Siba Smarak Panigrahi

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Education

Ph.D. in Computer Science **2024–Ongiong**
École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland *GPA: 5.5/6.0*

M.Sc. (Thesis) in Computer Science **2022–2024**
McGill University and Mila, Montréal, Canada *GPA: 4.0/4.0*
Thesis: Equivariance in the Era of Large Pretrained Models (Supervisor: Siamak Ravanbakhsh)

B.Tech. in Computer Science and Engineering **2018–2022**
Indian Institute of Technology, Kharagpur, India *GPA: 9.73/10*
Department Rank **2** in graduating batch of CSE students (Supervisor: Abir Das, Rameswar Panda).

All India Senior School Certificate Examination (AISSCE) **2018**
Kendriya Vidyalaya Sangathan (KVS), India *98.6%*
Secured AIR 3, Rank 1 in Bhubaneswar Region. Among the top 0.1% of the 1.16 million candidates.

Research Interests

LLM Agents, AI Co-scientist, AI for Single-cell biology, Geometric Deep Learning

Publications

[10] **HeurekaBench: A Benchmarking Framework for AI Co-scientist**
S. S. Panigrahi*, J. Videnovic*, M. Brbic
*Under submission at International Conference on Learning Representations (**ICLR**) 2026.*

[9] **BigDocs: An Open and Permissively-Licensed Dataset for Training Multimodal Models on Document and Code Tasks** (Paper | Dataset | Website)
J. A. Rodriguez*, X. Jian*, **S. S. Panigrahi***, et al.
*International Conference on Learning Representations (**ICLR**) 2025; **NeurIPS** 2024 - RBFM workshop.*

[8] **SymmCD: Symmetry-Preserving Crystal Generation with Diffusion Models** (Paper | Code)
D. Levy*, **S. S. Panigrahi***, S-O. Kaba, Q. Zhu, K. Lee, M. Galkin, S. Miret, S. Ravanbakhsh
*International Conference on Learning Representations (**ICLR**) 2025; **NeurIPS** 2024 - AI4Mat (spotlight).*

[7] **Improved Canonicalization for Equivariant Adaptation of Large Pretrained Models** (Paper | Code)
S. S. Panigrahi, A. K. Mondal
***CVPR** 2024 - Workshop on Equivariant Vision (**EquiVision**).*

[6] **Efficient Dynamics Modeling in Interactive Environments with Koopman Theory** (Paper)
A. K. Mondal, **S. S. Panigrahi**, S. Rajeswar, K. Siddiqi, S. Ravanbakhsh
*International Conference on Learning Representations (**ICLR**) 2024; **EWRL** 2023.*

[5] **Equivariant Adaptation of Large Pretrained Models** (Paper | Blogpost @ ICML'24 | Code)
A. K. Mondal*, **S. S. Panigrahi***, S-O. Kaba, S. Rajeswar, S. Ravanbakhsh
*Neural Information Processing Systems (**NeurIPS**) 2023, EquiVision (**CVPR**) 2024 (spotlight).*

[4] **Identifying bot activity using topology-aware techniques** (Patent)
G Choudhary, SI Rahaman, **S. S. Panigrahi**, P Bhutani, M Kilaru, K Singh, A Singhania
US Patent 2023.

[3] **[Re]: Value Alignment Verification** (Paper | Code)
S. S. Panigrahi*, S. Patnaik*
*ML Reproducibility Challenge (**MLRC**) 2021; **NeurIPS 2022 Spotlight** and Journal Showcase Track.*

[2] **Leveraging Pre-trained Language Models for Key Point Matching** (Paper | Code)
M. N. Kapadnis*, S. Patnaik*, **S. S. Panigrahi***, V. Madhavan*, A. Nandy
***EMNLP** Workshop - Workshop on Argument Mining, 2021.*

[1] **Multi-class Emotion Classification Using EEG Signals** (Paper | Code)
D. Acharya, R. Jain, **S. S. Panigrahi**, R. Sahni, S. Jain, S. P. Deshmukh, A. Bhardwaj
*International Advance Computing Conference (**IACC**), 2020.*

Highlighted Research Experience

Document Understanding with LLMs **ServiceNow Research**
Visiting Researcher | Multimodal Foundation Models team *Mar 2024 - Jul 2024*

Developed permissively-licensed open dataset and improved document understanding capabilities of pretrained LLMs [9].

