Jungtaek Kim

Personal Information

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Work Experiences

Nov 01, 2024 – Present	**Research Associate at University of Wisconsin–Madison** Madison, Wisconsin, United States of America I worked on the reasoning and search capabilities of large language models with Prof. Kangwook Lee.
Jul 01, 2022 – Oct 31, 2024	**Postdoctoral Associate at University of Pittsburgh** Pittsburgh, Pennsylvania, United States of America This position was supported by the Center for Materials Data Science for Reliability and Degradation, which is the National Science Foundation's Industry-University Cooperative Research Center. I worked with Prof. Paul W. Leu, Prof. Satish Iyengar, Prof. Lucas Mentch, and Prof. Oliver Hinder.
Feb 16, 2022 – Jun 20, 2022	**Postdoctoral Researcher** **at Pohang University of Science and Technology (POSTECH)** Pohang, Republic of Korea This position was supported by the BK21 FOUR, funded by the Ministry of Education of Korea and National Research Foundation of Korea. It has been carried out in the group of Prof. Minsu Cho.
Jun 07, 2021 – Oct 01, 2021 Oct 30, 2020 – Feb 05, 2021	**Research Intern at Vector Institute** Toronto, Ontario, Canada (Remote Research) I have developed a Bayesian optimization-based LEGO assembly baseline and a reinforcement learning-based LEGO assembly method, dubbed Brick-by-Brick, during this internship. It has been carried out under the supervision of Prof. Graham W. Taylor.
Jan 02, 2018 – Apr 27, 2018	**Research Engineering Intern at SigOpt Inc.** San Francisco, California, United States of America I have implemented a Bayesian optimization method for transferring prior trials via multi-task Gaussian process regression. I worked with Dr. Michael McCourt. SigOpt Inc. has been acquired by Intel Corporation.
Oct 30, 2017 – Dec 29, 2017	**Research Intern at AITRICS** Seoul, Republic of Korea I have implemented an attention model for a dataset of electronic health records and validated Bayesian optimization-based model tuning for clinical dataset. I worked with Dr. Saehoon Kim.
Jan 02, 2017 – Jan 26, 2017 Aug 01, 2016 – Aug 26, 2016	**Research Intern at Samsung Electronics** Hwaseong, Republic of Korea I have studied, designed, and developed a trend classification framework for hundreds million sensors of semiconductor manufacturing system using convolutional neural networks, a density estimator for defects on semiconductors, and an integrated anomaly detection system for hundreds million sensors of semiconductor manufacturing system using convolutional recurrent neural networks and generative adversarial networks.

Education

Mar 01, 2015 – Feb 11, 2022	Ph.D. in Computer Science and Engineering at **Pohang University of Science and Technology (POSTECH)** Pohang, Republic of Korea Supervisor: Prof. Seungjin Choi and Prof. Minsu Cho Dissertation: Efficient Bayesian Optimization: Algorithms, Approximation, and Regret Analysis Committee: Prof. Minsu Cho, Prof. Seungjin Choi, Prof. Dongwoo Kim, Dr. Michael McCourt, Prof. Jungseul Ok
Mar 01, 2010 – Feb 13, 2015	B.S. in Mechanical Engineering & Computer Science and Engineering at **Pohang University of Science and Technology (POSTECH)** Pohang, Republic of Korea
Jul 07, 2014 – Aug 15, 2014	Summer Session at **University of California, Berkeley** Berkeley, California, United States of America
Mar 01, 2007 – Feb 28, 2010	High School Graduate at **Hansung Science High School** Seoul, Republic of Korea

Research Interests

- Statistical machine learning

- Large language models

- Bayesian optimization

Publications, Peer-Reviewed Presentations & E-Prints

(* and $^+$ indicate equal contribution by representing co-first and co-corresponding authors, respectively.)

E-prints

1. **Jungtaek Kim**. Beyond regrets: Geometric metrics for Bayesian optimization. *arXiv e-prints*, arXiv:2401.01981, 2024.

2. **Jungtaek Kim** and Seungjin Choi. Practical Bayesian optimization with threshold-guided marginal likelihood maximization. *arXiv e-prints*, arXiv:1905.07540, 2019.

3. Minseop Park, **Jungtaek Kim**, Saehoon Kim, Yanbin Liu, and Seungjin Choi. MxML: Mixture of meta-learners for few-shot classification. *arXiv e-prints*, arXiv:1904.05658, 2019.

