Prashant Govindarajan

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Education

- **Mila and Polytechnique Montréal**, Montréal, Canada — *Aug'22-Present*
  PhD in Computer Engineering; Advisor: Sarath Chandar
- **Indian Institute of Technology Madras**, Chennai, India — *Jul'17-Jul'22*
  Bachelor of Science in Biological Sciences and Master of Technology in Data Science
  Minor: Computational Biology — *CGPA: 9.31/10.00*

Research Experience

- **AI-automated CAD object generation**
  Mentors: Sarath Chandar, Jay Pathak, Quentin Fournier — *Jun'24-Present*
  - Collaboration with Ansys: LLMs for automated generation of 3D Computer-Aided Design (CAD) objects
  - Published CADmium, an open-source dataset and LLM fine-tuning approach [Paper, Code, Website]
- **Reinforcement learning for material design**
  Mentors: Sarath Chandar, Mathieu Reymond, Santiago Miret, Mariano Phielipp — *Aug'22-Present*
  - Project with Intel on offline and online reinforcement learning approaches for generating new crystal structures
  - Integrated first-principles density functional theory with conservative Q-learning – accepted at MoML 2023, AI4Mat workshop at NeurIPS 2023, and Digital Discovery Journal [Paper, Code]
  - Released CrystalGym, the first online RL environment and benchmark for material discovery – Spotlight at AI4Mat-ICLR 2025 [Paper, Code]
- **Master's Thesis: Graph generative models for binding site-specific molecule generation**
  Guides: Balaraman Ravindran, Karthik Raman, IIT Madras [Thesis, Poster] — *Aug'21-Jun'22*
  - Designed graph variational autoencoder models for generation of drug molecules that can bind to a given binding site
  - Explored sequential models like RNN and LSTM for node and edge generation, and determined ways to mitigate order dependence during training
- **Analysis of drug response and gene expression data of AML cells**
  Guide: Brian Wilhelm, Université de Montréal (Virtual) — *Jun-Sep'21*
  - Performed analysis of drug response and gene expression data, focusing on Acute Myeloid Leukemia
  - Computational methods to identify drug-gene correlations and molecules that can induce leukemic cell maturation
- **Deep generative models for single-cell gene expression analysis**
  Guide: Hongyu Zhao, Yale University (Virtual) — *May-Jul'20*
  - Evaluated state-of-the-art unsupervised deep learning techniques including variational autoencoders for single-cell gene expression data analysis
- **RNA-seq data analysis of human oral squamous cell carcinoma**
  Guide: Debnath Pal, Indian Institute of Science Bangalore — *May-Jul'19*
  - Identified somatic mutations in RNA-sequencing data of human oral squamous cell carcinoma samples

Projects

- **Effects of visual representation for navigation control tasks**
  Robot Learning, Université de Montréal — *Jan-Apr'23*
  - Studied effects of contrastive learning and VAE-based pretraining strategies for RL-based visual navigation
- **Incorporating geometry into score-based model for crystal structure design**
  Geometry and Generative Models, McGill University — *Sep-Dec'22*
  - Attempted ways to incorporate crystal symmetry as an inductive bias into generative models for crystal structure design
- **Generating drug-like molecules from gene expression signatures using transformer**
  Algorithmic Approaches to Computational Biology, IIT Madras [Poster, Video, Report] — *Sep-Dec'20*
  - Designed an attention-based transformer model for *de novo* generation of drug-like molecules that can induce a desired transcriptomic profile. Accepted as poster at MLCSB COSI, ISMB 2022
  - Generated chemical compounds that were unique, valid, relevant, synthesizable and similar to known compounds
- **Parallel analyses of canonic polyadic tensor decomposition algorithm**
  Parallel Scientific Computing, IIT Madras [Report, Code] — *Feb-Jun'21*
  - CPU- and GPU-level parallelization of tensor decomposition algorithm using OpenMP and OpenACC
- **Deep generative approach to model single-cell data of human embryoid bodies**
  Computational Systems Biology, IIT Madras — *Jan'20-Jul'20*
  - Worked on using deep generative variational autoencoder model (scVI) to identify biologically relevant cell types of single-cell human embryoid bodies

Awards

- **PBEEE** – Merit scholarship for international students awarded by Fonds de recherche du Québec
- **Khorana Program for Scholars 2020**[1] – Awarded by Department of Biotechnology, Government of India
- **INSPIRE Scholar** – Awarded by Department of Science and Technology, Government of India

Publications (Google Scholar)

