NGOC-QUANG NGUYEN

Ph.D. Candidate in Computer Science

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EDUCATION

Korea University *Sep 2020 - Present*
Ph.D , Computer Science and Engineering, GPA: 93.5% Advisor: Jaewoo Kang

Gachon University *Sep 2017 - Jul 2019*
MSc, Computer Science and Engineering, GPA: 80.6% Advisor: Sangwoong Lee

Vietnam National University, Hanoi *Sep 2012 - Mar 2017*
BEng, Mechanical Engineering, GPA: 75.5%

EXPERIENCE

DMIS lab Sep 2020 – Present
Drug discovery *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 Aug 2019 - Jul 2020
Drug discovery *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 Sep 2017 - Jul 2019
Computer Vision *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 (adopted Google facenet to make output for Arduino kit to open the lab door).

NTQ Solution Jun 2015 - Sep 2015
Robotics *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.

Component neural networks: euclidean neural networks, multiplayer perception neural network.

MulinforCPI (2,5D), [Github_Here] 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.

Component neural networks:
Principal neighborhood aggregation graph neural network, message passing neural network, multiplayer perception neural network, 1D convolutional neural network, 2D convolutional neural network

PerceiverCPI (2D),[Github_Here] Duration: Sep.2021-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.

Component neural networks:
Directed message passing neural network, multiplayer perception neural network, 1D convolutional neural network

HONORS & AWARDS

Excellent paper award: [Here] Feb 2023, Korea University

Research scholarship: [Here] Sep 2020 - Sep 2022, BK21FOUR

Foreign natural sciences and engineering scholarship: [Here] Sep 2020 - Sep 2022, Korea University

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

SKILLS AND CERTIFICATES

Exploratory Data Analysis, Statistics, Modeling, Communication.
Certificates: AWS Fundamentals [Here], IBM Data Analyst [Here], Google Advanced Data Analytics [Here]
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.
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Letter of recommendation: upon request

Prof. Sangwoong Lee, Ph.D.
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Email: slee@gachon.ac.kr
Letter of recommendation: [Here]

Mujeen Sung, PhD.
Address: Korea University, Seoul, Korea.
Tel: (+82) 10-9073-3590
Email: mujeensung@korea.ac.kr
Letter of recommendation: [Here]