NGOC-QUANG NGUYEN

Ph.D. Candidate in Computer Science

✉ quangku12@korea.ac.kr   🏠 Home   in Linkedin   � GitHub   G Google Scholar

🎓 EDUCATION

Korea University
Ph.D , Computer Science and Engineering

Sep 2020 - Present
Advisor: Jaewoo Kang

Gachon University
MSc, Computer Science and Engineering

Sep 2017 - Jul 2019
Advisor: Sangwoong Lee

Vietnam National University, Hanoi
BEng, Mechanical Engineering

Sep 2012 - Mar 2017

💼 EXPERIENCE

DMIS lab
Drug discovery

Sep 2020 – Present
Machine learning and AI researcher

· May 2023 - Dec 2023: Collaborated with **AIGEN Sciences** on predicting compound-protein interactions utilizing multi-level features.
· Mar 2022 - Mar 2023: Collaborated with **SK-Nexilis** on predicting material properties and making recipe recommendation system.
· Analyzing large-scale datasets from various sources such as biochemical assays such as: BioLiP, PDBbind, DUD_E, Davis, KIBA, Metz.
· Building deep learning models and algorithms predict protein-compound interactions mainly focusing on multimodal learning.
· Developing models to capture 3D geometric information with Equivariant neural networks.

Voronoi Inc
Drug discovery

Aug 2019 - Jul 2020
Machine learning and AI researcher

· Developed and applied reinforcement learning techniques for small molecule generation with high binding affinity by ReLeaSE (Reinforcement Learning for Structural Evolution).
· Predicted compound properties by the deep directed message passing neural network.
· Predicted compound toxicity by deep neural neural network with multitask learning technique.
· Collaborated with biologists, chemists, and other researchers to design experiments, validate predictions, and optimize experimental conditions.

PRML lab
Computer Vision

Sep 2017 - Jul 2019
Machine learning and AI researcher

· Medical imaging analysis (image segmentation for seeking lung, colon, and breast tumors).
· Classified the breast cancer histology images using incremental boosting convolution networks.
· Face recognition: automatic door recognition (used face to open the lab door).

NTQ Solution
Robotics

Jun 2015 - Sep 2015
Robotic engineering intern

· Built a guidance robot using a Raspberry Pi kit, which is controlled by a gaming remote.
· Developed and programmed a quadcopter thesis using an Arduino kit, integrating a radio control system with a transmitter and receiver.

📖 PUBLICATIONS

Journal publications

MulinforCPI: enhancing precision of compound-protein interaction prediction through novel perspectives on multi-level information integration

Ngoc-Quang Nguyen; Sejeong Park; Mogan Gim; Jaewoo Kang   **Briefings in Bioinformatics, 2023**

PerceiverCPI: A nested cross-attention network for compound-protein interaction prediction

Ngoc-Quang Nguyen; Gwanghoon Jang; Hajung Kim; Jaewoo Kang   **Bioinformatics, 2022**

Contour-aware Polyp Segmentation in Colonoscopy Images using Detailed Upsampling Encoder-Decoder Networks

Ngoc-Quang Nguyen; Duc My Vo; Sang-Woong Lee   **IEEE Access, 2020**

Robust Boundary Segmentation in Medical Images Using a Consecutive Deep Encoder-Decoder Network

Ngoc-Quang Nguyen; Sang-Woong Lee   **IEEE Access, 2019**

Classification of breast cancer histology images using incremental boosting convolution networks

Duc My Vo; **Ngoc-Quang Nguyen**; Sang-Woong Lee   **Information Sciences, 2018**

Conference publications

Colorectal segmentation using multiple encoder-decoder network in colonoscopy images

Ngoc-Quang Nguyen; Sang-Woong Lee   **AIKE, Laguna Hills, 2018**

🤖 SELECTED PROJECTS

EquiCPI (3D), ongoing   Duration: Dec.2023-present

Project size: 2 members

Project description: Fully leveraging the 3D-generated structures derived from an existing sequence dataset with SE(3) neural networks enhances the accuracy of the CPI task.

Responsibilities:

- Researching and utilizing the Special Euclidean Group in three dimensions.
- Implementing SE(3) to effectively extract and learn information from 3D structures considering translation, rotation, reflection.

MulinforCPI (2,5D), Github   Duration: Jan.2023-Sep.2023

Project size: 3 members

Project description: Proposed a two-step deep learning strategy named MulinforCPI (utilizing multi-level information for compound–protein interaction prediction) that incorporates transfer learning techniques along with multi-level resolution features. The aim is to overcome the limitations associated with forecasting the interaction between compounds and proteins.

Responsibilities:

- Conducted an analysis of the impact of 3D information on the CPI task.
- Designed a cross-cluster validation strategy to comprehensively assess model performance, with a specific emphasis on evaluating its effectiveness in predicting interactions with novel scaffold compounds.
- Proposed and implemented a novel architecture to address the challenge of limited availability of comprehensive and well-structured datasets.

PerceiverCPI (2D),Github   Duration: Feb.2022-Sep.2022

Project size: 3 members

Project description: Proposed the Perceiver CPI network, which adopts a cross-attention mechanism to improve the learning ability of the representation of drug and target interactions and exploits the information obtained from extended-connectivity fingerprints to improve the performance of predicting binding free energy.

Responsibilities:

- Proposed main ideas to overcome the representation's simplification of molecular fingerprints and the current integration methods.
- Implemented the proposed architecture with directed message passing neural network and 1DCNN network.
- Analyzed the importance of atom features and bond features.
- Designed the performance evaluation strategies.

🏆 HONORS & AWARDS

Excellent paper award   Feb 2023, Korea University

Research scholarship   Sep 2020 - Sep 2022, BK21FOUR

Foreign natural sciences and engineering scholarship   Sep 2020 - Sep 2022, Korea University

Full scholarship covering living expenses and tuition fees   Sep 2017 - Jul 2019, Gachon University

🔧 SKILLS

Exploratory Data Analysis, Statistics, Modeling, Communication.
Technique Languages: Python, Java, C#.
Others: AWS Unix/Linux, working cross-functionally.
Source Code Management: GitHub, Gitlab.
Languages: English (advanced), Korean (beginner), Vietnamese (native).

👥 REFERENCES

Prof. Jaewoo Kang, Ph.D.   **Prof. Sangwoong Lee, Ph.D.**
Address: Korea University, Seoul, Korea.   Address: Gachon University, Gyeonggi, Korea.
Tel: (+82) 2-3290-4840   Tel: (+82) 3-1750-6918
Email: kangj@korea.ac.kr   Email: slee@gachon.ac.kr