Md Hossain Shuvo, Ph.D.
Assistant Professor

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EDUCATION

DEC 2023

Virginia Tech
Ph.D. in Computer Science
Advisor: Dr. Debswapna Bhattacharya
GPA: 3.88/4.0

JUL 2017

Alabama A&M University
M.Sc. in Computer Science
Advisor: Dr. Yujian Fu
GPA: 4.0/4.0

JUL 2014

Bangladesh University of Business and Technology
B.Sc. in Computer Science
Advisor: Mr. Md Saifur Rahman
CGPA: 3.86/4.0

RESEARCH INTERESTS

Computational Biology
Machine Learning
Data Analytics
Artificial Intelligence

RESEARCH EXPERIENCE

AUG 2021 – DEC 2023

Virginia Tech
Advisor: Dr. Debswapna Bhattacharya
Research direction: application of machine learning in developing computational methods for addressing problems related to protein complexes

JAN 2018 – JUL 2021

Auburn University
Advisor: Dr. Debswapna Bhattacharya

> **Research direction:** application of machine learning in developing computational methods for addressing problems related to protein structure prediction

AUG 2015 – JUL 2017   **Alabama A&M University**

> **Advisor:** Dr. Yujian Fu
>
> **Research direction:** development of tools for analyzing interactive behaviors in embedded and heterogeneous robotic systems

ACADEMIC EXPERIENCE

JAN 2024 - PRESENT   **Prairie View A&M University**

> **Position:** Assistant Professor, Dept. of CS

AUG 2018 – JAN 2020   **Auburn University**

> **Position:** Graduate Teaching Assistant, Dept of CSSE
>
> **Courses:**
> 1. **COMP 5970/6970:** Computational Biology
> 2. **COMP1210:** Fundamental of Computing I

MAY 2016 – JUL 2016   **North Alabama Center for Educational Excellence (NACEE)**

> **Position:** Assistant Mentor
>
> **Topic:** implementing multi-tasking and interactive behavior in NAO Humanoid robot

JAN 2015 – JUL 2015   **Dhaka Commerce College, Dhaka, Bangladesh**

> **Position:** Lecturer, Dept. of Stat, Math and COMP

JAN 2014 – DEC 2014   **Dhaka Cambrian College, Dhaka, Bangladesh**

> **Position:** Lecturer, Dept. of Information and Communication Technology

REFEREED PUBLICATIONS

2024

18. **M. H. Shuvo,** D. Bhattacharya, EquiRank: improved protein-protein interface quality estimation using protein-language-model-informed equivariant graph neural networks. Accepted to ICIBM 2024.

17. 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*, 2024 gkae039, 10.1093/nar/gkae039

2023

16. **M. H. Shuvo**, M. Karim, R. Roche, and D. Bhattacharya, "PIQLE: protein-protein interface quality estimation by deep graph learning of multimeric interaction geometries", Bioinformatics Advances, 2023, vbad070, 10.1093/bioadv070.

15. **M. H. Shuvo**, M. Karim, and D. Bhattacharya, "iQDeep: an integrated web server for protein scoring using multiscale deep learning models", Journal of Molecular Biology, 168057, 2023. doi: 10.1016/j.jmb.2023.168057

14. 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, doi: 10.1371/journal.pcbi.1011435

13. S. Bhattacharya, R. Roche, **M. H. Shuvo**, and D. Bhattacharya, "Contact-assisted threading in low-homology protein modeling", Methods in Molecular Biology book series, vol. 2627, 2023, doi: 10.1007/978-1-0716-2974-1 3

2022

12. R. Roche, S. Bhattacharya, **M. H. Shuvo**, and D. Bhattacharya, "rrQNet: Protein contact map quality estimation by deep evolutionary reconciliation", Proteins, Jun 2022, doi: 10.1002/prot.26394.

2021

11. **M. H. Shuvo**, M. Gulfam, and D. Bhattacharya, "DeepRefiner: high-accuracy protein structure refinement by deep network calibration", Nucleic Acids Research, vol. 49, no. W1, pp. W147–W152, Jul. 2021, doi: 10.1093/nar/gkab361

10. S. Bhattacharya, R. Roche, **M. H. Shuvo**, and D. Bhattacharya, "Recent Advances in Protein Homology Detection Propelled by Inter-Residue Interaction Map Threading", Front Mol Biosci, vol. 8, p. 643752, 2021, doi: 10.3389/fmolb.2021.643752.