4. **Jungtaek Kim**, Saehoon Kim, and Seungjin Choi. Learning to warm-start Bayesian hyperparameter optimization. *arXiv e-prints*, arXiv:1710.06219, 2017.

Conferences

1. **Jungtaek Kim**. Density ratio estimation-based Bayesian optimization with semi-supervised learning. In *Proceedings of the Forty-Second International Conference on Machine Learning (ICML-2025)*, Vancouver, British Columbia, Canada, July 13–19, 2025.

2. Thomas Zeng, Shuibai Zhang, Shutong Wu, Christian Classen, Daewon Chae, Ethan Ewer, Minjae Lee, Heeju Kim, Wonjun Kang, Jackson Kunde, Ying Fan, **Jungtaek Kim**, Hyung Il Koo, Kannan Ramchandran, Dimitris Papailiopoulos, and Kangwook Lee. VersaPRM: Multi-domain process reward model via synthetic reasoning data. In *Proceedings of the Forty-Second International Conference on Machine Learning (ICML-2025)*, Vancouver, British Columbia, Canada, July 13–19, 2025. *Oral Presentation*.

3. Chaeyun Jang*, Hyungi Lee*, **Jungtaek Kim**[+], and Juho Lee[+]. Model fusion through Bayesian optimization in language model fine-tuning. In *Advances in Neural Information Processing Systems 37 (NeurIPS-2024)*, Vancouver, British Columbia, Canada, December 10–15, 2024. *Spotlight Presentation.*

4. Hyunsoo Chung, **Jungtaek Kim**, Hyungeun Jo, and Hyungwon Choi. Exploiting preferences in loss functions for sequential recommendation via weak transitivity. In *Proceedings of the Thirty-Third ACM International Conference on Information and Knowledge Management (CIKM-2024)*, Boise, Idaho, USA, October 21–25, 2024. *Short Research Paper Track.*

5. Kwang-Sung Jun and **Jungtaek Kim**. Noise-adaptive confidence sets for linear bandits and application to Bayesian optimization. In *Proceedings of the Forty-First International Conference on Machine Learning (ICML-2024)*, Vienna, Austria, July 21–27, 2024.

6. **Jungtaek Kim**, Jeongbeen Yoon, and Minsu Cho. Generalized neural sorting networks with error-free differentiable swap functions. In *Proceedings of the Twelfth International Conference on Learning Representations (ICLR-2024)*, Vienna, Austria, May 7–11, 2024.

7. **Jungtaek Kim**, Mingxuan Li, Oliver Hinder, and Paul W. Leu. Datasets and benchmarks for nanophotonic structure and parametric design simulations. In *Advances in Neural Information Processing Systems 36 (NeurIPS-2023)*, New Orleans, Louisiana, USA, December 10–16, 2023. *Datasets and Benchmarks Track.*

8. Tackgeun You, Mijeong Kim, **Jungtaek Kim**, and Bohyung Han. Generative neural fields by mixtures of neural implicit functions. In *Advances in Neural Information Processing Systems 36 (NeurIPS-2023)*, New Orleans, Louisiana, USA, December 10–16, 2023.

9. **Jungtaek Kim**, Seungjin Choi[+], and Minsu Cho[+]. Combinatorial Bayesian optimization with random mapping functions to convex polytopes. In *Proceedings of the Thirty-Eighth Conference on Uncertainty in Artificial Intelligence (UAI-2022)*, Eindhoven, the Netherlands, August 1–5, 2022.

10. Jinhwi Lee*, **Jungtaek Kim***, Hyunsoo Chung, Jaesik Park, and Minsu Cho. Learning to assemble geometric shapes. In *Proceedings of the Thirty-First International Joint Conference on Artificial Intelligence (IJCAI-2022)*, Vienna, Austria, July 23–29, 2022.

11. Rylee Thompson, Boris Knyazev, Elahe Ghalebi, **Jungtaek Kim**, and Graham W. Taylor. On evaluation metrics for graph generative models. In *Proceedings of the Tenth International Conference on Learning Representations (ICLR-2022)*, Virtual, April 25–29, 2022.

12. **Jungtaek Kim** and Seungjin Choi. On uncertainty estimation by tree-based surrogate models in sequential model-based optimization. In *Proceedings of the Twenty-Fifth International Conference on Artificial Intelligence and Statistics (AISTATS-2022)*, Virtual, March 28–30, 2022.

