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Google Scholar Link: https://scholar.google.com/citations?user=wNEYBrAAAAAJ&hl=en

BIO AND RESEARCH SUMMARY

I am a tenure-track Assistant Professor in the Department of Computer Science and Engineering at University of Minnesota, Twin Cities.

My general research interests are in the areas of artificial intelligence (AI) and machine learning (ML) where I focus on advancing foundations of AI/ML to solve challenging real-world problems with high societal impact. The overarching theme of my research program is *AI to Accelerate Scientific Discovery and Engineering Design*. A large focus of my current work is on developing novel adaptive experimental design algorithms to optimize combinatorial spaces (e.g., sequences, trees, graphs, and mixture of discrete/continuous design variables) and applying them to solve high-impact engineering and science applications (e.g., drug/vaccine design, nanoporous materials design, biological sequence design, hardware design, and additive manufacturing). Specific topics include:

- Probabilistic modeling (Gaussian processes, deep models, and their combination) over structured data
- Methods to combine domain knowledge and experimental/observational data to create rich structured models
- Principled data acquisition strategies for diverse goals (e.g., optimization, discovery, and predictive models)
- Creating predictive models and sequential decision-making policies using small training data
- Accelerate the discovery of nanoporous materials for sustainability applications (e.g., storage and separation of gases); accelerate the design of effective, safe, and low-cost drugs and vaccines; biological sequence design (e.g., proteins) for health applications; design of high-performance and low-power hardware to overcome Moore's law; and improving additive manufacturing processes for their effectiveness.

PROFESSIONAL EXPERIENCE

Assistant Professor (Tenure Track) — **August 2024–**
Department of Computer Science and Engineering, University of Minnesota — *Minneapolis, Minnesota*

EDUCATION

Ph.D., Computer Science — **2018–2024**
Washington State University — *Pullman, Washington*
Advisor: Prof. Jana Doppa
Thesis: Adaptive Experimental Design for Optimizing Combinatorial Structures
2023 Voiland College of Engineering and Architecture, Outstanding PhD Dissertation Award

MS, Computer Science — **2018–2020**
Washington State University — *Pullman, Washington*
Thesis: A Learning to Search Framework for Multi-Objective Optimization of Manycore Systems Design
2020 WSU Outstanding Dissertation Award. (Nominated for WAGS Outstanding Innovation in Technology Award)

Bachelor of Technology, Mathematics and Computing — **2013–2017**
Delhi Technological University — *New Delhi, India*

INDUSTRIAL RESEARCH EXPERIENCE

Research Intern — **June 2023–August 2023**
Meta Research - Adaptive Experimentation Team — *San Francisco*

Research Intern — **June 2022–August 2022**
Meta Research - Adaptive Experimentation Team — *New York*

Research Intern — **May 2021–August 2021**
Google Research - Vizier Team — Remote

Research and Development Engineer — **October 2017–May 2018**

Works Applications *Tokyo, Japan*

Software Engineering Intern **June 2016–August 2016**
Samsung *Bengaluru, India*

AWARDS AND HONORS

- AAAI New Faculty Highlights Speaker, 2025
- Voiland College of Engineering, Outstanding PhD Dissertation Award, 2023
- Rising Stars in AI, KAUST AI Initiative, 2023
- Selected for Heidelberg Laureate Forum, 2022
- Voliand College of Engineering, Outstanding Graduate Research Assistant Award, 2022
- Top Reviewer Award, International Conference on Machine Learning (ICML), 2021
- Outstanding Reviewer Award, International Conference on Learning Representations (ICLR), 2021
- Top Reviewer Award, International Conference on Machine Learning (ICML), 2020
- WSU Outstanding Dissertation Award (Nominee for WAGS Outstanding Innovation in Tech. Award), 2020
- WSU GPSA Graduate Research Assistant Excellence Award, 2020
- Voiland College of Engineering, Outstanding Teaching Assistant in Computer Science Award, 2020
- Mahmoud Dillsi Graduate Fellowship, 2020
- Alfred Suksdorf Fellowship, Washington State University, 2018-2020

PUBLICATIONS

Conference Papers

18. [**AAAI'25**] Yassine Chemingui,Aryan Deshwal, Honghao Wei, Alan Fern, Janardhan Rao Doppa. Constraint-Adaptive Policy Switching for Offline Safe Reinforcement Learning. *Thirty-Ninth AAAI Conference on Artificial Intelligence (AAAI), 2025.*

17. [**ICML'24**] Minh Hoang, Azza Fadhel, Aryan Deshwal, Janardhan Rao Doppa, Nghia Hoang. Learning Surrogates for Offline Black-Box Optimization via Gradient Matching. *Forty-first International Conference on Machine Learning (ICML)*, 2024.

