

Website 
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### Research Interests

• Knowledge-Guided Machine Learning • Vision-Language Models • Generative AI • Graph Neural Networks • AI for Science • Explainable AI • Semantic Segmentation Models • Self-Supervised Learning • Recommender Systems

### Education

Virginia Tech December 2024

PhD, Computer Science

Blacksburg, USA

 $The sis:\ Learning\ without\ Expert\ Labels\ for\ Multimodal\ Data.$ 

Advisor: Dr. Anuj Karpatne

Virginia Tech May 2023

Master of Science, Computer Science, GPA: 4.0/4.0

Bangladesh University of Engineering and Technology (BUET)

March 2016

Bachelor of Science and Engineering, Computer Science, GPA: 3.86/4.0

Dhaka, Bangladesh

Blacksburg, USA

# Work Experience

Amazon AGI Seattle, WA

Applied Scientist II

December 2024 – Present

• Developing customer-centric multimodal LLMs.

Virginia Tech Blacksburg, VA

Graduate Research Assistant, Advisor: Dr. Anuj Karpatne

May 2019 – Dec 2024

- Enhanced the performance of large vision language models (VLMs) for discovering biological traits through prompting, in-context learning, and instruction tuning that leverages the scientific knowledge. Additionally, designed a multitask benchmark VQA dataset for scientific tasks on organismal images. See publication C1, C7, W1. (Publications at NeurIPS 2024, AAAI 2024)
- Developed a hierarchical prototype network to discover evolutionary traits directly from images as prototypes. Additionally, collaborated on accelerating trait discovery using conditional diffusion models with phylogenetic knowledge in the form of hierarchical embeddings. See publication C2, C3, W2. (Publications at AAAI 2024, ECCV 2024)
- Structured a thorough comparative analysis of **Weakly Supervised Semantic Segmentation** approaches, highlighting the superiority of saliency maps over class activation maps (CAMs) through novel evaluation metrics and introducing stochastic aggregation via random cropping to enhance saliency effectiveness. See publication **C8**.
- Developed Distance-aware Negative Sampling (DNS) for enhanced graph representation learning, optimizing cohesion and separation by considering node-pair distances, improving structural similarity in **Unsupervised Graph Representation Learning (GRL) project.** See publication **C6**, **W8**. (Publications at SDM 2021, PIML 2020)
- Innovated PID-GAN architecture merging physics insights into GAN training for robust uncertainty quantification and effective use of unlabeled data, advancing the **Physics Informed Discriminator (PID) Framework**. See publication **C5, W4, W7**. (Publications at KDD 2021, NeurIPS 2020, AAAI 2021)
- Implemented a single-stage structured pruning algorithm DAM that can enforce  $L_0$  sparsity. It achieves state-of-the-art performance not only on structured pruning for image classification tasks but also on dimensionality reduction and graph representation learning tasks. See publication C4. (Publications at NeurIPS 2021)

Amazon.com Bellevue, WA

Applied Scientist Intern, Advisor: Dr. Badrinath Srinivas

May 2022 - Aug 2022

• Developed a real-time delivery image ranking algorithm to help Amazon drivers improve package delivery. The algorithm utilizes object-detection models along with statistical methods that yield 70% improvement over prior baselines.

Qualcomm Inc Santa Clara, CA

Machine Learning Engineer Intern, Advisor: Dr. Will Morrison

June 2021 - Aug 2021

• Collaborated with the GNSS Location team on GPS-based position estimation problem. This project involves improving the performance of state-of-the-art Graph Neural Network (GNN) models on satellite-based position estimations.

# **Publications**

### Conference Proceedings/Preprints

- [C1] M. Maruf, A. Daw, K. Mehrab, A. Karpatne et al., "VLM4Bio: A Benchmark Dataset to Evaluate Pretrained Vision-Language Models for Trait Discovery from Biological Images", accepted at NeurIPS 2024. [PDF]
- [C2] H. Manogaran, M. Maruf, A. Daw, A. Karpatne et al., "What Do You See in Common? Learning Hierarchical Prototypes over Tree-of-Life to Discover Evolutionary Traits", under submission. [PDF]
- [C3] M. Khurana, A. Daw, M. Maruf, A. Karpatne et al., "Hierarchical Conditioning of Diffusion Models Using Tree-of-Life for Studying Species Evolution", in ECCV 2024. [PDF]

