Seul Lee

CONTACT INFORMATION

KAIST, South Korea
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Homepage: seullee05.github.io

RESEARCH INTERESTS

My research interest is mainly in developing generative models for graphs. I especially focus on molecule generation that can bridge the gap between real-world drug discovery and automatic drug discovery. I am currently interested in the following topics:

- Drug discovery
- Generative models, especially diffusion models
- Graph representation learning

EDUCATION

KAIST, Daejeon, South Korea

M.S., Graduate School of AI — **Mar. 2021 - Aug. 2022**

- Advisor: Prof. Sung Ju Hwang
- Area of study: Machine learning
- Anticipate proceeding to a Ph.D. degree under the supervision of Prof. Sung Ju Hwang.

B.S., Department of Aerospace Engineering — **Mar. 2015 - Aug. 2019**

B.S., Department of Biological Sciences — **Mar. 2015 - Aug. 2019**

RESEARCH EXPERIENCE

AITRICS, Seoul, South Korea

- Research topic: Docking-optimized molecule generation using reinforcement learning

CONFERENCE PUBLICATIONS

Score-based Generative Modeling of Graphs via the System of Stochastic Differential Equations

Jaehyeong Jo*, **Seul Lee***, and Sung Ju Hwang (*: equal contribution),
International Conference on Machine Learning **(ICML), 2022**.

Edge Representation Learning with Hypergraphs

Jaehyeong Jo*, Jinheon Baek*, **Seul Lee***, Dongki Kim, Minki Kang, and Sung Ju Hwang (*: equal contribution),
Conference on Neural Information Processing Systems **(NeurIPS), 2021**.

Hit and Lead Discovery with Explorative RL and Fragment-based Molecule Generation

Soojung Yang, Doyeong Hwang, **Seul Lee**, Seongok Ryu, and Sung Ju Hwang,
Conference on Neural Information Processing Systems **(NeurIPS), 2021**.

Journal Publications

Robotic Scanning Technology for Laser Pulse-Echo Inspection

Seul Lee, Jong-min Hyun, Hasan Ahmed, and Jung-ryul Lee,
Electronics Letters, 2020.

Preprints

Exploring Chemical Space with Score-based Out-of-distribution Generation

Seul Lee, Jaehyeong Jo, and Sung Ju Hwang,
arXiv:2206.07632, 2022.

Honors and Awards

- Boeing Undergraduate Scholarship **Feb. 2018 - Aug. 2019**
- KAIST Presidential Fellowship (KPF) **Mar. 2017 - Aug. 2019**
- National Science and Engineering Scholarship **Mar. 2015 - Feb. 2019.**

Skills

- Fluent in English
- Fluent in Python and PyTorch

References

- Prof. Sung Ju Hwang, Professor, KAIST
  E-mail: sjhwang82@kaist.ac.kr