16. [**IJCAI'24**] Mohammed Amine Gharsallaoui, Bhupinderjeet Singh, Aryan Deshwal, Yan Yan, Kirti Rajagopalan, Ananth Kalyanaraman, Janardhan Rao Doppa. Streamflow Prediction with Uncertainty Quantification for Water Management: A Neuro-Symbolic Learning Approach. *Thirty-Third International Joint Conference on Artificial Intelligence (IJCAI)* , 2024.

15. [**AAAI'24**] Yassine Chemigue, Aryan Deshwal, Nghia Hoang, Janardhan Rao Doppa. Offline Model-based Black-Box Optimization via Policy-guided Gradient Search. *Thirty-Eighth AAAI Conference on Artificial Intelligence (AAAI)*, 2024.

14. [**AISTATS'23**] Aryan Deshwal, Sebastian Ament, Maximilian Balandat, Eytan Bakshy, Janardhan Rao Doppa, and David Eriksson. Bayesian Optimization over High-Dimensional Combinatorial Spaces via Dictionary-based Embeddings. *Twenty-sixth International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2023.

13. [**AAAI'22**] Aryan Deshwal, Syrine Belakaria, Janardhan Rao Doppa, Dae Hyun Kim. Bayesian Optimization over Permutation Spaces. *Thirty-Sixth AAAI Conference on Artificial Intelligence (AAAI)*, 2022.

12. [**NeurIPS'21**] Aryan Deshwal, Janardhan Rao Doppa. Combining Latent Space and Structured Kernels for Bayesian Optimization over Combinatorial Spaces. *Thirty-Fifth Conference on Neural Information Processing Systems (NeurIPS)*, 2021.

11. [**ICML'21**] Aryan Deshwal, Syrine Belakaria, Janardhan Rao Doppa. Bayesian Optimization over Hybrid Spaces. *Proceedings of Thirty-eighth International Conference on Machine Learning (ICML), 2021.*

10. [**DAC'21**] Aryan Deshwal, Syrine Belakaria, Ganapati Bhat, Janardhan Rao Doppa, and Partha Pratim Pande. Learning Pareto-Frontier Resource Management Policies for Heterogeneous SoCs: An Information-Theoretic Approach. *Proceedings of 58th ACM/IEEE Design Automation Conference (DAC), 2021.*

9. [**AAAI'21**] Aryan Deshwal, Syrine Belakaria, Janardhan Rao Doppa. Mercer Features for Efficient Combinatorial Bayesian Optimization. *Proceedings of Thirty-Fifth AAAI Conference on Artificial Intelligence (AAAI), 2021.*

8. [**AAAI'20**] Aryan Deshwal, Syrine Belakaria, Janardhan Rao Doppa, and Alan Fern. Optimizing Discrete Spaces via Expensive Evaluations: A Learning to Search Framework. *Proceedings of Thirty-Fourth AAAI Conference on Artificial Intelligence (AAAI)*, 2020.

7. [**AAAI'20**] Syrine Belakaria, Aryan Deshwal, Nitthilan Kannappan Jayakodi, and Janardhan Rao Doppa. Uncertainty-Aware Search Framework for Multi-Objective Bayesian Optimization. *Proceedings of Thirty-Fourth AAAI Conference on Artificial Intelligence (AAAI)*, 2020.

6. [**AAAI'20**] Syrine Belakaria, Aryan Deshwal, and Janardhan Rao Doppa, Multi-Fidelity Multi-Objective Bayesian Optimization: An Output Space Entropy Search Approach. *Proceedings of Thirty-Fourth AAAI Conference on Artificial Intelligence (AAAI)*, 2020.