- [C4] J. Bu\*, A. Daw\*, M. Maruf\*, and A. Karpatne, "Learning Compact Representations of Neural Networks using DiscriminAtive Masking (DAM)", in NeurIPS 2021 (\* equal contribution). [PDF]
- [C5] A. Daw\*, M. Maruf\*, and A. Karpatne, "PID-GAN: A GAN Framework based on a Physics-informed Discriminator for Uncertainty Quantification with Physics", in KDD 2021 (\* equal contribution). [PDF]
- [C6] M. Maruf and A. Karpatne "Maximizing Cohesion and Separation in Graph Representation Learning: A Distance-aware Negative Sampling Approach", in SDM 2021. [PDF]
- [C7] K. Mehrab\*, M. Maruf\*, A. Daw\*, A. Karpatne et al., "Fish-Vista: A Multi-Purpose Dataset for Understanding & Identification of Traits from Images", under submission. (\* equal contribution). [PDF]
- [C8] M. Maruf, A. Daw, J. Bu, and A. Karpatne, "Beyond Discriminative Regions: Saliency maps as Alternatives to CAMs for Weakly Supervised Semantic Segmentation", in ArXiv:2308.11052. [PDF]

#### Journal Articles

- [J1] M. Balk, J. Bradley, M. Maruf, A. Karpatne et al., "A FAIR and Modular Image-based Workflow for Knowledge Discovery in the Emerging Field of Imageomics", in Methods in Ecology and Evolution 2024. [PDF]
- [J2] Y. Bakis, Y. Altintas, M. Maruf, A. Karpatne et al., "Extracting Landmark and Trait Information from Segmented Digital Specimen Images Generated by Artificial Neural Networks", in Biodiversity Information Science and Standards 2022.
- [J3] M. Maruf and S. Shatabda, "iRSpot-SF: Prediction of Recombination Hotspots by Incorporating Sequence-based Features into Pseudo Components", in Genomics 2019. [PDF]

#### Workshop Proceedings

- [W1] M. Maruf, A. Daw, and A. Karpatne, "Are Pre-trained Vision Language Models (VLMs) Decent Zero-shot Predictors in Scientific Contexts?", in Imageomics Workshop AAAI 2024.
- [W2] M. Khurana, A. Daw, M. Maruf, and A. Karpatne, "Conditioning Diffusion Models Using the Knowledge of Phylogeny for Understanding Species Evolution", in Imageomics Workshop AAAI 2024.
- [W3] K. Mehrab, A. Daw, M. Maruf, and A. Karpatne, "Phylo-GNN: Phylogeny-guided Graph Neural Network Approach for Fine-Grained Image Trait Identification", in Imageomics Workshop AAAI 2024.
- [W4] A. Daw\*, M. Maruf\*, and A. Karpatne, "PID-GAN: A gan framework based on a physics-informed discriminator for uncertainty quantification with physics", in SGAI AAAI 2021 (\* equal contribution).
- [W5] M. Maruf, M. Elhamod, P. Mandke, and A. Karpatne, "Biology-guided Neural Network for Fish Trait Discovery", in Integrative and Comparative Biology 2021.
- [W6] M. Elhamod, M. Maruf, P. Mandke, and A. Karpatne, "Biology-guided Neural Network for Species Classification", in Integrative and Comparative Biology 2021.
- [W7] A. Daw, M. Maruf, and A. Karpatne, "Physics-Informed Discriminator (PID) for Conditional Generative Adversarial Networks", in ML4PS NeurIPS 2020.
- [W8] M. Maruf and A. Karpatne, "Informing Neural Networks for Drug Effect Prediction Using Biological Knowledge of Protein-Protein Interactions", in PIML 2020.

# Academic Services, Honors & Awards

Reviewer: NeurIPS (2024), Dataset and Benchmark track NeurIPS (2024), ML4PS NeurIPS(2021-present), SGAI-AAAI (2021, 2022), PKDD (2023), KDD (2021, 2022).

PC Member: SGAI-AAAI (2021, 2022, 2024).

Session Chair: Spatiotemporal Data at SDM 2021.

Fellowship: Kafura Graduate Fellowship, Virginia Tech, 2023.

Award: SDM Doctoral Student Travel Award (2020), Dean's List Award (BUET 2011-16).

# Technical Skills

Python, C++, Java, PyTorch, Tensorflow, SageMaker, S2, S3, EC2, Deepspeed, LoRA.

## References

Dr. Anuj Karpatne, Associate Professor, Department of Computer Science, Virginia Tech.

More references will be provided upon request.