# JAEHYEONG JO

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#### RESEARCH INTERESTS

My research interest mainly focuses on understanding physical systems through the lens of graphstructured data and its geometric symmetries. In particular, I've been focusing on the generation of the graph with diffusion models and its applications to real-world tasks, for example, drug discovery or protein design.

#### **PUBLICATIONS**

## Graph Generation with Destination-Driven Diffusion Mixture

Jaehyeong Jo\*, Dongki Kim\*, and Sung Ju Hwang

Preprint, arXiv:2302.03596

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

Seul Lee, Jaehyeong Jo, and Sung Ju Hwang

Preprint, arXiv:2206.07632

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

Jaehyeong Jo\*, Seul Lee\*, and Sung Ju Hwang

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 Neural Information Processing Systems (NeurIPS), 2021

#### RESEARCH EXPERIENCE

#### MLAI (Machine Learning & Artificial Intelligence) Lab, KAIST

Seoul, Korea

Research Assistant (Advisor: Prof. Sung Ju Hwang)

Sep. 2021 - Present

Conducting research on graph generative model with applications to drug discovery.

Kimlab, UofT Toronto, Canada

Visiting student (Host: Prof. Philip Kim)

Feb. 2023 - Feb. 2023

· Conducting research on protein generative model with diffusion models.

#### PAI (Probability Artificial Intelligence) Lab, KAIST

Daejeon, Korea

Research Assistant (Advisor: Prof. Ganguk Hwang)

Mar. 2020 - Aug. 2021

· Conducted research on graphs (edge representation learning using hypergraph structure).

## **TALKS**

## Generation of Graph-Structured Data with Diffusion Models

Toronto, Canada

in University of Toronto (UofT)

Feb 2023

#### Score-based Generative Modeling of Graphs via the SDEs

in LoGaG: Learning on Graphs and Geometry Reading Group

Online Oct. 2022

#### Learning with Graph Structure Data

Pohang, Korea July 2022

in Pohang University of Science and Technology (POSTECH)

<sup>\*</sup> denotes equal contribution.

# Score-based Graph Generation for Material Design

in Samsung Advanced Institute of Technology (SAIT)

Suwon, Korea Jun. 2022

### **EDUCATION**

Korea Advanced Institute of Science and Technology (KAIST)

Ph.D. in Artificial Intelligence

Sep. 2021 - Present

Advisor: Proffesor Sung Ju Hwang

Korea Advanced Institute of Science and Technology (KAIST)

Daejeon, Korea

M.S. in Mathematical Sciences Mar. 2020 - Aug. 2021

Advisor: Professor Ganguk Hwang

Korea Advanced Institute of Science and Technology (KAIST)

Daejeon, Korea

B.S. in Mathematical Sciences

Mar. 2016 - Feb. 2020

Minor in Computer Science & Engineering

GPA: 3.75/4.3

#### ACADEMIC SERVICES

#### **Conference Reviewers**

- · Learning on Graphs Conference (LoG), 2022
- · Conference on Neural Information Processing Systems (NeurIPS), 2022
- · International Conference on Machine Learning (ICML), 2022, 2023