5. [**DATE'20**] Syrine Belakaria†, Zhiyuan Zhou†, Aryan Deshwal, Janardhan Rao Doppa, Deuk Heo, and Partha Pratim Pande. Design of Multi-Output Switched-Capacitor Voltage Regulator via Machine Learning. *Proceedings of Twenty-Third ACM/IEEE Design, Automation and Test in Europe Conference (DATE)*, 2020. † denotes equal contribution.

4. [**CODES'19**] Paul Bogdan, Fan Chen, Aryan Deshwal, Janardhan Rao Doppa, Biresh Kumar Joardar, Hai (Helen) Li, Shahin Nazarian, Linghao Song, Yao Xiao. Taming Extreme Heterogeneity via Machine Learning based Design of Autonomous Manycore Systems. *International Conference on Hardware/Software Codesign and System Synthesis Companion (CODES), pp 21:1-21:10*, 2019.

3. [**NeurIPS'19**] Syrine Belakaria, Aryan Deshwal, and Janardhan Rao Doppa.Max-value Entropy Search for Multi-Objective Bayesian Optimization. *Proceedings of Thirty-Third International Conference on Neural Information Processing Systems (NeurIPS), pp 7823-7833*, 2019.

2. [**IJCAI'19**] Aryan Deshwal, Janardhan Rao Doppa, and Dan Roth. Learning and Inference for Structured Prediction: A Unifying Perspective. *Proceedings of Twenty-Eighth International Joint Conference on Artificial Intelligence (IJCAI), pp 6291-6299*, 2019.

1. [**IJCAI'19**] Chao Ma, F A Rezaur Rahman Chowdhury, Aryan Deshwal, Md Rakibul Islam, Janardhan Rao Doppa, and Dan Roth. Randomized Greedy Search for Structured Prediction: Amortized Inference and Learning. *Proceedings of Twenty-Eighth International Joint Conference on Artificial Intelligence (IJCAI), pp 5130-5138*, 2019.

Journal Papers

8. [**Advanced Materials**] Eric Chen, Alaleh Ahmadian, Sonja Sparks, Aryan Deshwal, Janardhan Rao Doppa, Kaiyan Qiu. Machine Learning Enabled Design and Optimization for 3D-Printing of High-Fidelity Presurgical Organ Models. *Advanced Materials Journal*, 2024.

7. [**Digital Discovery'23**] Nickolas Gantzler, Aryan Deshwal, Janardhan Rao Doppa, Cory Simon. Multi-fidelity Bayesian Optimization of Covalent Organic Frameworks for Xenon/Krypton Separations. To appear in *Digital Discovery Journal, Royal Society of Chemistry*, 2023.

6. [**TODAES'23**] Gaurav Narang, Aryan Deshwal, Janardhan Rao Doppa, Raid Ayoub, Mike Kishnivesky, Partha Pratim Pande. Dynamic Power Management in Large Manycore Systems: A Learning-to-Search Framework. *ACM Transactions on Design Automation of Electronic Systems (TODAES), 28(5): 84:1-84:21*, 2023.

5. [**TCAD'22**] Biresh Kumar Joardar, Aryan Deshwal, Janardhan Rao Doppa, Partha Pratim Pande, Krishnendu Chakrabarty. High-Throughput Training of Deep CNNs on ReRAM-based Heterogeneous Architectures via Optimized Normalization Layers. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems (TCAD) 41(5): 1537-1549*, 2022.

4. [**MSDE'21**] Aryan Deshwal, Cory Simon, Janardhan Rao Doppa. Bayesian Optimization of Nanoporous Materials. *Molecular Systems Design and Engineering Journal, Royal Society of Chemistry, 6, 1066-1086*, 2021.

3. **[JAIR'21]** Syrine Belakaria, Aryan Deshwal, Janardhan Rao Doppa. Output Space Entropy Search Framework for Multi-Objective Bayesian Optimization. *Journal of Artificial Intelligence Research (JAIR), 72: 667-715*, 2021.

2. **[TECS'20]** Nitthilan K. Jayakodi, Syrine Belakaria, Aryan Deshwal, and Janardhan Rao Doppa. Design and Optimization Framework to Trade-off Energy and Accuracy of Inference on Mobile Platforms via Pretrained Neural Networks. *ACM Trans. on Embedded Computing Systems (TECS), 19(1): 4:1-4:24*, 2020.

