

Varun Madhavan

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EDUCATION

University of Michigan Ann Arbor

(Aug 25 - Present)

PhD in Chemical Engineering and Scientific Computing

PhD candidate at Goldsmith Lab ([Website](#))

Indian Institute of Technology Kharagpur

(Aug 18 - May 23)

Bachelor of Technology and Master of Technology (5 Year Dual Degree)

Major: Chemical Engineering; Minor: Computer Science

GPA: **9.15/10**; Class Rank **3**

PUBLICATIONS

Journals

- **Clarifying trust of materials property predictions using neural networks with distribution-specific uncertainty quantification**
C. J. Gruich, [V. Madhavan](#), Y. Wang, B. R. Goldsmith ([Paper](#))
Machine Learning: Science and Technology, Volume 4, Number 2 (April 2023)
- **Machine learning conservation laws from differential equations**
Z. Liu, [V. Madhavan](#), M. Tegmark ([Paper](#))
Physical Review E (October 2022)

Preprints

- **Self supervised pre-training for partial differential equations**
[V. Madhavan](#), A. S. Sebastian, B. Ramsundar, V. Viswanathan ([Preprint](#))

Conferences

- **Deep learning for spatially explicit emulation of epidemic agent-based models**
[V. Madhavan](#), A. Mitra, P. P. Chakrabarti ([AAMAS 2023](#)) ([AI4ABM at ICML 2022](#))
AI4ABM Workshop at the International Conference on Machine Learning (ICML) 2022
International Conference on Autonomous Agents and Multi-Agent Systems (AAMAS) 2023
- **RCTransformer: Unveiling the power of self-attention for shipping cost prediction**
P. A. Sreekar, S. Verma, [V. Madhavan](#), A. Persad ([Paper](#))
Asian Conference on Machine Learning (ACML) 2023
- **LiMPET: Language modeling for predicting events and times**
A. Gupta, S. Soni, [V. Madhavan](#), S. Bisht, S. Verma, A. Persad
Amazon Machine Learning Conference (AMLC) 2024
- **City scale simulation of pandemic intervention policies using agent-based models**
G. Suryawanshi, [V. Madhavan](#), A. Mitra, P. P. Chakrabarti ([Paper](#))
Winter Simulation Conference (WSC) 2021
- **Leveraging pre-trained language models for key point matching**
M. N. Kapadnis, S. Patnaik, S. S. Panigrahi, [V. Madhavan](#), A. Nandy. Link: ([Paper](#))
Empirical Methods in Natural Language Processing, Argument Mining Workshop (EMNLP) 2021

PROFESSIONAL EXPERIENCE

Applied Scientist | Amazon

(Jan 24 - Aug 25)

Improving downstream task performance with package level unsupervised pre-training

Designed a novel pre-training paradigm for package data with an unsupervised next-state prediction objective and an encoder for parsing variable length shipment plans, static metadata, and past scan sequences into a single general-purpose package representation. Enabled a step change improvement in model performance on downstream tasks like shipping cost prediction, delay prediction, identification of lost packages, etc., compared to similar architectures without pre-training.

Forecasting package demand for first-mile pickup planning and routing

Built a gradient boosting based forecasting model to predict the package demand for first-mile pickup planning and routing at different geographic and temporal granularities, enabling an estimated 20 cent reduction in pickup costs per package. Deployed this model with multi-threaded batch processing to enable high throughput inference of 10M packages per day.

RESEARCH EXPERIENCE

Electrochemical Energy Group | Carnegie Mellon University

(Jan - Oct 23)

Building foundational PDE solvers with self-supervised pre-training | Advisor: Dr. Venkat Viswanathan

Designed an algorithm to learn a foundational neural PDE solver from trajectory data by decomposing them into temporal chunks (n-dimensional patches) using convolutional blocks, and training a transformer to auto-regressively generate future chunks based on past chunks. Trained this model on multiple systems from PDEBench, demonstrating that the resulting model can generate full solutions from the initial state for both unseen trajectories and parameters.

