### Updated June 13, 2025

### Namuk Park

RESEARCH SUMMARY My research focuses on developing *foundation models for biology* to understand and design proteins through empirical analysis of neural network approaches. In particular, my key research has covered the following topics: (i) *Vision Transformers*, (ii) *representation learning*, and (iii) *AI for protein structures*.

INDUSTRY
EXPERIENCE

**Genentech**, New York, United States Postdoctoral Fellow at Prescient Design Mar 2023 - Present

▶ We aim to bring better medicines to patients faster by developing cutting-edge AI approach for drug discovery. (Research topic: Representation learning for 3D protein structures [5])

NAVER, Seongnam, South Korea

Feb 2022 - Nov 2022

Visiting Researcher at NAVER AI Lab

▶ We focus on conducting fundamental machine learning research and contributing to NAVER and AI communities (Research topic: Empirical analysis of self-supervised Vision Transformers [4])

### Probe Technology, Seoul, South Korea

Jul 2013 - Feb 2018

Co-founder and CEO

▶ We provided enterprise resource planning & machine-learning-based data analysis tool for small businesses.

#### **Publications**

- [5] Namuk Park, Pedro O. Pinheiro, Nathan C. Frey, Sidney L. Lisanza, Andrew M. Watkins, Arian R. Jamasb, Matthieu Kirchmeyer, Richard Bonneau, Saeed Saremi, and Vladimir Gligorijevic, "AtoMAE: Learning Protein Structure Representations from Atomic Voxel Grids via Masked Autoencoders", ICMLW 2025.
- ▶ We demonstrate that neural networks with minimal domain-specific inductive bias can acquire biological knowledge through representation learning. In particular, we introduce AtoMAE—an atomistic voxel-based Transformer pre-trained via Masked Autoencoder for protein structure representation learning. Despite relying only on raw atomic information, AtoMAE scales efficiently and surpasses both protein language modeling and graph neural networks.
- [4] Namuk Park, Wonjae Kim, Byeongho Heo, Taekyung Kim, and Sangdoo Yun. "What Do Self-Supervised Vision Transformers Learn?", ICLR 2023. arXiv, code.
- ▶ We show that self-supervised Vision Transformers trained with contrastive learning (CL) and masked image modeling (MIM) exploit opposite behaviours: (i) CL primarily captures global patterns compared with MIM, (ii) CL is more shape-oriented whereas MIM is more texture-oriented, and (iii) CL plays a key role in the later layers while MIM focuses on the early layers.
- [3] Namuk Park and Songkuk Kim. "How Do Vision Transformers Work?", ICLR 2022. Spotlight. Top 100 Most Cited AI Papers for 2022. [article] Top 100 AI Achievements From 2022 to 2023. [article] arXiv, code.

▶ We show that the success of "multi-head self-attentions" (MSAs) lies in the "spatial smoothing" of feature maps, not in the capturing of long-range dependencies. In particular, we demonstrate that MSAs (i) flatten the loss landscapes, (ii) are low-pass filters, contrary to Convs, and (iii) significantly improve accuracy when positioned at the end of a stage. See also [2].

# [2] Namuk Park and Songkuk Kim. "Blurs Behave Like Ensembles: Spatial Smoothings to Improve Accuracy, Uncertainty, and Robustness.", ICML 2022. Winner of Qualcomm Innovative Fellowship South Korea. arXiv, code.

▶ We show that "spatial smoothing" (a simple blur filter) improves the accuracy, uncertainty, and robustness of CNNs, all at the same time. This is primarily due to that spatial smoothing flattens the loss landscapes by "spatially ensembling" neighboring feature maps of CNNs. See also [1].

## [1] Namuk Park, Taekyu Lee, and Songkuk Kim. "Vector Quantized Bayesian Neural Network Inference for Data Streams." AAAI 2021. arXiv, code.

▶ We show that "temporal smoothing" (moving average of recent predictions) significantly improves the computational performance of Bayesian NN inference without loss of accuracy. To do so, we propose "ensembles for proximate data points" as an alternative to ensembles for a single data point.

#### **EDUCATION**

### Yonsei University, Incheon, South Korea

Mar 2011 – Feb 2022

M.S. and Ph.D. in School of Integrated Technology (Computer Science)

▶ Thesis: "Practical Bayesian Neural Networks: A Data Uncertainty Perspective"

▶ Advisor: Prof. Songkuk Kim<sup>[mail]</sup>

### Yonsei University<sup>[wiki]</sup>, Seoul, South Korea

Mar 2008 - Feb 2011

B.S. in Physics

▶ *GPA*: 4.18/4.30., Valedictorian of the College of Sciences & 1 year early graduation based on academic excellence.

Daejeon Science High School [wiki], Daejeon, South Korea

Mar 2006 - Feb 2008

▶ 1 year early graduation based on academic excellence.

### Awards & Honors

Outstanding Thesis Award, Third prize (Yonsei University)

Jun 2022

Winner of Qualcomm Innovative Fellowship South Korea (Qualcomm)

Nov 2021

Research Grant Support for Ph.D. Students (National Research Foundation of

South Korea) Jun 2021 - Feb 2022

National Fellowship from Global Open Source Frontier (NIPA<sup>1</sup>) Jun 2019 – Dec 2020

China-Japan-South Korea OSS Award (The Organizing Committee of

the CJK OSS Award) Nov 2019

OSS Competition, Honorable mention (NAVER Corporation) Feb 2019

OSS Challenge, First prize—the Award From the Minister of Science and ICT Nov 2018

OSS Competition (2<sup>nd</sup> phase), First prize (NAVER Corporation)

Aug 2018

OSS Competition (1st phase), Second prize (NAVER Corporation) Feb 2018

National Ph.D. Full Ride Fellowship (Institute for Information and Communications

Technology Promotion of South Korea) Mar 2011 – Feb 2016

 $<sup>^1</sup>$ National IT Industry Promotion Agency, an IT industry promotion organization operated by the Government of South Korea

Yonsei University Alumni Full Ride Scholarship, GE Scholarship, National Scholarship for Science and Engineering, and other merit-based scholarships Sep 2008 – Feb 2011

Invited	"How Do Vision Transformers Work?"	
Talks	▶ Seminar at SeoulTech	Aug 2022
	▶ AI Seminar at UNIST	Mar 2022
	▶ Tech talk at NAVER WEBTOON	Jan 2022
	▶ NAVER Tech Talk at NAVER Corporation	Dec 2021
	"Uncertainty in AI: Deep Learning Is Not Good Enough for Safe AI"	
	⊳ Keras Korea Meetup at AI Yangjae Hub	Dec 2019
	▶ OSS Contribution Festival organized by NIPA	Dec 2019
	⊳ South Korea-Uzbekistan SW Technology Seminar at Tashkent University of	
	Information Technologies	Oct 2019
	"A Fast and Lightweight Probability Tool for AI in Scala"	
	▶ North-East Asia OSS Forum organized by NIPA	Nov 2019
	▶ OSS Day (Keynote) organized by NIPA	Nov 2018
	▶ Scala Night Korea organized by Scala User Group Korea	Apr 2018
Reviewer	ICML 2022, 2023 & 2024, NeurIPS 2022, 2023 ( <i>Top reviewer</i> ), & 2024, ICLR 2024 & 2025, AAAI 2023 & 2024, IJCAI 2024, CVIU	