1. **[TECS'19]** Aryan Deshwal, Nitthilan K. Jayakodi, Biresh Joardar, Janardhan Rao Doppa, Partha Pratim Pande. MOOS: A Multi-Objective Design Space Exploration and Optimization Framework for NoC enabled Manycore Systems. *ACM Transactions on Embedded Computing Systems (TECS), 18(5s): 77:1-77:23*, 2019.

Workshop Papers

7. Aryan Deshwal, Sait Cakmak, Yuhou Xia, David Eriksson. Sample-Efficient Bayesian Optimization with Transfer Learning for Heterogeneous Search Spaces. *AutoML Conference 2024 (Workshop Track)*.

6. Aryan Deshwal, Syrine Belakaria, Janardhan Rao Doppa. Scalable Combinatorial Bayesian Optimization with Tractable Statistical models. *Proceedings of NeurIPS Workshop on Engineering Modeling, Simulation, and Design, 2020*.

5. Syrine Belakaria, Aryan Deshwal, Janardhan Rao Doppa. Information-Theoretic Multi-Objective Bayesian Optimization with Continuous Approximations. *Proceedings of NeurIPS Workshop on Engineering Modeling, Simulation, and Design, 2020*.

4. Syrine Belakaria, Aryan Deshwal, Janardhan Rao Doppa. Max-value Entropy Search for Multi-Objective Bayesian Optimization with Constraints. *Proceedings of NeurIPS Workshop on Machine Learning and the Physical Sciences, 2020*.

3. Aryan Deshwal, Syrine Belakaria, Janardhan Rao Doppa, and Alan Fern. Optimizing Discrete Spaces via Expensive Evaluations: A Learning to Search Framework. *ICML Workshop on Real World Experiment Design and Active Learning*, 2020.

2. Syrine Belakaria, Aryan Deshwal, and Janardhan Rao Doppa. Max-value Entropy Search for Multi-Objective Bayesian Optimization. *ICML Workshop on Real World Experiment Design and Active Learning*, 2020.

1. Syrine Belakaria, Aryan Deshwal, and Janardhan Rao Doppa. Uncertainty aware Search framework for Multi-Objective Bayesian Optimization with Constraints. *ICML Workshop on Automated Machine Learning (AutoML)*, 2020.

CONFERENCE/INVITED TALKS

- Adaptive Experimental Design To Accelerate Scientific Discovery and Engineering Design @ Oregon State University, 2024.
- Adaptive Experimental Design to Accelerate Scientific Discovery and Engineering Design @ Indian Institute of Science, 2024.
- Adaptive Experimental Design to Accelerate Scientific Discovery and Engineering Design @ Indian Institute of Technology, Roorkee, 2024.
- Adaptive Experimental Design to Accelerate Scientific Discovery and Engineering Design @ Indian Institute of Technology, Delhi, 2024.
- Invited Talk, Bayesian Optimization over Combinatorial Structures @ INFORMS Conference, 2023.
- Invited Talk, Bayesian Optimization over Combinatorial Structures @ Amazon Science Seminar, 2023.
- Bayesian Optimization over High-Dimensional Combinatorial Spaces via Dictionary-based Randomized Continuous Embeddings @ AISTATS, 2023.
- Invited Talk, Bayesian Optimization over Combinatorial Structures @ Secondmind, 2022.
- Invited Talk, Bayesian Optimization over Combinatorial Structures @ Valence Labs, 2022.
- Invited Talk, Bayesian Optimization over Combinatorial Structures, Invited Talk @ Argonne National Laboratory, 2022.
- Bayesian Optimization over Permutation Spaces @ AAAI, 2022.

- Bayesian Optimization over Hybrid Spaces @ ICML, 2021.
- Mercer Features for Efficient Combinatorial Bayesian Optimization @ AAAI, 2021.
- Optimizing Discrete Spaces via Expensive Evaluations: A Learning to Search Framework @ AAAI, 2020.
- MOOS: A Multi-Objective Design Space Exploration and Optimization Framework for NoC enabled Many-core Systems @ Embedded Systems Week Conference, 2019.
- Randomized Greedy Search for Structured Prediction: Amortized Inference and Learning @ IJCAI, 2019.
- Learning and Inference for Structured Prediction: A Unifying Perspective @ IJCAI, 2019.

