# Jungtaek Kim

#### Personal Information

Nationality: Republic of Korea

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# Work Experience

Feb 16, 2022 – Present | 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.

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.

Jul 25, 2017 – Oct 20, 2017 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 <b>Hansung Science High School</b> Seoul, Republic of Korea

#### Research Interest

- Statistical machine learning
- Bayesian optimization
- Hyperparameter optimization
- Automated machine learning
- Sequential assembly

# Publication & Peer-Reviewed Presentation

(\* indicates equal contribution.)

#### E-print

- 1. **Jungtaek Kim**, Minsu Cho, and Seungjin Choi. Combinatorial Bayesian optimization with random mapping functions to convex polytopes. *arXiv e-prints*, arXiv:2011.13094, 2020.
- 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.

#### Conference

- 1. 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.
- 2. **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.

- 3. 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.
- 4. 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.
- 5. **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.
- 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.
- 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.
- 8. **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.
- 9. 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.

#### Journal

1. **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.

#### Workshop

- 1. **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.
- 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.
- 3. **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
- 4. 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.
- 5. **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.
- 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.
- 7. **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. Additionally, BayesO Benchmarks is a Python package that implements benchmark functions for Bayesian optimization.
- Combinatorial 3D Shape Dataset: Dataset of sequences of volumetric primitive placement, composed of 406 instances of 14 classes.

#### Honor and Award

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 Service

### Program Committee Member & Reviewer

- NeurIPS (2021, 2020, 2019), ICML (2022, 2021, 2020, 2019), AISTATS (2022, 2021), UAI (2022, 2020, 2019), ICLR (2022), ECML-PKDD (2020), ACML (2021, 2020, 2019, 2018), AutoML-Conf (2022), AutoML (2021, 2020, 2019, 2018), AAAI (2022, 2021, 2020), IJCAI (2022, 2021), NAS (2020), IJCNN (2019, 2018, 2017)
- Machine Learning, Journal of Open Source Software, Journal of Artificial Intelligence Research

#### Talk & Non-Peer Reviewed Presentation

• 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**

#### Teaching Assistant

- 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

# Language

Korean: Native

English: Full professional proficiency

# Technical Skill

Intermediate: HTML, CSS, Javascript, Django

Advanced: Python, Matlab, TensorFlow, scikit-learn, Most of the scientific packages in Python, LATEX