

Sahil Manchanda

Research Interests

Learning Combinatorial optimization, Graph generative modeling, Mixed Integer Programs, Few-Shot learning, Continual learning, AI for material science

Publications

- AAAI 2023 **Lifelong Learning to Solve Mixed Integer Programs** [pdf]
S Manchanda, S Ranu
- ECML **On the Generalization of Neural Combinatorial Optimization Heuristics** [pdf]
-PKDD 2022 S Manchanda, S Michel, D Drakulic, J Andreoli
- AAAI 2022 **TIGGER: Scalable Generative Modelling for Temporal Interaction Graphs** [pdf]
S Gupta, S Manchanda, S Ranu, S Bedathur
- NeurIPS 2021 **NeuroMLR: Robust and Reliable Route Recommendation on Road Networks** [pdf]
J Jain, V Bagadia, S Manchanda and S Ranu
- NeurIPS 2020 **GCOMB: Learning Budget-constrained Combinatorial Algorithms over Billion-sized Graphs** [pdf]
S Manchanda, A Mittal, A Dhawan, S Medya, S Ranu and A Singh
- CYBCONF 2017 **Representation learning of drug and disease terms for drug repositioning** [pdf]
S Manchanda, A Anand

PrePrint

- arxiv 2023 **StriderNET: A Graph Reinforcement Learning Approach to Optimize Atomic Structures on Rough Energy Landscapes** [pdf]
V Bihani, S Manchanda, S Sastry, S Ranu, NM Krishnan
- arxiv 2022 **Unsupervised Graph Neural Network Reveals the Structure–Dynamics Correlation in Disordered Systems** [pdf]
V Bihani, S Manchanda, S Ranu, NM Krishnan

Patent

- Granted in 2022 **US Patent: Trained pattern analyzer for roll out decision**
S Manchanda, A Rajkumar, S Kaur, N Unny. ([Link](#))

Education

- 2019 – Cont **Ph.D, Computer Science and Engineering, Indian Institute of Technology Delhi**, 8.73/10.0
- 2015 – 2017 **Master, Computer Science and Engineering, Indian Institute of Technology Guwahati**, 9.14/10.0
- 2010 – 2014 **Bachelor, Information Technology, Indraprastha University, Delhi**, 78.4%
- 2010 **Senior Secondary Education, CBSE New Delhi**, 97%
- 2008 **Secondary Education, CBSE New Delhi**, 91.8%

Work Experience

- Dec 2022 **University of Tokyo, Japan**
Visiting Researcher, Graph Neural Networks, Advisor: Prof. Toyotaro Suzumura
- Sep 2020 – **NAVER Labs, France**
- Mar 2021 Research intern, Machine Learning and Optimization
- Aug 2017 – **Conduent Labs India/Xerox Research Centre India, Bangalore, India**
- Jan 2019 Research Engineer, Machine Learning and Statistics
- June 2014 – **Adobe Systems, India**
- July 2015 Adobe Acrobat Team

Technical Skills

- Languages Python, C++
- Tools PyTorch, Torch-geometric, Git, CPLEX, SCIP, NumPy, SciPy, Scikit-learn, Pandas

Research Projects

- 2021-2022 **StriderNET: A Graph Reinforcement Learning Approach to Optimize Atomic Structures on Rough Energy Landscapes**
Advisor: *Prof.Sayan Ranu and Prof.Anoop Krishnan*, IIT Delhi.
- Learned reinforcement learning based Graph policy network to displace atoms to low energy configuration.
 - Model generalizes to unseen atomistic system sizes.
 - Achieved significantly better results compared to existing baselines.
- 2021-2022 **LifeLong learning to solve Mixed Integer Programs**
Advisor: *Prof.Sayan Ranu*, IIT Delhi.
- Analysed catastrophic forgetting in SoA methods in the continual setup.
 - Developed method to learn to solve MIPs in continual fashion. Tackled forgetting using Elastic Weight Consolidation and Knowledge distillation.
 - Achieved significantly better results compared to existing baselines.
- 2021-2022 **Unsupervised Graph Neural Network Reveals the Structure–Dynamics Correlation in Disordered System**
Advisor: *Prof.Anoop Krishnan and Prof.Sayan Ranu*, IIT Delhi.
- Developed unsupervised graph neural networks (GNN) for learning local structure of disordered system which in turn govern their dynamics.
 - Results show unsupervised graph neural networks can enable the discovery of local motifs in glasses, which exhibit dynamical heterogeneity. Analysis showed the such embeddings can reveal the structure-dynamics correlation in disordered systems.
- 2021-2022 **Few-Shot generative modeling of labeled graphs**
Advisor: *Prof.Sayan Ranu and Prof.Srikanta Bedathur*, IIT Delhi.
- Analyzed limitations of existing deep graph generative methods on *extremely low volume* of training datasets such as AIDS active molecules, rare cancer active molecule datasets etc.
 - Developed a Few-shot learning method to tackle this problem which learns to transfer knowledge from auxiliary datasets from similar domains.
 - Improved over SoA baselines by over 50% on various graph metrics on different domains such as Chemical, Molecular and Physical simulation systems.
- 2020-2021 **Generalization of Neural Combinatorial Optimization Heuristics**
Advisor: *Dr. Jean-Marc Andreoli and Dr. Sofia Michel*, NAVER Labs, Europe.
- Analyzed limitations of existing deep NCO methods on the generalization aspect.
 - Developed a decaying step-size-based meta-learning framework to tackle generalization issue.
 - The proposed framework adapts to out-of-distribution instances quickly with an extremely small number of fine-tuning instances.
- 2020-2021 **Robust and reliable route recommendation in road networks**
Advisor: *Prof.Sayan Ranu*, IIT Delhi.
- Developed an inductive model using Lipschitz embeddings on GCN to learn road embeddings.
 - Explored the importance of local-learning over end-to-end learning for enhancing the adversarial robustness of the model.
 - Model improved over existing work by 25% in terms of accuracy 25% in and 20% in terms of reachability. More effective in terms of answering queries over unseen data.
- 2020-2021 **Learning Budget-constrained Combinatorial Algorithms over Billion-sized Graphs**
Advisor: *Prof.Sayan Ranu*, IIT Delhi.
- Predict individual quality of nodes using Graph convolution network(GCN) and identify potential nodes.
 - Deep Q network to predict nodes that collectively form a good solution by using GCN scores and locality of nodes as features. Importance Sampling for fast locality computation.
 - Achieved quality similar to the state of the art while being more than 2 orders of magnitude faster.