9. A. Kryshtafovych, . . . , **M. H. Shuvo**, . . . , "Modeling SARS-CoV-2 proteins in the CASP-commons experiment", Proteins, vol. 89, no. 12, pp. 1987–1996, Dec. 2021, doi: 10.1002/prot.26231.

2020

8. **M. H. Shuvo**, S. Bhattacharya, and D. Bhattacharya, "QDeep: distance-based protein model quality estimation by residue-level ensemble error classifications using stacked deep residual neural networks", Bioinformatics, vol. 36, no. Suppl 1, pp. i285–i291, Jul. 2020, doi: 10.1093/bioinformatics/btaa455

7. R. Alapati, **M. H. Shuvo**, and D. Bhattacharya, "SPECS: Integration of side-chain orientation and global distance-based measures for improved evaluation of protein structural models", PLoS One, vol. 15, no. 2, p. e0228245, 2020, doi: 10.1371/journal.pone.0228245

2016

6. **M.H. Shuvo**, Y. Fu, "Sonar sensor virtualization for object detection and localization", SoutheastCon 2016, 1–8. doi: 10.1109/SECON.2016.7506699

5. Y. Fu, **M.H. Shuvo**, "An approach to analyzing adaptive intelligent vehicle system using SMT solver", In 2016 International Conference on Control, Decision and Information Technologies", (CoDIT)., pp. 313–319, doi: 10.1109/CoDIT.2016.7593580

4. Y. Fu, **M.H. Shuvo**, "Android-Based Remote Robot Control System". In, 2016 ASEE Annual Conference & Exposition Proceedings. ASEE Conferences, New Orleans, Louisiana, p.26251, doi: 10.18260/p.26251

2015

3. S. Rahman, **M.H. Shuvo**, "Advancement of Information System in the Health Sphere in Rural-Urban Areas of Developing Countries: A Case Study of Bangladesh". IJIRSET, Vol. 4, Issue 6, June 2015, doi: 10.15680/IJIRSET.2015.0406131

2. **M.H. Shuvo,** T. Haque, "Suspicious Behavior Detection Framework for Social Networking Sites Using Hidden Markov Model", 2015 Dhaka Commerce College Journal, Vol 7, Issue 1, P. 173 – 192

2014

1. M.M. Rahman, S. Ahmed, **M.H. Shuvo**, "Nearest Neighbor Classifier Method for Making Loan Decision in Commercial Bank". IJISA, 6, 60–68, doi: 10.5815/ijisa.2014.08.07

ABSTRACTS AND POSTERS

Abstracts

9. **M. H. Shuvo**, M. Karim, and D. Bhattacharya, "Protein modeling and accuracy estimation by Bhattacharya group in CASP15," CASP15 abstract, p. 35, 2022.

8. **M. H. Shuvo**, M. Gulfam, and D. Bhattacharya, "Deep network calibration for protein structure refinement," 13th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics, ACM-BCB 2022.

7. **M. H. Shuvo**, S. Bhattacharya, R. Roche, and D. Bhattacharya, "Protein tertiary structure prediction by Bhattacharya group in CASP14," CASP14 abstract, p. 38, 2020.

6. **M. H. Shuvo**, and D. Bhattacharya, "Protein model accuracy estimation by Bhattacharya groups in CASP14," CASP14 abstract, p. 39, 2020.

5. **M. H. Shuvo**, and D. Bhattacharya, "Protein structure refinement by Bhattacharya groups in CASP14," CASP14 abstract, pp. 40–41, 2020.

4. D. Bhattacharya, R. Alapati, and **M. H. Shuvo**, "Protein structure prediction and refinement by Bhattacharya human group in CASP13," CASP13 abstract, pp. 29-30, 2018.

