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 $[\underline{pdf}]$ 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 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 Representation learning of drug and disease terms for drug repositioning [pdf] 2017 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 US Patent: Trained pattern analyzer for roll out decision
 - 2022 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%.

$2017\text{-}2018 \quad \textbf{Mobility Analytics Platform - Descriptive platform for transportation network}$

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 across 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

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

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