Sumit Tarafder

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Research Interests

Topics 3D structure prediction, refinement or quality estimation of protein, RNA and associated complexes
Areas 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, Bangladesh*

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 *Blacksburg, VA*

- **CS 5914 TS: Warehouse Scale Computing (Fall 2022)**
  - Graded multiple paper review and summary writings for individual students and conducted office hours.
- **CS 5805 Advanced Machine Learning (Fall 2025)**
  - Responsible fo assignment design & grading, project proposal & report evaluation (in-class sessions).

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. "*PARSEbp: Pairwise Agreement-based RNA Scoring with Emphasis on Base Pairings",*", **2025**. [**Under Review**]
- **Sumit Tarafder**, Debswapna Bhattacharya. "*RNAbpFlow: Base pair-augmented SE(3)-flow matching for conditional RNA 3D structure generation*", **2025**. [**Under Review**]
- **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**, Xinyu Wang, Rahmatullah Roche, Debswapna Bhattacharya. "*Advances in Language-Model-Informed Protein–Nucleic Acid Binding Site Prediction*", Methods in Molecular Biology, Page 139-151, **July 2025**. Impact Factor: 1.3
- **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, **Sumit Tarafder**, Debswapna Bhattacharya. "*Single-sequence protein-RNA complex structure prediction by geometric attention-enabled pairing of biological language models*", Cell Systems, **2025**. IF: 7.7.
- 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* at *ISMB '24* (Montreal, CA)
- Presented "*lociPARSE*" as a full-length talk at *GLBIO conference* (Minnestota, USA)

Awards

Pratt Fellowship	Department of Computer Science, Virginia Tech — awarded in *2024* and *2025*.
Travel Grant	Department of Computer Science, Virginia Tech — supported participation at *ISMB 2024*.
Travel Grant	ISCB and GLBC — supported presentation at *GLBIO 2025*.
Dean's List Award	University Merit Scholarship and Dean's List, *(BUET)*.

Services

- Reviewer at IEEE/ACM Transactions on Computational Biology and Bioinformatics
- Sub-reviewer at ISMB 2025, IEE BIBM 2025, IEE BIBM 2024, BIOKDD 2024

Skills

Languages: Python, Java, C, C++, HTML/CSS
Tools: Git, Docker, Chimera, PyMOL, VS Code
Frameworks: PyTorch, PyTorch Lightning, Matplotlib, Scikit-learn, LangChain