RAHMATULLAH ROCHE

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RESEARCH INTERESTS

Applied Machine Learning, Computational Biology, Data Science and Human Computer Interaction

EDUCATION

Ph.D. in Computer Science August 2021 – July 2024
Virginia Tech Blacksburg, Virginia, USA

Master of Science in Computer Science and Software Engineering August 2018 – August 2021
Auburn University Auburn, Alabama, USA

Bachelor of Science in Computer Science and Engineering February 2011 – March 2016
Bangladesh University of Engineering and Technology (BUET) Dhaka, Bangladesh

AWARDS

NSF ACCESS Explore Resources 2024-Ongoing
PI, ”Advanced computational prediction of biomolecular properties and interactions”

Turner College Research Award 2025
Columbus State University

Core Course Design Institution Professional Development Award 2024, 2025
Columbus State University

Experiential Field Trip Grant Spring’24, Fall’24
Columbus State University

Travel award and YSEA Finalist 2024
20th Annual meeting of MCBIOS

Pratt Fellowship Award 2023-2024
Virginia Tech

Invited for Highlight Talk 2021
12th ACM-BCB conference

Best Poster Award for ‘PolyFold’ 2020
ACM Bioinformatics and Computational Biology

RESEARCH AND TEACHING EXPERIENCE

Assistant Professor August 2024 – Ongoing
Computer Science, Columbus State University

- Conducting research in Deep Learning and Computational Biology
- Teaching Computer Science courses

Research Assistant August 2018 – July 2024
Advisor: Dr. Debswapna Bhattacharya, Department of CS, Virginia Tech

- Employed deep learning techniques for predictive modeling
- Developed methods for protein 3D structure prediction and visualization

Teaching Assistant August 2018 – December 2020
Department of CSSE, Auburn University Auburn, Alabama, USA

- Evaluated projects and assignments
- Conducted question answering sessions and office hours

Lecturer September 2016 – July 2018
Department of CSE, Eastern University Dhaka, Bangladesh

- Taught computer science courses
- Supervised and monitored undergraduate student projects
- Prepared report for quality assessment of learning processes

Publications

[13] **R. Roche**, S. Tarafder, D. Bhattacharya. Single-sequence protein-RNA complex structure prediction by geometric attention-enabled pairing of biological language models. *Cell Systems (2025).* doi: 10.1016/j.cels.2025.101400

[12] S. Tarafder, X. Wang, **R. Roche**, D. Bhattacharya. Advances in Language-Model-Informed Protein–Nucleic Acid Binding Site Prediction. *Methods Mol Biol, 2941, 139-151 (2025).* doi: 10.1007/978-1-0716-4623-6_9 [Springer Nature Book Chapter]

[11] **R. Roche**, B. Moussad, M. H. Shuvo, S. Tarafder, D. Bhattacharya. EquiPNAS: improved protein–nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks. *Nucleic Acids Research,Volume 52, Issue 5 (2024).* doi: 10.1093/nar/gkae039

[10] S. Tarafder, **R. Roche**, D. Bhattacharya. The landscape of RNA 3D structure modeling with transformer networks *Biology Methods and Protocols, Volume 9, Issue 1 (2024).* doi: 10.1093/biomethods/bpae047

[9] **R. Roche**, B. Moussad, M. H. Shuvo, D. Bhattacharya. E (3) equivariant graph neural networks for robust and accurate protein-protein interaction site prediction. *PLOS Computational Biology 19, e1011435 (2023).* doi: 10.1371/journal.pcbi.1011435

[8] B. Moussad*, **R. Roche***, D. Bhattacharya. The transformative power of transformers in protein structure prediction. *Proceedings of the National Academy of Sciences 120, e2303499120 (2023).* doi: 10.1073/pnas.2303499120 [*Equally contributed]

[7] M. H. Shuvo, M. Karim, **R. Roche**, D. Bhattacharya. PIQLE: protein–protein interface quality estimation by deep graph learning of multimeric interaction geometries. *Bioinformatics Advances 3, (2023).* doi: 10.1093/bioadv/vbad070