3. R. Alapati, **M. H. Shuvo**, and D. Bhattacharya, "clustQ: Multi-model QA using superposition-free weighted internal distance comparisons," CASP13 abstract, p. 31, 2018

2. D. Bhattacharya and **M. H. Shuvo**, "refineD: Protein structure refinement using machine learning guided restrained relaxation," CASP13 abstract, p. 32, 2018

1. D. Bhattacharya and **M. H. Shuvo**, "scoreD: Estimating Global Distance Test using deep discriminative binary classifier ensemble," CASP13 abstract, p. 33

Posters

1. **M. H. Shuvo**, S. Bhattacharya, D. Bhattacharya, "QDeep: distance-based protein model quality estimation by residue-level ensemble error classifications using stacked deep residual neural networks", ISMB 2020

PARTICIPATION IN COMMUNITY-WIDE ASSESSMENT

APR 2022 – AUG 2022	**15th Critical Assessment of Protein Structure Prediction (CASP15) challenge**
	Role: method development, technical support for double-blind testing of our developed methods in both server and human pipelines
MAY 2020 – SEP 2020	**14th Critical Assessment of Protein Structure Prediction (CASP14) challenge**

	Role: method development, technical support for double-blind testing of our developed methods in both server and human pipelines
APR 2020	**CASP Commons (COVID-19, 2020), a collaborative initiative for modeling the SARS-2-CoV structure** **Role:** Provided technical support for testing our developed methods in predicting and assessing SARS-2-CoV target
MAY 2018 – AUG 2018	**13th Critical Assessment of Protein Structure Prediction (CASP13) challenge** **Role:** method development, technical support for double-blind testing of our developed methods in both server and human pipelines

HONORS AND AWARDS

Faculty Enhancement Program award	Awarded by the Roy G. Perry College of Engineering at PVAMU
NSF NDSA PFx instructor	Selected to be a PFx instructor
NSF NDSA RESEARCH AFFINITY COHORT	Selected as 1 of the 20 researchers
GOOGLE TEC EQUITY IMPACT FUND	$50,000 non-dilutive funding, led jointly with Dr. Wang at PVAMU
ACCESS ALLOCATIONS	Principal Investigator (PI), NSF - XSEDE Research Allocation
PRATT FELLOWSHIP AWARD	Awarded Pratt Fellowship at Virginia Tech, 2023
YOUNG SCIENTIST EXCELLENCE AWARDS	Awarded 1st place prize at 18th annual MCBIOS conference, 2022
CONFERENCE FELLOWSHIP	I. Received fellowship award for MCBIOS 2022 II. Received ISMB 2020 fellowship award
PUBLICATION RECOGNITION	DeepRefiner paper accepted for ACM-BCB 2022 Highlights track
TRAVEL FELLOWSHIP	Received travel grant for IEEE SoutheastCon 2016
POSTER AWARD	Awarded 2nd place prize at AAMU STEM Day 2016

SCIENTIFIC SOFTWARE DEVELOPMENT

PIQLE	Protein-protein interface quality estimation method [GitHub]
iQDeep	Integrated protein scoring server [Server]
DeepRefiner	High-accuracy protein structure refinement server [Server]
QDeep	Single-model protein quality estimation method [GitHub]
SPECS	Improved evaluation method for protein structures [Github]
EquiPPIS	E(3) equivariant graph neural networks for robust and accurate protein-protein interaction site prediction [Github]

EquiPNAS	EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks [GitHub]
rrQNet	Protein contact map evaluation method [Github]

TECHNICAL SKILLS

PROGRAMMING SKILLS	Python, R, Java, C, C++, PHP, ASP, Apache Cordova MySQL, MSSQL
APP DEVELOPMENT	I. Standalone application development with Java EE II. Mobile applications development in both Android and iOS III. Platforms Web applications development IV. Robotic applications development for EV3, NAO, and UAV

SERVICES AND OUTREACH

DIVISION OF RESEARCH AND INNOVATION COMMITTEE	Serving as a member of the Division of Research and Innovation Committee for Computer Science at PVAMU
FACULTY SEARCH COMMITTEE	Served as a member of the PVAMU faculty search committee
REVIEWER	Served as a sub-reviewer for BIOKDD 2021, 2023, 2024, IEEE ACM/Transaction
EVENT MANAGEMENT	i. Provided logistic support on E-day 2020 at Auburn University ii. Provided logistic support on AAMU Senior High School Day 2016
TECHNICAL COMMITTEE MEMBER	Provided technical support by developing the complete submission management system for AAMU STEM Day 2016