TEACHING EXPERIENCE

Tutorial Instructor

- Lead organizer of *AAAI Tutorial on Recent Advances in Bayesian Optimization* at AAAI-2023. Slides Link.
- Lead organizer of *IJCAI Tutorial on Bayesian Optimization: From Foundations to Advanced Topics* at IJCAI-2022.
- Lead organizer of *AAAI Tutorial on Bayesian Optimization: From Foundations to Advanced Topics* at AAAI-2022.

Teaching Assistant and Guest Lecturer

- Teaching Assistant for CptS 570: Introduction to Machine Learning (Fall-2019). Outstanding TA Award.
- Guest lecturer for CptS 570 (Introduction to Machine learning), CptS 577 (Structured Prediction and Intelligent Decision-Making), and CptS 315 (Introduction to Data Mining).

CONFERENCE/WORKSHOP ORGANIZATION

- Lead organizer of *4th Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI for Biological Sciences Theme)* upcoming at AAAI-2025. Website Link.
- Lead organizer of *3rd Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI for Materials and Manufacturing Theme)* at AAAI-2024. Website Link.
- Lead organizer of *2nd Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI for Earth and Environment Science Theme)* at AAAI-2023. Website Link.
- Lead organizer of *1st Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI for Chemistry Theme)* at AAAI-2022. Website Link.

PROFESSIONAL SERVICE AND OUTREACH ACTIVITIES

Area Chair and Senior Program Committee Member

- Forty-second International Conference on Machine Learning (ICML), 2025
- Twenty-Eighth International Conference on Artificial Intelligence and Statistics (AISTATS), 2025
- Thirteenth International Conference on Learning Representations (ICLR), 2025
- Thirty-Ninth AAAI Conference on Artificial Intelligence (AAAI), 2025
- Thirty-Eighth AAAI Conference on Artificial Intelligence (AAAI), 2024
- Thirty-Seventh AAAI Conference on Artificial Intelligence (AAAI), 2023

Program Committee Member

- Thirty-eighth Conference on Neural Information Processing Systems (NeurIPS), 2024 (Top Reviewer award)
- Forty-first International Conference on Machine Learning (ICML), 2024
- Twelfth International Conference on Learning Representations (ICLR), 2024
- Thirty-Eighth AAAI Conference on Artificial Intelligence (AAAI), AI for Social Impact Track, 2024
- Thirty-Seventh Conference on Neural Information Processing Systems (NeurIPS), 2023

- Fortieth International Conference on Machine Learning (ICML), 2023
- International Conference on Learning Representations (ICLR), 2023
- Twenty-Sixth International Conference on Artificial Intelligence and Statistics (AISTATS), 2023
- Thirty-Sixth Conference on Neural Information Processing Systems (NeurIPS), 2022
- Thirty-Ninth International Conference on Machine Learning (ICML), 2022
- Thirty-Fifth Conference on Neural Information Processing Systems (NeurIPS), 2021
- Thirty-Eighth International Conference on Machine Learning (ICML), 2021 Top Reviewer Award, Expert Reviewer
- Thirty-Fifth AAAI Conference on Artificial Intelligence (AAAI), 2021
- International Conference on Learning Representations (ICLR), 2021 Outstanding Reviewer Award
- Thirty-Fourth Conference on Neural Information Processing Systems (NeurIPS), 2020
- Thirty-Seventh International Conference on Machine Learning (ICML), 2020 Top Reviewer Award
- Twenty-Ninth International Joint Conference on Artificial Intelligence (IJCAI), 2020

Conference and Journal Reviewer

- Reviewer for NeurIPS-2019, UAI-2019, KDD-2019, AISTATS-2019, ESWEEK-2019, AAAI-2020, AISTATS-2020, UAI-2020, KDD-2020, UAI-2021, AISTATS-2022, NeurIPS-2022, ICLR-2023, AISTATS-2023
- Transactions on Machine Learning Research (TMLR), 2022
- Journal of Artificial Intelligence Research (JAIR), 2019, 2021

OPEN-SOURCE SOFTWARE

- GAUCHE: Gaussian process library for chemistry.
- Bayesian Optimization Software: PSR, MerCBO, HyBO, BOPS, BODi, BO_of_COFS, LADDER, and Heterogeneous_botl.