Diffusion Models for Materials Generation **Mila and McGill University**
Supervisor(s): Prof. Siamak Ravanbakhsh, Santiago Miret (Intel Labs) *Sep 2023 - Aug 2024*

Building **conditional diffusion models** for **materials generation** and **crystal structure prediction** task. Proposed meaningful representations for space groups and atom site symmetries for conditioning and **interpretability** [8].

Equivariant Adaptation of Large Pretrained and Foundation Models **Mila and McGill University**
Supervisor(s): Prof. Siamak Ravanbakhsh *Feb 2023 - Sep 2023*

Designed **equivariant canonicalization networks** to orient inputs to a canonical form, with a regularization loss, before passing through large pretrained/foundation models, effectively eliminating the requirement for designing and training extensive equivariant architectures from scratch [5, 7]. The research paper [5] was accepted to **NeurIPS 2023**.

Contextual Bias in Visual Recognition Models **IIT Kharagpur**
Supervisor(s): Prof. Abir Das, Dr. Rameswar Panda (MIT-IBM Watson AI Lab) *Apr 2021 - Dec 2021*

Evaluated **mAP** and used **GradCAM** with state-of-the-art computer vision models to quantitatively and qualitatively determine the contextual bias in images containing exclusive and co-occurring biased pairs. Proposed shallow models to capture contextual bias and **knowledge distillation** approaches for automated bias mitigation to improve.

Key Projects

CausalBench: Inferring gene regulatory network with factor graphs **Mila**
Causal Inference and ML Course Project | Instructor: Prof. Dhanya Sridhar

Studied the computational advantages and scalability potential of **factor graphs** in **causal discovery** (DCD-FG) for inferring **Gene Regulatory Networks** (GRNs). As per the CausalBench Challenge metrics, observed ∼**2x increase** with factor-graphs and further improvements with higher number of factors and matrix threshold values. (Code)

Crystal Symmetry aware framework for material generation **McGill University and Mila**
GGM Course Project | Instructor: Joey Bose and Prof. Prakash Panangaden

Incorporated Bravais lattice information and implemented **equivariant message-passing** in DimeNet graph encoder to integrate crystal symmetry information for **material generation**. **Reduced** the Wasserstein distance between generated and ground truth distribution for property and density by **more than 10%** from CDVAE in the MP-20 dataset. (Code)

Study of Facebook posts during elections **MIT, USA**
Data Analytics Intern | Supervisor(s): Dr. Kiran Garimella (IDSS, MIT)
Prof. Aaditya Dar (ISB), & Vasundhara Sirnate (The Polis Project)

Designed a complete framework to simplify the study of Facebook posts during elections. Analyzed page characteristics and post reactions from various politics-related Facebook pages and their correlation with election results. Trained simple classification pipelines with features from **TF-IDF** to predict the political party associated with a post. (Code)

