Vinayak Gupta

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RESEARCH INTERESTS

Designing ML models, LLMs, and benchmarks for text + time-series tasks on medical, wearable, and digital health data. Also training de novo foundation models for biological sequences, purchase records, and spatial data to advance genomics, drug discovery, and personalized recommendations.

EXPERIENCE

Lawrence Livermore National Laboratory   Aug. 2024 – Present
Machine Learning Researcher
Working on several DOE-funded projects at the intersection of time-series modeling, health data, and foundation models, driving innovations in predictive analytics and AI for healthcare.
- Developing and training foundation models on bio-sequences and multi-million patient health records, given by Kaiser Permanente, to forecast temporal patterns and early disease diagnosis.
- Designing self-improving LLM-based agents to detect defects in 3D-printed structures using multi-angle image analysis and multi-variate time-series data from manufacturing processes.
- Managing training and optimization of large-scale foundation models (de novo) national lab GPU clusters such as Tuolumne cluster (among the most powerful supercomputers globally).

Paul G. Allen School of Computer Science & Engineering   Apr. 2023 – May 2024
Postdoctoral Researcher - University of Washington
Researcher under Prof. Tim Althoff (Behavioral Data Science Group), focusing on LLMs capable of understanding and reasoning with multi-modal time-series data, including both images and text.
- Worked on applying LLMs to time-series forecasting, identifying limitations in existing models and proposing simpler, scalable architectures. Awarded NeurIPS 2024 Spotlight and featured in multiple articles, including IBM blogs, referred as "*One of the biggest revelations of 2024*".
- Released a benchmark time-series understanding dataset, adopted by companies like Apple and ByteDance to evaluate LLM reasoning over temporal and textual data.
- Developed a LLM prompt-injection dataset (7K+ monthly downloads on HuggingFace) and a defense framework treating prompts as programs, influencing GitHub's test-case generator.

IBM Research   Aug. 2022 – Mar. 2023
Research Scientist
With the WatsonX Data & AI team, I worked on enabling Watson-Core to perform business intelligence tasks such as data denoising, feature aggregation, etc., using only text commands over IBM cloud. Developed the first functional prototype replacing Watson-Core with an LLM-powered backend for business tasks and led a tutorial on automated intelligence agents at a major NLP event.

Amazon   Jan. 2022 – Jun. 2022
Applied Scientist-II Intern
Analyzed Amazon Pay records to model user-item preferences and predict future purchases for personalized and well-timed coupon recommendations, and tested methods to handle missing events.

Siemens Healthcare   May 2016 – Jan. 2017
Research Intern
Developed computer vision models, including video-frame super-resolution, to enhance radiographic imaging on Siemens Multimobil 5C X-Ray equipment. Tech-Intern Rating: 1 (Highest Possible).

EDUCATION

Indian Institute of Technology (IIT) Delhi
Ph.D. in Computer Science & Engineering.
- Institute Nominee for ACM SIGKDD and ACM Doctoral Dissertation Awards.
- Institute-wide Distinction in Doctoral Research Award.

Indian Institute of Information Technology (IIIT) Jabalpur
B.S. in Computer Science & Engineering.
- Silver Medal Nominee for Best Undergraduate Thesis.

PREPRINTS OR UNDER REVIEW

Geno-Prot: A Benchmark for Multimodal Genomic–Proteomic Modeling.
V. Gupta*, J. Wakim*, J. Marti, J. Allen, B. Bartoldson, B. Kailkhura.

Closing the Omics Gap: Unified Modeling for Biomolecular Foundation Models.
V. Gupta*, J. Wakim*, J. Marti, J. Allen, B. Bartoldson, B. Kailkhura.

Efficient and Responsible Adaptation of LLMs for Equitable Top-k Recommendations.
K. Kaur, M. Chadha, **V. Gupta**, and C. Shah.

SPML: A DSL for Defending Language Models Against Prompt Attacks.
R. Sharma, **V. Gupta**, and D. Grossman.

<div style="float:left">CONFERENCE, JOURNAL, AND NOTABLE WORKSHOP PUBLICATIONS</div>

Differentiable Adversarial Attacks for Marked Temporal Point Processes.
V. Gupta*, P. Chakraborty*, R. Rahul, S. Bedathur, and A. De.
AAAI Conference on Artificial Intelligence (**AAAI**), 2025.

Cost-Effective Biological Data Analysis via a Benchmark and Ensemble of LLMs.
V. Gupta, B. Bartoldson, J. Wakim, J. Allen, J. M. Marti, T. Chen, and B. Kailkhura.
U.S. Office of Scientific and Technical Information (**OSTI**), 2025. (Limited Release)

Enhancing Biological Insights with Knowledge-Driven Multi-Modal RNA Models.
M. Qiu, ..., **V. Gupta**, B. Bartoldson, B. Kailkhura, T. Chen.
U.S. Office of Scientific and Technical Information (**OSTI**), 2025. (Limited Release)

Are Language Models Actually Useful for Time Series Forecasting?
M. Tan, M. Merill, **V. Gupta**, T. Althoff, and T. Hartvigsen.
Neural Information Processing Systems (**NeurIPS**), 2024. **(Spotlight)**

Language Models Still Struggle to Zero-shot Reason about Time Series.
M. Merill, M. Tan, **V. Gupta**, T. Hartvigsen, and T. Althoff.
Empirical Methods in Natural Language Processing (**EMNLP**) Findings, 2024.

Defending Multi-modal Language Models Against Image-Based Prompt Attacks.
R. Sharma, **V. Gupta**, and D. Grossman.
Workshop on Security Architectures for Generative AI (**SAGAI**), IEEE S&P 2024.

Modeling Human Activity Sequences using Temporal Point Process Flows.
V. Gupta and S. Bedathur.
ACM Transactions on Intelligent Systems and Technology (**TIST**), 2023.