2019 **Labeled Graph generative modeling**

Advisor: *Prof. Sayan Ranu*, IIT Delhi.

- Extended GraphRNN(NeurIPS 2018) for graph generative modeling for handling node and edge labels.
- Developed domain-agnostic method which works on different domains such as social networks, biological, chemical etc.

2017-2018 **Vehicle Health Monitoring**

Advisor: *Dr. Arun Rajkumar*, Conduent Labs.

- Developed item-set mining based model for recommending rollout of vehicles for a US based fleet agency.
- The method mines defect patterns which led to failures in the past when fleet supervisors made rollout decision.
- Showed performance improvement of over 15%.

2017-2018 **Mobility Analytics Platform - Descriptive platform for transportation network**

Advisor: *Dr. Narayanan Unny*, Conduent Labs.

- Developed algorithms for estimating passenger alighting in bus/metro network using check-in data in a flat fare environment.
- Designed solution to support heterogeneous data -fare collection(paper ticket /smart card) and vehicle location data.
- Developed various functionalities using fare collection data and GTFS(vehicle schedule) such as estimating direction of vehicles, identification of missing vehicle stop times, alignment of real trips to scheduled trips.

2016-2017 **Representation learning of drug and disease terms for drug repositioning**

Advisor: *Prof. Ashish Anand*, IIT Guwahati.

- Learned word vector representation of drug and disease terms from unstructured bio-medical text(PubMed)
- Enhanced vector representations using similarity information from structured data such as side-effect based drug similarity and gene based disease similarity etc.
- Used matrix completion approach to predict drug-disease associations.

Achievements

- 2023 Among top 200 young researchers from the world selected to attend the Heidelberg Laureate Forum 2023 in Germany.
- 2023 Outstanding Teaching Assistanship Award: Computer Networks course(UG + PG) at IIT Delhi
- 2022 Qualcomm Innovation Fellowship Recipient
- 2015 Graduate Aptitude Test in Engineering : All India rank 273 among 115425 candidates.
- 2010 CBSE Merit certificate : Received Merit Certificates for Computer Science and Mathematics for being in top 0.1 % of the successful candidates all over India.

Miscellaneous

- 2020-2021 Student member, PhD interviews organizing team, CSE, IIT Delhi
- 2019-Cont Teaching assistant at IIT Delhi - Computer networks, Data Structures and Algorithms, Database systems
- PC Chair KDD Applied Data Science Track.
- Reviewer AAAI, LoG, ECML-PKDD, AutoML, AISTATS, TKDD, KDD, TKDE, and WSDM
- Subreviewer SIGMOD, VLDB, EDBT, AAAI, WSDM, ICLR, CODS-COMAD,ICDM, KDD, ICDE, TKDE
- 2016-2017 Student representative (M.Tech) - Department Post Graduate Programme Committee, Dept. of CSE, IIT, Guwahati.

References

- Prof. Sayan Ranu, Associate Professor, IIT Delhi sayanranu@iitd.ac.in
- Prof. Srikanta Bedathur, Associate Professor, IIT Delhi srikanta@iitd.ac.in
- Dr. Jean-Marc Andreoli, Principal Scientist, NAVER Labs, Europe jean-marc.andreoli@naverlabs.com
- Dr. Narayanan Unny, Director, Big Data Labs, American Express, narayanan.unny@gmail.com
- Prof. Ashish Anand, Associate professor, IIT Guwahati anand.ashish@iitg.ernet.in
- Dr. Sofia Michel, Scientist, NAVER Labs, Europe, sofia.michel@naverlabs.com

- Dr. Sourav Medya, Post-doctoral fellow, Northwestern University sourav.medya@kellogg.northwestern.edu