13. Hyunsoo Chung*, **Jungtaek Kim***, Boris Knyazev, Jinhwi Lee, Graham W. Taylor, Jaesik Park, and Minsu Cho. Brick-by-Brick: Combinatorial construction with deep reinforcement learning. In *Advances in Neural Information Processing Systems 34 (NeurIPS-2021)*, Virtual, December 6–14, 2021.

14. Juho Lee*, Yoonho Lee*, **Jungtaek Kim**, Eunho Yang, Sung Ju Hwang, and Yee Whye Teh. Bootstrapping neural processes. In *Advances in Neural Information Processing Systems 33 (NeurIPS-2020)*, Virtual, December 6–12, 2020.

15. **Jungtaek Kim** and Seungjin Choi. On local optimizers of acquisition functions in Bayesian optimization. In *Proceedings of the European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML-PKDD-2020)*, Virtual, September 14–18, 2020.

16. Juho Lee, Yoonho Lee, **Jungtaek Kim**, Adam R. Kosiorek, Seungjin Choi, and Yee Whye Teh. Set Transformer: A framework for attention-based permutation-invariant neural networks. In *Proceedings of the Thirty-Sixth International Conference on Machine Learning (ICML-2019)*, Long Beach, California, USA, June 9–15, 2019.

17. Inhyuk Jo, **Jungtaek Kim**, Hyohyeong Kang, Yong-Deok Kim, and Seungjin Choi. Open set recognition by regularizing classifier with fake data generated by generative adversarial networks. In *Proceedings of the Forty-Third IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP-2018)*, Calgary, Alberta, Canada, April 15–20, 2018.

18. **Jungtaek Kim** and Seungjin Choi. Clustering-guided GP-UCB for Bayesian optimization. In *Proceedings of the Forty-Third IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP-2018)*, Calgary, Alberta, Canada, April 15–20, 2018.

19. Saehoon Kim, **Jungtaek Kim**, and Seungjin Choi. On the optimal bit complexity of circulant binary embedding. In *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence (AAAI-2018)*, New Orleans, Louisiana, USA, February 2–7, 2018.

Journals

1. Mingxuan Li*, **Jungtaek Kim***, and Paul W. Leu. JaxLayerLumos: A JAX-based differentiable optical and radio frequency simulator for multilayer structures. *Journal of Open Source Software*, vol. 10, no. 114, p. 8572, 2025.

2. Seokjun Ahn*, **Jungtaek Kim***, Minsu Cho, and Jaesik Park. Budget-aware sequential brick assembly with efficient constraint satisfaction. *Transactions on Machine Learning Research*, 2024.

3. Karinna Martin, Katie Shanks, Yipeng Liu, **Jungtaek Kim**, Sajad Haghanifar, Mehdi Zarei, Sooraj Sharma, and Paul W. Leu. Minimizing annual reflection loss in fixed-tilt photovoltaic modules using graded refractive index (GRIN) anti-reflective glass. *Solar Energy*, vol. 272, p. 112424, 2024.

4. Mehdi Zarei, Mingxuan Li, Elizabeth E. Medvedeva, Sooraj Sharma, **Jungtaek Kim**, Zefan Shao, S. Brett Walker, Melbs LeMieux, Qihan Liu, and Paul W. Leu. Flexible embedded metal meshes by sputter-free crack lithography for transparent electrodes and electromagnetic interference shielding. *ACS Applied Materials & Interfaces*, vol. 16, no. 5, pp. 6382–6393, 2024.

5. **Jungtaek Kim**, Mingxuan Li, Yirong Li, Andrés Gómez, Oliver Hinder, and Paul W. Leu. Multi-BOWS: Multi-fidelity multi-objective Bayesian optimization with warm starts for nanophotonic structure design. *Digital Discovery*, vol. 3, no. 2, pp. 381–391, 2024.

6. **Jungtaek Kim** and Seungjin Choi. BayesO: A Bayesian optimization framework in Python. *Journal of Open Source Software*, vol. 8, no. 90, p. 5320, 2023.

7. **Jungtaek Kim**, Michael McCourt, Tackgeun You, Saehoon Kim, and Seungjin Choi. Bayesian optimization with approximate set kernels. *Machine Learning*, vol. 110, no. 5, pp. 857–879, 2021.