Academic Achievements & Honors

- **Amii Upper Bound** bursary to attend Upper Bound AI conference (2025)
- **EDIC Fellowship** for starting Ph.D. at EPFL (2024)
- **Mitacs Accelerate Fellowship** at ServiceNow Research (2024)
- **Graduate Research Enhancement and Travel** (GREAT) Award, McGill University (2024)
- **Oxford ML Summer School** (OxML) (Representation Learning & Generative AI track) (2024)
- **Google's CS Research Mentorship Program** (CSRMP) Class of 2023b (2023)
- **CIFAR Deep Learning + Reinforcement Learning** (DLRL) **Summer School** (2023)
- **The Cornell, Maryland, Max Planck Pre-doctoral Research School** (CMMRS) (2023)
- **Jamsetji Nusserwanji Tata** (JN Tata) **Scholar** (endowment for higher studies) (2022)
- **Eastern European Machine Learning** (EEML) **Summer School** (selected for poster presentation) (2022)
- **Research Week with Google (Computer Vision track)** (1 of 150 selected students) (2022)
- **Prof. J.C. Ghosh Memorial Endowment Prize** (highest CGPA after semester VI) (2021)
- **Indo-US Science and Technology Forum (IUSSTF) - Viterbi** Award (1 of 15 awardees) (2021)
- **DAAD-WISE scholarship**, **University of Freiburg** (declined) (2021)
- **Technology Alumni Association (Delhi Chapter) Award** (highest CGPA after semester II) (2019)
- **Jagadis Bose National Science Talent Search Examination** (Rank 2 of 173 awardees) (2018)
- **Guest of the Hon'ble Prime Minister of India** to witness Republic Day Parade (2017)
- **KVS Junior Mathematical Olympiad** (Rank 6 in India; Rank 1 in Bhubaneswar region) (2016)
- **Exchange Student, Sakura Exchange Program in Science** (1 of 90 selected students) (2016)

Relevant Coursework

Mathematics - Linear Algebra, Calculus, Probability, and Statistics
Computer Science - Training Large Language Models, Geometry and Generative Models (GGM), Probabilistic Graphical Models, Network Science, Causal Inference and ML, Deep Learning, Machine Learning, Reinforcement Learning, Natural Language Processing (NLP), Information Retrieval, Principles of Programming Languages, Computer Networks*, Operating Systems*, Algorithms - I* & II, Cryptography & Network Security, Theory of Computation, Compilers*, Software Engineering* (* includes lab component)

Skills

- **Programming Languages** - Python, C, Java, LaTeX, Verilog, MIPS
- **Libraries** - PyTorch, PyTorch Lightning, PyTorch Geometric, Jax, NumPy, Pandas, Huggingface, Hydra
- **Web Development** - Django, HTML, CSS, Bootstrap, PostgreSQL

Activities and Leadership

Member, Mental Health Committee, Mila
Head, Kharagpur Data Analytics Group (KDAG), IIT Kharagpur (Reading-sessions)
Head, Institute Wellness Group, IIT Kharagpur (Facebook)
Head Boy, Student Council, KV No.2 CRPF Campus, Bhubaneswar

Professional Services

- **Organizing**:
  - ML Reproducibility Challenge (MLRC) 2023
  - CampusPulse (sponsored **CA$ 6000** GCP credits)
  - Molecular ML Conference (MoML) 2024, MoML 2023
- **Posters/Talks**:
  - International Conference on Learning Representations (ICLR) 2025, Singapore (Posters, 2025)
  - EquiVision workshop, Computer Vision and Pattern Recognition (CVPR) 2024, Seattle (Talk, 2024)
  - Google Research, Bengaluru (Talk, 2024)
  - International Conference on Learning Representations (ICLR) 2024, Vienna (Poster, 2024)
  - Conference on Neural Information Processing Systems (NeurIPS), New Orleans (Poster, 2023)
  - European Workshop on Reinforcement Learning (EWRL) 2023, VU Brussel (Poster, 2023)
  - NeurIPS 2022 Journal Showcase Track (and Spotlight lightning talk) (Poster & Talk, 2022)
  - 50^{th} Anniversary of School of Computer Science, McGill University (Poster, 2022)
  - KDAG Winter Workshop, lecture on Support Vector Machines (Talk, 2020)
- **Teaching Assistant (TA)**: CS401 (Head TA, EPFL, Autumn 2025), CS250 (EPFL, Spring 2025)
- **Volunteering**: DNetCV 2022 (CVPR-Workshop), EMNLP 2021
- **Reviewer**: NeurIPS (2024, 2025), ICLR (2025, 2026), AI4Mat (ICLR 2025, NeurIPS 2024 Workshop), GRaM 2024 (ICML-Workshop), NeurReps (2023, 2024) (NeurIPS-Workshop), MoML (2023, 2024), MLRC 2022 (Outstanding Reviewer), DNetCV 2022 (CVPR-W)