating material characterization with Machine learning. GPA: 3.95/4 — *Aug 2023 - going on*
  Supervisor: Sergei Kalinin
  - Wrote the server-client ( ) code to control Transmission electron micrscope from high performance computing to leverage compute intensive ML models for live decision making. (Publication link)
  - Deployed initial version of human in the loop material characterization on electron microscopy(Publication link). (Demo link)
  - Deployed segment anything segmentation model by Meta for automated particle characterization on electron microscope in realtime. (Demo link)

- **Indian Institute of Science** — Bangalore, India
  Bachelors + Masters in Computational material Science, GPA: 8.05/10 — *Aug 2015 - July 2020*
  - As bachelors thesis - Used Density functional theory to study band structure and defect level in Lanthana, a potential replacement for Silicon dioxide for semiconductors. Conducted simulation in quantum espresso (open source package). Furthermore we did electrostatic correction in the formation energy of the charged defects.
  - As masters thesis - Worked on using dimensionality reduction to detect patterns in sensor data to **characterize ions**. Developed and deployed the code on server using flask, javascript, html and css.Web app link:

Industry Experience

- **Mindtree Ltd.** — Bangalore, India
  Research Engineer, Machine Learning — *Aug 2020 - Jul 2022*
  - Developed physics-informed neural network (PINN) models in PyTorch for solving a) wave equations and b) Lotka-Volterra equations (Code link:). Implemented Neural ODEs for time series forecasting using both Julia and Python (torchdyn package).Gained hands-on experience with NVIDIA Modulus by solving basic dynamical systems using the PINN package (link:).
  - Implemented a research paper (Paper link:) using **PyTorch**.The trained language model(**Neural Network based- BERT**) became better at downstream task with an increase in F1 score from 0.69 to 0.79 on a product classification task.
  - Explored transformers(Neural Network) based time-series model (Link:).Thought about various features like holiday, weather and region based special occasions to encode in model for better forecasting. Finally improved bias by 7 percent and accuracy by 8 percent.

- **Vijna Labs** Bangalore, India
  Research Intern, Deep Learning for Computer Vision *Jul 2019 - Dec 2020*
  - Worked on estimation of obstacle dimensions and depth using a object detection **deep learning model**, YOLOv3. The accuracy percentage to detect objects was doubled.

Research Experience

- **Indian Institute of Technology (IIT Delhi)** Delhi, India
  Research Associate, M3RG Lab *Jan 2023 - Jul 2023*
  Supervisors: Dr. NM Anoop Krishnan, Dr. Sayan Ranu
  - Published in Neurips AI4MAT- Atomistic modelling using **Equivariant Graph Neural Networks**.(Code link:).We evaluate them on several complex tasks such as evaluation of the structure and dynamics on forward simulations at different temperatures, compositions, and crystal structures. We evaluate the quality of simulations by new metrics on structure, and dynamics.
- **Indian Institute of Science (IISc)** Bangalore, India
  Research Associate, Deep Representation Learning Lab *Aug 2022 - Dec 2022*
  Supervisors: Prof. Prathosh AP, Prof. Vishweshwa Guttal
  - Implemented the induction of grammatical information tags and knowledge distillation in translation model. (Code link:).The trained language model(**Neural Network based - BART**) showed 20 percent increase in Bleu score. It was also deployed on **Huggingface**
  - Studying the behaviour of collective behaviour of fishes using a **stochastic differential equation**.(Code link:). Used **neural networks**, to fit drift and diffusion function of the sde.The implemented code has potential to study dependence of other factors, like position of fishes in determining the sde thus helping in studying boundary effects(one of the applications).
- **Japan Advanced Institute of Science and Technology (JAIST)** Ishikawa, Japan
  Research Intern, Drug Discovery *Jun 2017 - Aug 2017*
  - I was funded by Jasso as an international student to conduct research in Japan. I worked on synthesizing nanomaterials for drug delivery to cancerous cells. Did NMR and confocal laser scanning microscopy to characterize the material.

Patent

Kalinin, S.; Liu, Y.; Biswas, A.; Duscher, G.; **Pratiush, U.**; Roccapriore, K.; Ziatdinov, M.; Vasudevan, R.; mani, V.; Ahmadi, M. *Human-in-the-loop machine learning for automated experiment in computation, synthesis, microscopy, and characterization.*

Skills Summary

- **Languages**: Python, Shell scripting, C++, Julia(light), Javascript, CSS, HTML.
- **Tools**: GIT, PyTorch, Tensorflow, relevant python packages(Numpy, Pandas, Flask, Scipy, Scikit-learn), Docker.

Courses

Material characterization methods, Condensed matter physics, Modelling and simulation in material science, Statistical mechanics, Advance software engineering, Deep learning, Computer vision, Natural language processing, Reinforcement learning

Honors and Awards

- Got **selected** to URSSI Research Software + Open Science Summer school at UIUC(sponsored by NASA) with full funding.
- Our project came **1st** in LLM for materials and chemistry hackathon 2024 [Link to demo]
- Got **promoted** in Jan'2022 for achieving excellent performance rating at Mindtree.
- Recipient of research scholarship for carrying out undergraduate research..
- Recipient of JASSO scholarship for carrying out a summer research project at Japan Advanced Institute of Science and Technology (JAIST), Japan
- Secured above 99.5 percentile in **IIT** entrance exam 2015 more than a million students appear for it in india.

Selected Publications

Please see Google Scholar for an updated list: Google Scholar

- **Realizing smart scanning transmission electron microscopy using high performance computing**
  U Pratiush, Austin Houston, Sergei V Kalinin, Gerd Duscher
  [Link to Article]

- **Co-orchestration of multiple instruments to uncover structure–property relationships in combinatorial libraries**
  Boris N. Slautin, **Utkarsh Pratiush**, Ilia N. Ivanov, Yongtao Liu, Rohit Pant, Xiaohang Zhang, Ichiro Takeuchi, Maxim A. Ziatdinov, Sergei V. Kalinin
  [Link to Article]

- **EGraFFBench: Evaluation of Equivariant Graph Neural Network Force Fields for Atomistic Simulations**
  V Bihani, **U Pratiush**, Sajid Mannan, Tao Du, Zhimin Chen, Santiago Miret, Matthieu Micoulaut, Morten M Smedskjaer, Sayan Ranu, NM Krishnan
  [Link to Article]
  arXiv preprint arXiv:2310.02428
  [Neurips AI4MAT spotlight]

- **Discovering mesoscopic descriptions of collective movement with neural stochastic modelling**
  U Pratiush, A Nabeel, V Guttal, P AP
  [Link to Article]
  arXiv preprint arXiv:2303.09906