

HUIYU CAI

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EDUCATION

Quebec AI Institute (Mila) & University of Montreal (UdeM)

Sep. 2021 - Present

Department of Computer Science and Operations Research

First year PhD Student supervised by Prof. Jian Tang

Peking University (PKU)

Sep. 2017 - Jul. 2021

School of Electronic Engineering and Computer Science (EECS)

Overall GPA: 3.60/4

Awarded **Excellent Graduate in Beijing**

Core Courses (Grades): Signal and Systems (99), Machine Perception Lab (98), Mathematical Foundations for the Information Age (96), Deep Learning (93), Introduction to Pattern Recognition (93), Machine Learning (92), Algorithm Design and Analysis (87), Computer Net And Web Technology (87), Data Structure and Algorithms (87), Introduction to Parallel and Distributed Computing (86.5), Introduction to Computer Systems (85), Algorithms in Game AI (85), Information Theory

Peking University (PKU)

Sep. 2016 - Jun. 2017

College of Chemistry and Molecular Engineering (CCME)

Overall GPA: 3.68/4

Ranking: Top 5% in CCME, 2016-2017

Core Courses (Grades): General Chemistry (93), Organic Chemistry (95.5), Quantitative Chemical Analysis (95), General Chemistry Lab (89), Comprehensive Analytical Chemistry Lab (89)

TECHNICAL STRENGTHS

Computer Languages

C/C++ (gdb), Assembly Language, Python (pdb), 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

Mathematics

Mathematical Analysis, Set and Graph Theory, Probability Theory and Statistics, Linear Algebra, Stochastic Processes, Convex Analysis and Optimization Methods, Machine Learning Theory

PUBLICATIONS

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

Graph Neural Networks, Representation Learning, Bioinformatics, Drug discovery, Natural Language Processing, Music Processing/Generation

RESEARCH EXPERIENCE

Inductive Node Classification with StructGNN

Oct. 2020 – Feb. 2021

Submitted to NIPS 2021 (Second 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

Submitted to ICLR 2021 (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× running speed and 1/3 memory requirement
- Practiced various scRNA-seq preprocessing and visualization techniques.
- Formed a comprehensive understanding of scRNA-seq data mining.

Robustness Study of Neural Code Comment Generation Systems

Jun. 2019 – Aug. 2019

Submitted to ICSE 2020 (Second Author)

- Designed and implemented multiple ways of attacking a neural code comment generation model while fully preserving the syntactic correctness and semantic integrity of the code blocks.
- Conducted human evaluation study on adversarial-trained and vanilla models, proving (1) vanilla seq2seq models are extremely vulnerable under adversarial attacks, (2) adversarial training significantly improves model robustness.

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.

TEMPO and Its Derivatives in Organic Redox-Flow Batteries

Apr. 2017 – Oct. 2017

Accepted by University Chemistry, 2017 (Third Author)

- Read, categorized and summarized previous literature on inorganic redox-flow batteries (RFBs).
- Compared inorganic RFBs to organic ones, highlighting the advantages of the latter.

PROJECTS

Music Source Separation: Theory and Applications

Apr. 2020 – Jun. 2020

Class project, Machine Perception Lab (Individual project)

- Reviewed and benchmarked six influential algorithms for music source separation.
- Used the SOTA method, Demucs, to remix two songs with similar chord progressions, by extracting the voice of one song and pasting it to the extracted background music of the other song.

Raiden Game Implementation in Java

Jan. 2020 – Jun. 2020

Class project, Java Programming (First Author)

- Designed and implemented (with graceful object-oriented programming) a vertical shooting game similar to Raiden in Java from scratch, with delicate visual & sound effects.
- Led and coordinated my group via GitHub.

Fine-grained Face Manipulation via DLGAN

Oct. 2019 – Jan. 2020

Class project, Introduction to Artificial Intelligence (Second Author)

- Co-built a GUI program which takes a photo of the user, then manipulates its face using Disentangled Label-specific GAN (DLGAN).
- Implemented network modules between server (hosts DLGAN model) and client (requests DLGAN service).

Bird Sound Classification

Mar. 2019 – Jun. 2019

Class project, Algorithm Design and Analysis (First Author)

- Led a three-member group to build an end-to-end model for bird sound classification.
- Proposed and tuned a convolution network specifically for bird sound spectrogram classification on a subset of *Bird-CLEF 2016*. Implemented multiple data augmentation techniques to boost the robustness of the model.

TEACHING EXPERIENCE

Teaching Assistant, Introduction to Computer Systems

Sep. 2019 - Jan. 2020

- Organized a 2-hour seminar per week where students present class reviews which I then comment and supplement to deepen their understanding of course materials.
- Answered student questions and guided them in completing lab assignments.
- Graded assignments and exams.

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

EXTRA-CURRICULAR ACTIVITIES

Student Acappella Club, Peking University

Oct. 2016 - Jul. 2021

President of Club Council

Deputy director of Department of Music Research and Training

Music director of Paca Vocal Group

Standing Committee of EECS Student Representative Assembly
Representative of Class 3

Sep. 2017 - Sep. 2020