Retrieving Continuous Time Sequences using Point Processes with Learnable Hashing.
V. Gupta, S. Bedathur, and A. De.
ACM Transactions on Intelligent Systems and Technology (**TIST**), 2023.

Modeling Spatial Trajectories using Coarse-Grained Smartphone Logs.
V. Gupta and S. Bedathur.
IEEE Transactions on Big Data (**TBD**), 2023.

Teaching Old DB Neural Tricks: Learning Embeddings on Multi-tabular Databases.
G. Gaur, R. Singh, S. Arora, **V. Gupta**, and S. Bedathur.
International Conference on Data Science & Management of Data (**CODS-COMAD**), 2023.

Learning Point Processes for Efficient Retrieval of Continuous Time Event Sequences.
V. Gupta, S. Bedathur, and A. De.
AAAI Conference on Artificial Intelligence (**AAAI**), 2022.

ProActive: Self-Attentive Temporal Point Process Flows for Activity Sequences.
V. Gupta and S. Bedathur.
ACM SIGKDD Conference on Knowledge Discovery and Data Mining (**KDD**), 2022.

Modeling Continuous Time Sequences with Missing Events using Point Processes.
V. Gupta, S. Bedathur, S. Bhattacharya, and A. De.
ACM Transactions on Intelligent Systems and Technology (**TIST**), 2022.

Overcoming Data Scarcity for POI Recommendation via Cross-Region Transfer.
V. Gupta and S. Bedathur.
ACM Transactions on Intelligent Systems and Technology (**TIST**), 2022.

IBM Tutorial on Advances in NLP Research for Automated Business Intelligence.
V. Gupta, C. Rajmohan, R. Chaudhuri, A. Gupta, B. Ganesan, A. Agarwal, S. Mehta.
International Conference on Natural Language Processing (**ICON**). 2022.

Modeling Human Actions in Time-Stamped Activity Sequences.
V. Gupta and S. Bedathur.
Workshop on Applied ML for Time-Series Forecasting (**AMLTS**), colocated with CIKM 2022.

Learning Temporal Point Processes with Intermittent Observations.
V. Gupta, S. Bedathur, S. Bhattacharya, and A. De.
Conference on Artificial Intelligence and Statistics (**AISTATS**), 2021

Region Invariant Normalizing Flows for Mobility Transfer.
V. Gupta and S. Bedathur.
Conference on Information and Knowledge Management (**CIKM**), 2021.

Modeling Implicit Communities from Geo-tagged Events using Spatial Processes.
A. Likhyani*, **V. Gupta***, P. K. Srijith, P. Deepak, and S. Bedathur.
Conference on Web Information Systems Engineering (**WISE**), 2020.

Load Balanced Ring Routing Protocol for Heterogeneous Networks with Sink Mobility.
S Maurya*, **V. Gupta***, and V. K. Jain.
IEEE Wireless Communications and Networking Conference (**WCNC**), 2017.

GRANTS	Microsoft Accelerate Foundation Models Research Program	2024
	UW eScience Institute: Azure Cloud Credits for Research	2024
GOVERNMENT RECOGNITION	**AI Experts at IndiaAI**: Initiative by Ministry of IT, Govt. of India.	Oct. 2022
	Article: "Read and Watch Lectures to Build a Foundation".	
OTHER AWARDS	NASSCOM AI Game-Changers of India: Runner-Up in ML Fundamentals Category.	2022
	Expert Talk at IndiaAI: Organized by NASSCOM and Ministry of IT – Govt. of India.	2022
	Outstanding Doctoral Paper Award: The First Intl. Conference on AI-ML Systems.	2021
	All India 9th Rank in ABU Asia-Pacific Robocon (Asia's largest robotics competition).	2015
	Project selected for 'Make In India' – Govt. of India's Flagship Manufacturing Initiative.	2015
SKILLS	**Proficient**: Python, PyTorch, and IBM Cloud.	
	Intermediate: Tensorflow, Langchain/Langraph, AutoGen, MATLAB, PySpark, Azure, and AWS.	

SELECTED
TALKS

"Do we need Large Language models for Time Series"
- AI Seminar: University of Southern California, LA. (▶ Video Link) — Nov. 2024
- Allen Institute, Seattle and Snap Inc, Seattle. — Apr. 2024

"Modeling Time Series for Recommendation and Other Applications"
- Georgia Institute of Technology, Atlanta and University of Michigan, Ann Arbor. — Oct. 2022
- University of California, San Diego and University of Notre Dame, Indiana. — Sep. 2022
- Technical University of Munich, Germany and IBM Research. — Jun. 2022

"Neural Temporal Models for Predicting Missing Events and Scaling Retrieval"
- ACM India Research and Careers for Students Symposium (Oral). — Feb. 2022
- Amazon Research Days and Doctoral Symposium: Conference on AI-ML Systems. — Nov. 2021
- MIT-IBM Watson AI Lab, Boston. — Sep. 2019

"Maxima: Electronic Mask for Patients with Exercise-Induced Asthma"
- Siemens Research Exhibition and Make-In-India Quality Improvement Program. — Jul. 2016

Invited Panelist
- Career Mentorship Program at Machine Learning for Health (ML4H). — Dec. 2023

MENTORING

University of Washington
(PhD) Reshabh K. Sharma and Mike A. Merill → Stanford University.

Indian Institute of Technology Delhi/Bombay
(PhD) Pritish Chakraborty and Rajat Singh. Siddhant Arora → CMU and Ritvik Vij → Amazon.

PC MEMBER AAAI, IJCAI, SIGIR, WSDM, WWW, ACM TOIS, IEEE TPAMI, TSP, and NeurIPS/ICML-W.