Yogesh Verma | Ph.D.

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Education

Ph.D. Computer Science | Nokia Scholar — Aalto University, Finland 2025
— Supervisor: Prof. Vikas Garg, Dr. Markus Heinonen, and Prof. Samuel Kaski
— Thesis: *Developing Continuous-time and Geometric ML Methods for Science*

B.S. - M.S. Physics | INSPIRE Fellow — IISER Mohali, India 2021
— Supervisor: Prof. Satyajit Jena
— Thesis: *Applications of Deep Learning Techniques in Characterizing Quark-Gluon Plasma*

Experience

Ph.D. Researcher | Prof. Vikas Garg lab — Aalto University, Finland 2022–2025
— Ph.D. Researcher in the HEALED Project
— Generative and Geometric ML models for drug discovery applications; Biomolecular modeling

Visiting Researcher | Device Concept lab — Huawei, Finland 2024
— Bayesian Inference for personalized healthcare monitoring; hemodynamic simulations

Research Associate | Prof. Ben Kilminster lab — University of Zurich & CERN, Switzerland, 2021
— ML Researcher for the Leptoquark Project in the CMS Experiment, CERN
— Graph Neural Networks for Leptoquark event detection; sensitivity analysis

Publications

Conference Publications:

1. **Y. Verma**, A. H. Souza, and V. Garg. "Persistent Homology meets Positional Encoding on Graphs". In: *International Conference on Machine Learning* (ICML) (2025).
2. **Y. Verma**, A. Bharti, and V. Garg. "Robust Simulation-Based Inference under Missing Data via Neural Processes". In: *International Conference on Learning Representations* (ICLR) (2025).
3. A. Dumitrescu, D. Korpela, M. Heinonen, **Y. Verma**, V. Iakovlev, H. Lahdesmåki, and V. Garg. "E(3)-equivariant models cannot learn chirality: Field-based molecular generation". In: *International Conference on Learning Representations* (ICLR) (2025).
4. **Y. Verma***, G. Mercatali*, A. Freitas, and V. Garg. "Diffusion Twigs with Loop Guidance for Conditional Graph Generation". In: *Advances in Neural Information Processing Systems* (NeurIPS) (2024).
5. **Y. Verma**, A. H. Souza, and V. Garg. "Topological Neural Networks go Persistent, Equivariant, and Continuous". In: *International Conference on Machine Learning* (ICML) (2024).
6. **Y. Verma**, M. Heinonen, and V. Garg. "ClimODE: Climate and Weather Forecasting With Physics-informed Neural ODEs". In: *International Conference on Learning Representations* (ICLR) (2024). — Oral Presentaion Top 1%
7. **Y. Verma**, M. Heinonen, and V. Garg. "AbODE: Ab initio Antibody Design using Conjoined ODEs". In: *International Conference on Machine Learning* (ICML) (2023).
8. **Y. Verma**, S. Kaski, M. Heinonen, and V. Garg, "Modular Flows: Differential Molecular Generation". In: *Advances in Neural Information Processing Systems* (NeurIPS) (2022).

Workshop Publications:

1. **Y. Verma**, A. H. Souza and V. Garg."Topological Neural Networks go Persistent, Equivariant, and Continuous". In: *ML for Life and Material Science* and *AI for Science Workshop*, 2024.
2. **Y. Verma**, M. Heinonen and V. Garg. "AbODE: Ab initio Antibody Design using Conjoined

ODEs". In: *New Frontiers in Learning, Control, and Dynamical Systems*, 2023.
3. **Y. Verma**, S. Kaski, M. Heinonen and V. Garg, "Modular Flows: Differential Molecular Generation" In: *New Frontiers in Graph Learning* and *Symbiosis of Deep Learning and Differential Equations Workshop*, 2022.
4. **Y. Verma**, and S. Jena. "Shower Identification in Calorimeter using Deep Learning", In: *DAE-HEP Symposium*, 2022.
5. **Y. Verma**, and S. Jena. "Particle Track Reconstruction using Geometric Deep Learning", In: *DAE-HEP Symposium*, 2021.

In review:

1. **Y. Verma**, M. Heinonen, and V. Garg. "Let Physics Guide Your Protein Flows: Topology-aware Unfolding and Generation", 2025.
2. Victor Pescaru, **Y. Verma**, and V. Garg. "Scratchpad increases the power of Transformers. Provably", 2025.

Other Publications and Preprints:

1. **Y. Verma**, and S. Jena. "Jet characterization in heavy ion collisions by QCD-aware graph neural networks", 2022.
2. **Y. Verma**, M. Aggarwal, V. Joshi and A. Sharma. "Characterization Study of a Button BPM with an approach to Automated Measurements", In: *IBIC*, 2020.

Research supervision

Summer internship (advisor)
Anna Parilova (2024), Eeshan Jain (2023), Julia Ripatti (2023), Victor Pescaru (2023)

Master's Project (advisor)
Hieu Pham (2025), Priscilla Ong (2024), Dawei Jiao (2023)

Bachelor's Project (advisor)
San Koktas (2024), Ritoban Dutta (2021)

Teaching Experience

- Course on Diffusion Models (guest lecturer) — Aalto University, 2025
- Deep Generative Models (guest lecturer & TA) — Aalto University, 2025
- Quantum Machine Learning (guest lecturer & TA) — Aalto University, 2023
- Modeling Biological Networks (TA) — Aalto University, 2022
- Computational Methods in Physics (TA) — IISER Mohali, 2021
- Experimental Particle Physics Lab (TA) — IISER Mohali, 2021

Awards and honours

- Encouragement Grant, Finnish Foundation for Technology Promotion — 2025
- Nokia Scholarship, Nokia Foundation — 2024
- DAAD AInet Fellow, DAAD — 2024
- Oral presentation: ICLR 2024 — 2024
- INSPIRE Scholarship, Government of India — 2016-2021

Academic service

Organiser

- FCAI Machine Learning Coffee Weekly Seminar — 2023 - 2025

- AI Day, FCAI 2024, 2025

Volunteer

- ICML, ICLR 2024, 2025
- ELLIS Robust ML Workshop 2023, 2024
- Foundation Day, IISER Mohali 2018, 2019

Reviewer

NeurIPS, ICML, ICLR, AAAI, AISTATS, TMLR, JMLR, AABI

Invited Talks

- Mathematical Perspective on Machine Learning Seminar — University of Helsinki, 2025
- Keynote, FCAI FAME SIG Meeting — FCAI, Espoo, 2025
- Math+ML+X Seminar — Tsinghua University, China, 2025
- ELLIS Advanced Probabilistic Machine Learning Seminar — Aalto University, Espoo, 2024
- Keynote, Workshop on Physics-Informed Learning — ELISE Conference, Helsinki, 2024
- AI4Science Seminar Talk — University of Stuttgart, 2024
- Research Seminar — MLLS Institute, Denmark, 2023