

HUIYU CAI

Mila & University of Montreal

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EDUCATION

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|--|------------------------------|
| Quebec AI Institute (Mila) & University of Montreal (UdeM) | <i>Sep. 2021 - Present</i> |
| Department of Computer Science and Operations Research (DIRO) | Overall GPA: 4.30/4.30 |
| First year PhD Student supervised by Prof. Jian Tang, working on deep generative models and representation learning on graphs. | |
| Peking University (PKU) | <i>Sep. 2017 - Jul. 2021</i> |
| School of Electronic Engineering and Computer Science (EECS) | Overall GPA: 3.60/4.00 |
| Awarded Excellent Graduate in Beijing . | |
| Peking University (PKU) | <i>Sep. 2016 - Jun. 2017</i> |
| College of Chemistry and Molecular Engineering (CCME) | Overall GPA: 3.68/4.00 |
| Ranking: Top 5% in CCME, 2016-2017. Note: I changed major to EECS after one year of study. | |

TECHNICAL STRENGTHS

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| Computer Languages | C/C++ (gdb), Python (pdb), Assembly Language, Java, R, JavaScript, Bash, Matlab |
| Computing Frameworks | Spark, MapReduce, OpenMP, MPI |
| Python Libraries | Re, NumPy, Sci-kit Learn, Pandas, Matplotlib, Seaborn, Sympy, TensorFlow, Pytorch, BeautifulSoup, Selenium, RDKit, ScanPy |
| English Fluency | TOEFL iBT 114 (Reading 30, Listening 30, Speaking 27, Writing 27) GRE Verbal 157, Quantitative 170, Analytical Writing 3.5 IELTS 8.0 (Listening 8.5, Reading 8.0, Writing 7.0, Speaking 7.5) |
| Mathematics | Mathematical Analysis, Set and Graph Theory, Probability Theory and Statistics, Linear Algebra, Stochastic Processes, Convex Analysis and Optimization Methods, Machine Learning Theory |

PUBLICATIONS

- Shengchao Liu, Meng Qu, Zuobai Zhang, **Huiyu Cai**, Jian Tang. Structured Multi-task Learning for Molecular Property Prediction, *AISTATS*, **2022**.
- Meng Qu*, **Huiyu Cai***, Jian Tang. Neural Structured Prediction for Inductive Node Classification. *ICLR*, **2022** (oral). *Equal contribution
- Yifan Zhao*, **Huiyu Cai***, Zuobai Zhang, Jian Tang, Yue Li. Learning interpretable cellular and gene signature embeddings from single-cell transcriptomic data, *Nature Communications*, **2021**. *Equal contribution
- Yitao Cai, **Huiyu Cai**, Xiaojun Wan. Multi-Modal Sarcasm Detection in Twitter with Hierarchical Fusion Model, *ACL*, **2019**.
- Jingjia Liu, Yuting Zhang, **Huiyu Cai**, Juan Yang. TEMPO and Its Derivatives in Organic Redox-Flow Batteries, *University Chemistry*, **2017**, 32(11): 32-44.

RESEARCH INTERESTS

Deep Generative Models, Graph Neural Networks, Representation Learning, AI for drug discovery

RESEARCH EXPERIENCE

Inductive Node Classification with StructGNN

Oct. 2020 – Feb. 2021

Accepted by ICLR 2022 (Co-first Author)

- Co-designed and implemented StructGNN, which combines graph neural networks and conditional random fields for efficient label-dependent inductive node classification
- Conducted extensive benchmarks showing the consistent improvement of StructGNN compared to GNNs or naive GNN+CRF models.
- Studied the effect of GNN architecture on the model performance, and pointed out future directions.

Massively Multi-Task Molecular Property Prediction with Explicit Task Relation Graph

Oct. 2020 – Feb. 2021

Accepted by AISTATS 2022 (Third Author)

- Constructed and cleaned a new drug target prediction dataset with explicit task relation graph.
- Co-developed the GNN-EBM model, which models the label dependency between tasks in both the latent space and the output space, uses Gibbs sampling for inference and noise contrastive estimation for learning.

Unsupervised scRNA-seq Data Mining via Embedded Topic Model

Jan. 2020 – Oct. 2020

Accepted by Nature Communications (First Author)

- Designed, tuned and benchmarked several models for scRNA-seq data modeling, including a joint graph-community learning model (vGraph) and an embedded topic model with batch correction (scETM).
- Optimized the scalability of scETM and gained 10 \times running speed and 1/3 memory requirement
- Practiced various scRNA-seq preprocessing and visualization techniques.
- Formed a comprehensive understanding of scRNA-seq data mining.

Multimodal Sarcasm Detection in Twitter

Apr. 2018 – Oct. 2018

Accepted by ACL 2019 (Second Author)

- Co-developed and implemented a hierarchical fusion model for multimodal (image + text + image attributes generated from image) sarcasm detection. This is the first approach of deep representation fusion for Twitter sarcasm detection.
- Labeled and cleaned noisy Twitter data. This dataset is now publicly available.

AWARDS AND HONORS

Excellent Graduate in Beijing, 2021

Excellent Graduate of Peking University, 2021

Leo Koguan Scholarship (1 out of 150), 2017

Leo Koguan Scholarship (1 out of 62), 2020

Founder Scholarship (2 out of 61), 2019

Second Prize, ACM-ICPC PKU campus competition, 2018

First Prize, 29th Chinese Chemistry Olympiad (Preliminary), 2015

First Prize, 28th Chinese Chemistry Olympiad (Preliminary), 2014

HOBBIES

Singing acappella (I was the music director of Paca Vocal School at Peking University)

Watching Sci-Fi (especially the Star Trek series)

Hiking / Swimming / Travelling / Ping pong