ARYAN DESHWAL

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RESEARCH SUMMARY

My research develops novel machine learning and data science algorithms for *adaptive experiment design* to optimize combinatorial structures (e.g., sequences, trees, and graphs), and applies them to solve high-impact science and engineering applications. Specific topics include:

- Learning probabilistic models over structured data
- Methods to combine domain knowledge and experimental data to create rich models
- Knowledge representation and machine learning for tractable reasoning
- Design of high-performance and low-power manycore systems to overcome Moore's law
- Nanoporous materials design for sustainability applications (e.g., storage and separation of gases)
- Accelerating the design of effective, safe, and low-cost drugs and vaccines

EDUCATION

Ph.D. Student, Computer Science, 4.0 GPA **2018–Present**
Washington State University *Pullman, Washington*
Advisor: Prof. Jana Doppa

MS, Computer Science **2018–2020**
Washington State University *Pullman, Washington*
Thesis: A Learning to Search Framework for Multi-Objective Optimization of Manycore Systems Design

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

RESEARCH EXPERIENCE

Research Assistant **August 2018–Present**
EECS Department, Washington State University *Pullman, Washington*

Undergraduate Research Intern **June 2017–August 2017**
Department of Biotechnology, I.I.T. Roorkee *Roorkee, India*

TEACHING EXPERIENCE

Teaching Assistant
EECS Department, Washington State University *Pullman, Washington*

- CptS 570: Introduction to Machine Learning (Fall-2019)

INDUSTRIAL EXPERIENCE

Research Intern **June 2023–August 2023**
Meta Research - BoTorch Team

Research Intern **June 2022–August 2022**
Meta Research - BoTorch Team

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

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

- Voiland College of Engineering, Outstanding Dissertation Award, 2023 [1]
- Rising Stars in AI, KAUST AI Initiative, 2023
- Selected for Heidelberg Laureatte Forum, 2022 [2]
- Voiland College of Engineering, Outstanding Graduate Research Assistant Award, 2022 [3]
- 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 Innovation in Technology Award (for my MS Dissertation), 2020
- WSU GPSA Graduate Research Assistant Excellence Award, 2020
- Voiland College of Engineering, Outstanding Teaching Assistant in Computer Science Award, 2020
- School of EECS, Outstanding Teaching Assistant in Computer Science Award, 2020
- Mahmoud Dillsi Graduate Fellowship, 2020
- Alfred Suksdorf Fellowship, Washington State University, 2018-2020

PUBLICATIONS

Conference Papers

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

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

3. **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.

4. **Aryan Deshwal**, Syrine Belakaria, Jana Doppa. Bayesian Optimization over Hybrid Spaces. *Proceedings of Thirty-eighth International Conference on Machine Learning (ICML), 2021.*

[1] https://vcea.wsu.edu/faculty-staff/awards/vcea-dissertation-award/
[2] https://www.heidelberg-laureate-forum.org/forum/9th-hlf-2022.html
[3] https://vcea.wsu.edu/faculty-staff/awards/outstanding-student-awards/

5. **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. To appear in *Proceedings of 58th IEEE/ACM Design Automation Conference (DAC), 2021.*

6. **Aryan Deshwal**, Syrine Belakaria, Jana Doppa. Mercer Features for Efficient Combinatorial Bayesian Optimization. *Proceedings of Thirty-Fifth AAAI Conference on Artificial Intelligence (AAAI), 2021.*

7. **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.

8. 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.

9. 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.

10. 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 IEEE/ACM Design, Automation and Test in Europe Conference (DATE)*, 2020. † denotes equal contribution.

11. 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.

12. 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.

13. **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.

14. 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

1. Nickolas Gantzler, **Aryan Deshwal**, Janardhan Rao Doppa, Cory Simon. Multi-fidelity Bayesian Optimization of Covalent Organic Frameworks for Xenon/Krypton Separations. *Digital Discovery*, 2023.

2. 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)*, 2023.

3. **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.

4. 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.

5. 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.

6. **Aryan Deshwal**, Nitthilan Kannappan 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.

7. Nitthilan Kannappan 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 Transactions on Embedded Computing Systems (TECS), 19(1): 4:1-4:24*, 2020.