- **Govindarajan, Prashant**, Davide Baldelli, Jay Pathak, Quentin Fournier, and Sarath Chandar. **"CADmium: Fine-Tuning Code Language Models for Text-Driven Sequential CAD Design."** arXiv preprint arXiv:2507.09792 (2025).
- **Govindarajan, Prashant**, Mathieu Reymond, Antoine Clavaud, Mariano Phielipp, Santiago Miret, and Sarath Chandar. **"CrystalGym: A New Benchmark for Materials Discovery Using Reinforcement Learning."** arXiv preprint arXiv:2509.23156 (2025).
- **Govindarajan, Prashant**, Mathieu Reymond, Santiago Miret, Mariano Phielipp, and Sarath Chandar. **"Crystal Design Amidst Noisy DFT Signals: A Reinforcement Learning Approach."** In AI for Accelerated Materials Design-NeurIPS 2024.
- **Govindarajan, Prashant**, Mathieu Reymond, Santiago Miret, Antoine Clavaud, Mariano Phielipp, and Sarath Chandar. **"A Reinforcement Learning Pipeline for Band Gap-directed Crystal Generation."** In AI for Accelerated Materials Design-Vienna 2024.
- **Govindarajan, Prashant**, Santiago Miret, Jarrid Rector-Brooks, Mariano Phielipp, Janarthanan Rajendran, and Sarath Chandar. **"Learning Conditional Policies for Crystal Design Using Offline Reinforcement Learning."** Digital Discovery (2024).
- **Govindarajan, Prashant**, Santiago Miret, Jarrid Rector-Brooks, Mariano Phielipp, Janarthanan Rajendran, and Sarath Chandar. **"Behavioral Cloning for Crystal Design."** In Workshop on "*Machine Learning for Materials*" *ICLR 2023*. 2023.

  Accepted Posters: AI4Mat workshop (ICLR 2025, Vienna 2024, NeurIPS 2023 & 2024), ML4Materials workshop at ICLR 2023, Molecular Machine Learning Conference (MoML 2023 at MIT), Intelligent Systems for Molecular Biology (ISMB 2022)

Research Areas and Interests

Reinforcement Learning, Large Language Models, AI-based Drug and Material Design, Geometric Deep Learning, and Computational Biology

Relevant Coursework & Skills

Courses

Geometry and Generative Models, Reinforcement Learning, Representation Learning, Robot Learning, Parameter and State Estimation, Parallel Scientific Computing, Algorithmic Approaches to Computational Biology, Pattern Recognition and Machine Learning

Skills

Python (PyTorch, Tensorflow), R, MATLAB, C/C++ (OpenMP, MPI, OpenACC), Matter Modeling (DFT)

Activities & Extra-curriculars

Teaching

- Machine Learning, Polytechnique Montréal, Fall 2025
- Reinforcement Learning, Polytechnique Montréal, Fall 2023
- Reinforcement Learning, IIT Madras, Spring 2022
- DSA for Biology, IIT Madras, Fall 2021

Activities

- Organizer of "AI for Materials" reading group at Mila.
- Instructor for Chandar Lab's High School Internship Program
- Volunteer for Graduate Application Assistance Program for Underrepresented Students in AI
- Social events organizer at Chandar Research Lab
- Organizer of Molecular ML Conference (MoML 2023 and MoML 2024 at Mila)
- Talk on "Deep Learning in Genomics and Drug Discovery", IIT Madras
- Volunteered to anchor in High Performance Computing Symposium, IIT Madras

[1] Fellowship awarded to biotechnology students to undertake research internship in the USA [Link]

- Former student member at the New York Academy of Sciences (NYAS)

Reviewing
- TMLR (2025)
- AI4Mat workshop (Vienna 2024, NeurIPS 2023 & 2024)
- MoML (2023-25)
- Deployable AI workshop (AAAI 2023)

Competitions
- First prize in start-up pitch competition at Sciencepreneurship, EPFL, Switzerland
- Winning team, MIT COVID-19 Challenge (wastewater biosensor to track COVID-19)
- Finalist, Tracking Coronavirus Challenge organized by NYAS

Sports
- Ultimate Frisbee under National Sports Organization scheme at IIT Madras

Others
- Summer Schools: Oxford ML (2024)[2], Sciencepreneurship (2024), Amii AI Week (2022)
- Coordinator, Sponsorship and Public Relations team, Shaastra[3] 2019, IIT Madras
- Coordinator, Analytics Club, Center For Innovation[4], IIT Madras

[2] Declined
[3] Annual technical fest of IIT Madras
[4] Student-run innovation lab of IIT Madras