[6] S. Bhattacharya, **R. Roche**, M. H. Shuvo, B. Moussad, D. Bhattacharya. Contact-Assisted Threading in Low-Homology Protein Modeling. *Methods Mol Biol 2627, 41-59 (2023).* doi: 10.1007/978-1-0716-2974-1_3 [*Springer Nature* Book Chapter]

[5] **R. Roche**, S. Bhattacharya, M. H. Shuvo, D. Bhattacharya. rrQNet: Protein contact map quality estimation by deep evolutionary reconciliation. *Proteins: Structure, Function, and Bioinformatics 90, 2023-2034 (2022).* doi: 10.1002/prot.26394

[4] S. Bhattacharya, **R. Roche**, B. Moussad, D. Bhattacharya. DisCovER: distance-and orientation-based covariational threading for weakly homologous proteins. *Proteins: Structure, Function, and Bioinformatics 90, 579-588 (2022).* doi: https://doi.org/10.1002/prot.26254

[3] **R. Roche**, S. Bhattacharya, D. Bhattacharya. Hybridized distance-and contact-based hierarchical structure modeling for folding soluble and membrane proteins. *PLOS Computational Biology 17, e1008753 (2021).* doi: 10.1371/journal.pcbi.1008753

[2] S. Bhattacharya, **R. Roche**, M. H. Shuvo, D. Bhattacharya. Recent advances in protein homology detection propelled by inter-residue interaction map threading. *Frontiers in Molecular Biosciences 8, 643752 (2021).* doi: 10.3389/fmolb.2021.643752

[1] A. J. McGehee, S. Bhattacharya, **R. Roche**, D. Bhattacharya. PolyFold: An interactive visual simulator for distance-based protein folding. *PLOS ONE 15, e0243331 (2020).* doi: 10.1371/journal.pone.0243331

Posters and Presentations

[3] **R. Roche**, S. Bhattacharya, D. Bhattacharya. Folding soluble and membrane proteins via hybridized distance and contact-based hierarchical structure modeling. (Highlight Talk)
ACM Bioinformatics Computational Biology, 2021.

[2] S. Bhattacharya, **R. Roche**, B. Moussad, D. Bhattacharya. DisCovER: distance- and orientation-based covariational threading for weakly homologous proteins.
29th ISMB/ECCB conference, 2021.

[1] A. J. McGehee, S. Bhattacharya, **R. Roche**, D. Bhattacharya. PolyFold: an interactive visual simulator for distance-based protein folding.
ACM Bioinformatics Computational Biology, 2020.

Abstracts

[3] S. Tarafder, **R. Roche**, D. Bhattacharya. Scoring-guided RNA Structure and Integrative Protein-RNA Complex Prediction by Bhattacharya group in CASP16. *CASP16 Abstract, 2024.*

[2] **R. Roche**, S. Bhattacharya, D. Bhattacharya. Hybridized distance- and contact- based hierarchical protein structure modeling using DConStruct.
Proceedings of the 12th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics, 2021.
doi: 10.1145/3459930.3469491

[1] M. H. Shuvo, S. Bhattacharya, **R. Roche**, D. Bhattacharya. Protein tertiary structure prediction by Bhattacharya group in CASP14. *CASP14 Abstract, 2020.*

Scientific Software Development and Dissemination

ProRNA3D-single 2024
Single-sequence protein-RNA complex structure prediction [GitHub]

EquiPNAS 2023
Protein–nucleic acid binding site prediction [GitHub]

EquiPPIS 2023
Protein–protein interaction site prediction [GitHub]

PIQLE 2023
Protein-protein interface quality estimation method [GitHub]

rrQNet 2022
Protein contact map quality estimation [GitHub]

DConStruct 2021
Hybridized distance- and contact-based hierarchical protein folding [GitHub]

DisCovER 2021
Distance- and orientation-based Covariational threadER [GitHub]

Services and Community Involvement

Discipline Coordinator for Computer Science (BS) - Web Development 2024-Ongoing
Columbus State University Columbus, GA

Reviewer 2023, 2024, 2025
BIBM, Briefings in Bioinformatics, Nature Scientific Reports, IEEE/ACM TCCB