Workshop Papers

1. **Aryan Deshwal**, Syrine Belakaria, Janardhan Rao Doppa. Scalable Combinatorial Bayesian Optimization with Tractable Statistical models, 2020. `https://arxiv.org/abs/2008.08177`. *Proceedings of NeurIPS Workshop on Engineering Modeling, Simulation, and Design, 2020.*

2. Syrine Belakaria, **Aryan Deshwal**, Janardhan Rao Doppa. Information-Theoretic Multi-Objective Bayesian Optimization with Continuous Approximations, 2020. `https://arxiv.org/abs/2009.05700`. *Proceedings of NeurIPS Workshop on Engineering Modeling, Simulation, and Design, 2020.*

3. Syrine Belakaria, **Aryan Deshwal**, Janardhan Rao Doppa. Max-value Entropy Search for Multi-Objective Bayesian Optimization with Constraints, 2020. `https://arxiv.org/abs/2009.01721`. *Proceedings of NeurIPS Workshop on Machine Learning and the Physical Sciences, 2020.*

4. **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.

5. 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.

6. 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

- Learning and Inference for Structured Prediction: A Unifying Perspective @ IJCAI Conference, 2019.
- Randomized Greedy Search for Structured Prediction: Amortized Inference and Learning @ IJCAI Conference, 2019.
- MOOS: A Multi-Objective Design Space Exploration and Optimization Frame-work for NoC enabled Manycore Systems @ Embedded Systems Week Conference, 2019.
- Optimizing Discrete Spaces via Expensive Evaluations: A Learning to Search Framework @ AAAI Conference, 2020.

- Mercer Features for Efficient Combinatorial Bayesian Optimization @ AAAI Conference, 2021.
- Bayesian Optimization over Hybrid Spaces @ ICML Conference, 2021.
- Bayesian Optimization over Permutation Spaces @ AAAI Conference, 2022.
- Bayesian Optimization over Combinatorial Structures @ Valence Labs, 2022.
- Bayesian Optimization over Combinatorial Structures @ Secondmind, 2022.
- Bayesian Optimization over High-Dimensional Combinatorial Spaces via Dictionary-based Randomized Continuous Embeddings @ AISTATS Conference, 2023.
- Bayesian Optimization over Combinatorial Structures @ Amazon Science Seminar, 2023.
- Bayesian Optimization over Combinatorial Structures @ INFORMS Conference, 2023.

PROFESSIONAL AND OUTREACH ACTIVITIES

Workshop and Tutorial Organization

- Lead organizer of *3rd Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI for Materials and Manufacturing Theme)* upcoming at AAAI-2024.
- Lead organizer of *2nd Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI for Earth and Environment Science Theme)* at AAAI-2023.
- Lead organizer of *AAAI Tutorial on Recent Advances in Bayesian Optimization* at AAAI-2023.
- Lead organizer of *1st Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI for Chemistry Theme)* at AAAI-2022.
- Lead organizer of *AAAI Tutorial on Bayesian Optimization: From Foundations to Advanced Topics* at AAAI-2022.

Senior Program Committee Member

- Thirty-Eighth AAAI Conference on Artificial Intelligence (AAAI), 2024
- Thirty-Seventh AAAI Conference on Artificial Intelligence (AAAI), 2023

Program Committee Member

- Twelfth International Conference on Learning Representations (ICLR), 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
- Thirty-Fifth AAAI Conference on Artificial Intelligence (AAAI), 2021
- International Conference on Learning Representations (ICLR), 2021
- Thirty-Fourth Conference on Neural Information Processing Systems (NeurIPS), 2020

- Thirty-Seventh International Conference on Machine Learning (ICML), 2020
- Twenty-Ninth International Joint Conference on Artificial Intelligence (IJCAI), 2020

Conference and Journal Reviewer

- Reviewer for NeurIPS-2019, UAI-2019, IJCAI-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
- IEEE Journal of Selected Topics in Signal Processing, 2019

SKILLS

- **Programming Languages.** Python, Bash, C/C++, HTML/CSS, LaTeX, Java, MATLAB
- **Tools/Packages.** Git, SQL, PyTorch, TensorFlow, Python data science tools