Goldsmith Lab | University of Michigan, Ann Arbor

(May - Aug 22)

Enabling uncertainty-aware catalyst search and discovery with Machine Learning | Advisor: Dr. Bryan Goldsmith

Explored the efficacy of various uncertainty quantification techniques applied to a Crystal Graph Convolutional Neural Network trained to predict the adsorption energies of molecules over alloy catalysts (OC20 IS2RE dataset). Identified accuracy, calibration, and dispersion as key uncertainty metrics for guiding high-throughput catalyst search, and designed a novel approach for uncertainty quantification based on Evidential Regression, outperforming benchmark approaches like Monte Carlo dropout and k-fold ensembling on these metrics.

Tegmark Group | Massachusetts Institute of Technology

(Apr - Aug 21)

Automating the discovery of conservation laws using Machine Learning | Advisor: Dr. Max Tegmark, Ziming Liu

Designed AI Poincaré, an algorithm to auto-discover conservation laws for any dynamical system from the governing partial differential equations both numerically (parameterized as neural networks) and symbolically, eliminating the need for ergodic trajectory data. Demonstrated that AI Poincaré can robustly identify conservation laws in test systems including the 3-body problem, the KdV equation, and the non-linear Schrodinger equation. Implemented a brute force search algorithm with fast rejection to efficiently find symbolic formulae for the discovered conservation laws.

THESIS

Master's Thesis | Chemical Engineering, IIT Kharagpur

(Aug 22 - Apr 23)

A molecular investigation of pattern recognition in polyelectrolyte adsorption | Advisor: Dr. Monojit Chakrabarty

Modeled the adsorption of polyelectrolyte molecules on patterned surfaces using molecular dynamics simulations, studying the effect of parameters like polyelectrolyte concentration, bond stiffness, pattern size, charge density, and pattern periodicity on the nature and extent of adsorption on charged surfaces.

Bachelor's Thesis | Centre of Excellence in Artificial Intelligence, IIT Kharagpur

(Aug 21 - Apr 22)

Accelerating agent-based pandemic spread simulators with machine learning based surrogates | Advisors: Dr. Partha Pratim Chakrabarti & Dr. Adway Mitra

Designed a machine learning based surrogate for computationally expensive agent-based pandemic spread simulators, enabling a 50x speedup in the simulation of counter-factual intervention scenarios like effective masking, contact tracing, vaccination, etc., while maintaining $\leq 5\%$ prediction error. Presented a poster on this work at the AI4ABM Workshop in the International Conference on Machine Learning (ICML) 2023, and published a full manuscript at the International Conference on Autonomous Agents and Multi-Agent Systems (AAMAS) 2023.

INTERNSHIP EXPERIENCE

Machine Learning Engineer Intern | Prodigal | Y Combinator S18

(Aug - Dec 23)

Minimizing call wrap time for customer support agents using natural language processing

Developed a system to minimize the time spent per customer for support agents by automatically generating summaries and identifying the main issues discussed in the call, by fine-tuning LLaMA 2 on a GPT4 annotated instruction dataset. Applied zero redundancy optimizers and flash attention to reduce fine-tuning time by 62%.

Applied Scientist Intern | Amazon

(Jan - Jul 23)

Estimating the shipping cost for last-mile shipments based on package route plans and rate cards

Designed the RCTransformer, a novel transformer-based architecture to utilize package plan data to estimate shipping costs, demonstrating superior performance against state-of-the-art tabular models FT-Transformer and TabTransformer. Presented this work as a poster at the Amazon Machine Learning Conference, and published a full manuscript in the Asian Conference on Machine Learning 2023.

COMPETITIONS

DevRev's Domain-Specific QA Challenge | Inter IIT Tech Meet 11.0

(Feb 23)

Represented IIT Kharagpur at the Inter IIT Tech Meet as the captain of the natural language processing team. Built a retrieval augmented generation (RAG) based chat interface for question answering over any given corpora by combining a DrQA retriever with an encoder language model. Optimized the system for on-device CPU-only inference, achieving an inference time $\leq 100\text{ms}/\text{query}$ with $\leq 1\text{GB}$ of RAM usage using a fast retriever, model distillation, and ONNX runtimes. Awarded second place amongst 21 participating IITs.