Peer-Reviewed Workshops

1. **Jungtaek Kim**, Ziqian Lin, Thomas Zeng, Minjae Lee, Chungpa Lee, Jy-yong Sohn, Hyung Il Koo, and Kangwook Lee. Transformers in the Dark: Navigating unknown search spaces via noisy feedback. *NeurIPS Workshop on What Can('t) Transformers Do? (WCTD-2025)*, San Diego, California, USA, December 7, 2025.

2. Mingxuan Li, **Jungtaek Kim**, Oliver Hinder, and Paul W. Leu. CHROMA: Conversational human-readable optical multilayer assembly for natural language-driven inverse design of structural coloration. *NeurIPS Workshop on AI for Accelerated Materials Design (AI4Mat-2025)*, San Diego, California, USA, December 6, 2025.

3. Mingxuan Li, **Jungtaek Kim**, and Paul W. Leu. Discovering multi-layer films for electromagnetic interference shielding and passive cooling with multi-objective active learning. *NeurIPS Workshop on AI for Accelerated Materials Design (AI4Mat-2024)*, Vancouver, British Columbia, Canada, December 14, 2024.

4. Chaeyun Jang, **Jungtaek Kim**, Hyungi Lee, and Juho Lee. Model fusion through Bayesian optimization in language model fine-tuning. *NeurIPS Workshop on Efficient Natural Language and Speech Processing (ENLSP-2023)*, New Orleans, Louisiana, USA, December 16, 2023.

5. Hyunsoo Chung and **Jungtaek Kim**. Leveraging uniformity of normalized embeddings for sequential recommendation. *NeurIPS Workshop on Self-Supervised Learning - Theory and Practice (SSL-TP-2023)*, New Orleans, Louisiana, USA, December 16, 2023.

6. **Jungtaek Kim**, Hyunsoo Chung, Jinhwi Lee, Minsu Cho, and Jaesik Park. Combinatorial 3D shape generation via sequential assembly. *NeurIPS Workshop on Machine Learning for Engineering Modeling, Simulation, and Design (ML4Eng-2020)*, Virtual, December 12, 2020.

7. Jinhwi Lee*, **Jungtaek Kim***, Hyunsoo Chung, Jaesik Park, and Minsu Cho. Fragment relation networks for geometric shape assembly. *NeurIPS Workshop on Learning Meets Combinatorial Algorithms (LMCA-2020)*, Virtual, December 12, 2020.

8. **Jungtaek Kim**, Michael McCourt, Tackgeun You, Saehoon Kim, and Seungjin Choi. Bayesian optimization over sets. *ICML Workshop on Automated Machine Learning (AutoML-2019)*, Long Beach, California, USA, June 14, 2019.

9. Minseop Park, Saehoon Kim, **Jungtaek Kim**, Yanbin Liu, and Seungjin Choi. TAEML: Task-adaptive ensemble of meta-learners. *NeurIPS Workshop on Meta-Learning (MetaLearn-2018)*, Montreal, Quebec, Canada, December 8, 2018.

10. **Jungtaek Kim** and Seungjin Choi. Automated machine learning for soft voting in an ensemble of tree-based classifiers. *ICML Workshop on Automatic Machine Learning (AutoML-2018)*, Stockholm, Sweden, July 14, 2018.

11. **Jungtaek Kim**, Saehoon Kim, and Seungjin Choi. Learning to transfer initializations for Bayesian hyperparameter optimization. *NeurIPS Workshop on Bayesian Optimization (BayesOpt-2017)*, Long Beach, California, USA, December 9, 2017.

12. **Jungtaek Kim**, Jongheon Jeong, and Seungjin Choi. AutoML Challenge: AutoML framework using random space partitioning optimizer. *ICML Workshop on Automatic Machine Learning (AutoML-2016)*, New York, New York, USA, June 24, 2016.

Selected Software

- BayesO: A Bayesian optimization framework in Python.
  - BayesO, BayesO Benchmarks, Batch BayesO, BayesO Metrics
- Combinatorial 3D Shape Dataset: Dataset for the sequences of volumetric primitives, i.e., LEGO bricks, composed of 406 instances of 14 classes.
- Nanophotonic Structures: Datasets and benchmarks for nanophotonic structure and parametric design simulations.
- JaxLayerLumos: A JAX-based differentiable optical and radio frequency simulator for multilayer structures.

Funding

1. Understanding the Importance of Reasoning Ability in Large Language Models for Scientific Discovery, Google Cloud Research Credits Program, $5,000, March 2025 – March 2026.

