SUMIT TARAFDER.

Research Interests

Topics Areas

3D structure prediction, refinement or quality estimation of protein, RNA and associated complexes Structural bioinformatics, deep learning

Education

Virginia Tech

Aug. 2022 - Present

Ph.D. student in Computer Science

Blacksburg, VA

Bangladesh University of Engineering & Technology (BUET)

Jan. 2022

M.Sc. in Computer Science and Engineering

Dhaka, Bangladesh

Bangladesh University of Engineering & Technology (BUET)

Feb. 2017

B.Sc. in Computer Science and Engineering

Dhaka, Banqladesh

Experience

Virginia Tech

Aug. 2022 - Present

Graduate Research Assistant, Bhattacharya Lab

Blacksburg, VA

- Focused on projects related to the prediction and quality estimation of RNA 3D structures and protein-RNA complexes.
- Recently implemented research projects are available in GitHub.

Virginia Tech

Aug. 2022 - Dec. 2022

Graduate Teaching Assistant, CS 5914 -TS: Warehouse Scale Computing

Blacksburg, VA

• Graded multiple paper review and summary writings for individual students and conducted office hours.

United International University

May 2017 - Oct. 2021

Lecturer, Department of Computer Science and Engineering

Dhaka, Bangladesh

• I was the instructor and coordinator for a wide range of undergraduate-level theory and practical courses.

Publications

- Sumit Tarafder, Debswapna Bhattacharya. "RNAbpFlow: Base pair-augmented SE(3)-flow matching for conditional RNA 3D structure generation", 2025. [Under Submission]
- Sumit Tarafder, Debswapna Bhattacharya. "lociPARSE: a locality-aware invariant point attention model for scoring RNA 3D structures", Journal of Chemical Information and Modeling, Volume 64, Issue 22, Pages 8655–8664, November 2024. Impact Factor: 5.7
- Sumit Tarafder, Rahmatullah Roche, Debswapna Bhattacharya. "The landscape of RNA 3D structure modeling with transformer networks", Biology Methods and Protocols, Volume 9, Page 47, Issue 1, July 2024. Impact Factor: 2.5
- Sumit Tarafder, Mazharul Islam, Swakkhar Shatabda, Atif Rahman. "Figbird: A probabilistic method for filling gaps in genome assemblies", Bioinformatics, Volume 38, August 2022, Pages 3717–3724, Issue 15. Impact factor: 6.9
- Sumit Tarafder, Md. Toukir Ahmed, Sumaiya Iqbal, Md Tamjidul Hoque, M. Sohel Rahman. "RBSURFpred: Modeling Protein Accessible Surface Area in Real and Binary Space using Regularized and Optimized Regression", Journal of Theoretical Biology, Volume 441, January 2018, Pages 44 - 57. Impact factor: 2.0
- Rahmatullah Roche, <u>Sumit Tarafder</u>, Debswapna Bhattacharya. "Single-sequence protein-RNA complex structure prediction by geometric attention-enabled pairing of biological language models", 2024. [Under Submission]
- Rahmatullah Roche, Bernard Moussad, Md Hossain Shuvo, Sumit Tarafder, Debswapna Bhattacharya. "EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks", NAR, volume 52, Page e27, Issue 5, January 2024. Impact Factor: 14.9

Talks

• Presented our work "lociPARSE" as a poster and flash talk at ISMB '24 (Montreal, CA)

Awards

Travel Grant Fellowship

Awarded by Department of Computer Science, Virginia Tech for ISMB '24 Pratt Fellowship from Department of Computer Science, Virginia Tech in '24

Dean's List Award University Merit Scholarship & Dean's List from BUET

Services

- $\bullet\,$ Sub-reviwer at ISMB 2025
- Reviwer at IEEE/ACM Transactions on Computational Biology and Bioinformatics
- $\bullet\,$ Sub-reviwer at IEE BIBM 2024
- Sub-reviwer at BIOKDD 2024

Skills

Languages: Python, Java, C, C++, HTML/CSS Tools: Git, Docker, Chimera, PyMOL, VS Code

Frameworks: PyTorch, PyTorch Lightning, Matplotlib, Scikit-learn, Linux