Key Point Matching Shared Task | Argument Mining Workshop, EMNLP 2021

(Aug 21)

Implemented a system for identifying key points in debates by predicting the semantic overlap score between a given argument and a ground truth key point, by decomposing each sentence into the constituent parts-of-speech and applying the pre-trained language model DeBERTa to classify the resulting sequence. Achieved a mean average precision score of 89.2% and second place in the global leaderboard.

TEACHING

- **Teaching Assistant:** Computer Aided Process Engineering Lab, Autumn 2022 & Spring 2023. Responsibilities: assisting in lab sessions, creating practice problem sets for review, holding weekly office hours to assist students with their queries, and grading weekly assignments and exams.
- **Kharagpur Data Analytics Group:** Taught an introductory machine learning curriculum to junior undergrads, covering the basics of Python programming, statistical data analysis techniques, and classical ML algorithms.

AWARDS & ACHIEVEMENTS

- **Ranked 1st** amongst all 120 ChemE undergraduates at the end of my first year at IIT Kharagpur, and **3rd** upon graduation. Ranked in the **top 10%** of the batch of **1400+** undergraduates across all majors throughout.
- Awarded the **Institute Honorable Mention** by the Technology Students Gymkhana for outstanding performance in science and technology activities amongst the entire graduating batch of 2023.
- Awarded the **Silver Medal** at the Inter IIT Technology Meet 2023, representing IIT Kharagpur as the NLP team captain.

COURSEWORK

- **Chemical Engineering:** Fluid Mechanics I* & II, Heat Transfer I* & II, Mass Transfer I* & II, Thermodynamics, Reaction Engineering*, Instrumentation & Process Control*, Process Equipment Design I & II, Computer Aided Process Engineering*, Advanced Mathematics for Chemical Engineering
- **Math:** Engineering Mathematics I & II, Transform Calculus, Numerical Solutions for PDEs, Probability & Statistics
- **Computer Science:** Algorithms I*, Switching Circuits & Logic Design*, Computer Architecture & Operating Systems, Image Processing, Big Data Processing, Scalable Data Mining
- **Artificial Intelligence:** Machine Learning Foundations & Applications*, Artificial Intelligence Foundations & Applications, Deep Learning, Natural Language Processing, Generative Graphical Models for Machine Learning, Symbolic Logic
(includes lab component)*

SKILLS

- **Programming Languages:** C | C++ | Python | PySpark | SQL | MATLAB | $\text{\LaTeX}$
- **Engineering / Simulators:** LAMMPS | DWSIM
- **Deep Learning Frameworks:** PyTorch | PyTorch Lightning | Keras
- **Python Libraries:** Huggingface | spaCy | sklearn | LightGBM | polars | pandas | numpy

VOLUNTEERING

- **Editor at IIT Tech Ambit:** Authored articles for the campus science newsletter IIT Tech Ambit covering on-campus research at IIT Kharagpur, including the rapid Covid-19 testing kit COVIRAP designed by Dr. Suman Chakraborty, low-cost electric cycles for campus mobility, and funding opportunities for budding startups on campus.
- **National Cadet Corps:** Cadet at the local Air Wing chapter of the National Cadet Corps, organizing social awareness camps, tree plantation drives, and the annual Republic Day parade.
- **Student Mentor:** Mentored five first-year undergraduates as part of the Student Welfare Program, guiding them in choosing their coursework and keeping them informed of campus activities and opportunities.
- **Conference Volunteer:** Actively contributed to the virtual organization of conferences COLING 2020 and EMNLP 2021 by coordinating workshop schedules, ensuring smooth virtual sessions, and providing support to presenters throughout the duration of the conferences.