2. Machine Learning Methods for Optimizing and Innovating Structural Color Paints and Coatings (PI: Paul W. Leu, Oliver Hinder, and Jungtaek Kim), PI, MDS-Rely, $48,220.4, January 2024 – August 2025.

Honors and Awards

Jun 09, 2019	ICML Travel Award for ICML-2019
Jun 06, 2018	2nd place in AutoML Challenge 2018 (PAKDD-2018 Data Competition)
Apr 15, 2018	IEEE Signal Processing Society Travel Grant for ICASSP-2018
Nov 18, 2016	Best Paper Runner-Up Award (supported by LG U+) in 2016 Fall Conference of Korea Business Intelligence Data Mining Society
Jun 24, 2016	3rd place in AutoML5 Phase of AutoML Challenge
Jul 03, 2014	Software Maestro (organized by Ministry of Science, ICT and Future Planning, Republic of Korea & National IT Promotion Agency, Republic of Korea)
Mar 02, 2010	Presidential Science Scholarship (awarded by the President of the Republic of Korea)

Professional Services

Program Committee Members & Reviewers

- NeurIPS (2025, 2024, 2023, 2022, 2021, 2020, 2019), ICML (2025, 2024, 2023, 2022, 2021, 2020, 2019), AISTATS (2026, 2025, 2024, 2023, 2022, 2021), UAI (2025, 2024, 2023, 2022, 2020, 2019), ICLR (2025, 2024, 2023, 2022), ECML-PKDD (2020), ACML (2022, 2021, 2020, 2019, 2018), AutoML-Conf (2022), CVPR (2023), ICCV (2025), AAAI (2023, 2022, 2021, 2020), IJCAI (2022, 2021), IJCNN (2019, 2018, 2017)

- Transactions on Machine Learning Research, Machine Learning, Journal of Open Source Software, Journal of Artificial Intelligence Research, IEEE Transactions on Image Processing, International Journal of Computer Vision

- NeurIPSW WCTD (2025), NeurIPSW SSL-TP (2023), ICLRW NAS (2020), ICMLW AutoML (2021, 2020, 2019, 2018)

- Directorate for Geosciences (GEO), U.S. NSF (2025)

Talks & Non-Peer Reviewed Presentations

- MOGAM Institute for Biomedical Research (September 5, 2023), Sequential Decision Making for Optimization, Learning and Search, The Tenth International Congress on Industrial and Applied Mathematics (August 24, 2023), BIRS Workshop on 3D Generative Models (July 12, 2023), Computer Science and Engineering Department Seminar, Washington University in St. Louis (May 5, 2023), Technical Seminar, MDS-Rely (September 15, 2022), The Eighth Annual Data Science in Engineering and Life Sciences Symposium (August 8, 2022), Graph Representation Learning Reading Group, Mila (April 14, 2022), KIRO (June 18, 2021), LIM Lab., UNIST (April 22, 2021), Vector Institute Research Symposium (February 16, 2021), Tutorial at KSC-2020 (December 23, 2020), COSEAL-2019 (August 26, 2019), AI Korea 2019 (July 26, 2019), Semiconductor Research Center, Samsung Electronics (June 28, 2019), Samsung Advanced Institute of Technology, Samsung Electronics (December 13, 2018), Naver Corporation (June 12, 2018), SigOpt Inc. (January 04, 2018), Yonsei University Health System (December 15, 2017), Software R&D Center, Samsung Electronics (October 11, 2017), Manufacturing Technology Center, Samsung Electronics (April 14, 2017), Chemical Engineering Department, Yeungnam University (October 05, 2016), The Fifteenth KYUTECH-POSTECH Joint Workshop on Neuroinformatics (August 23, 2016), XBrain Inc. (January 03, 2016)

Teaching

Courses

- Spring 2022, Recent Trends in Machine Learning: A Large-Scale Perspective @ POSTECH

Teaching Assistants

- Artificial Intelligence, Probabilistic Graphical Models, Automata & Formal Languages, Machine Learning

- Hyundai Steel Company ML Course, SK Hynix ML Course, Samsung Electronics Device Solutions Business ML Course, POSCO Group ML Course

Languages

Korean:	Native
English:	Full professional proficiency

Technical Skills

Intermediate:	HTML, CSS, Javascript, Django
Advanced:	Python, Matlab, TensorFlow, PyTorch, JAX, scikit-learn, Most of the scientific packages in Python, LaTeX