Yifei Wang

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Research Topics

Deep Learning, Efficiency, Optimization, Graph Neural Networks, Multimodal Learning, Generative AI, Large Language Model, Fairness, AI4Science, Healthcare Informatics.

Education

- **Brandeis University** *Jan 2020 - Jan 2025 (estimated)*

  Ph.D. student in Computer Science Massachusetts, USA
  - GPA: 4.0/4.0. GSAS Fellowship, Travel and Research Grant.
  - Research Focus: Graph Neural Network, Multimodal Learning, Fairness, AI4Science, AI4Healthcare, Generative AI.
  - Dissertation: Human-Knowledge Integrated Method for Learning with Small Data Challenges.
  - Core Courses: Statistical Machine Learning, Natural Language Processing, Learning on Graphs, Operation System.

- **Tsinghua University** *Aug 2015 - Jul 2019*

  Bachelor of Pure and Applied Mathematics advised by Prof. Chenglong Bao and Prof. Chunping Li. Beijing, China
  - GPA: 3.6/4.0. Top 10% Undergraduate Thesis.
  - Major Focus: Mathematics, Statistics, Optimization.
  - Thesis: An Improved Spectral Clustering Method by Enhancing Sparsity.
  - Core Courses: Statistical Inference, Numerical Analysis, Algorithm Analysis and Design, Optimization.

Experience

- **Brigham and Woman's Hospital & Harvard Medical School** *Aug 2022 - current*

  Research Trainee part-time advised by Li Zhou, Ph.D., M.D. and Liqin Wang, Ph.D. Boston, USA
  - Studied racial bias in the heathcare system using EHR data.
  - Proposed a counterpart-based fairness metric for mortality prediction models.

- **XtalPi Inc.** *July 2019 - Dec 2019*

  Algorithm Intern for AI-aided drug discovery Shenzhen, China
  - Implemented a transformer-like architecture for retrosynthetic reaction path prediction.
  - Improved model architectures and training strategies. Refined the pipeline of reaction prediction.

Publications and Preprints

[1] **Wang, Yifei**, Liqin Wang, Zhengyang Zhou, John Laurentiev, Joshua R. Lakin, Li Zhou, and Pengyu Hong. "Assessing fairness in machine learning models: A study of racial bias using matched counterparts in mortality prediction for patients with chronic diseases." *Journal of Biomedical Informatics*, 2024.

[2] **Wang, Yifei***, Zhengyang Zhou*, Liqin Wang, John Laurentiev, Peter Hou, Li Zhou, Pengyu Hong. "Counterpart Fairness – Addressing Systematic Between-group Differences in Fairness Evaluation" In *NeurIPS* Workshop, 2024.

[3] **Wang, Yifei**, Shiyang Chen, Guobin Chen, Ethan Shurberg, Hang Liu, and Pengyu Hong. "Motif-Based Graph Representation Learning with Application to Chemical Molecules." *Informatics*, vol. 10, no. 1, p. 8. MDPI, 2023.

[4] Yang, Tong*, **Yifei Wang***, Long Sha*, Jan Engelbrecht, and Pengyu Hong. "Knowledgebra: An Algebraic Learning Framework for Knowledge Graph." *Machine Learning and Knowledge Extraction* 4, no. 2 (2022): 432-445.

[5] Li, Peizhao, **Yifei Wang**, Han Zhao, Pengyu Hong, and Hongfu Liu. "On dyadic fairness: Exploring and mitigating bias in graph connections." In *International Conference on Learning Representations (ICLR)*, 2021.

[6] Hao Xu*, **Yifei Wang***, Yunrui Li*, Pengyu Hong. "Asymmetric Contrastive Multimodal Learning for Advancing Chemical Understanding"(preprint).

[7] Du, Xinsong, Zhengyang Zhou, **Yifei Wang**, Ya-Wen Chuang, Li Zhou et al. "Generative Large Language Models in Electronic Health Records for Patient Care Since 2023: A Systematic Review." (preprint)

[8] **Wang, Yifei**, Hao Peng, Long Sha, Zheyuan Liu, and Pengyu Hong. "State-level COVID-19 Trend Forecasting Using Mobility and Policy Data." (preprint)

*Equal contribution.

PROJECTS

View A: Graph Representational Learning, Multimodal Learning, AI for drug discovery.

- **Project 1: An Algebraic Learning Framework for Knowledge Graph** *[Paper] [Code]*
  - Developed an algebraic framework for learning consistent relation embeddings in knowledge graphs and proposed an algebraic-based instantiation for a knowledge graph embedding model.
  - Proposed simplified variants for learning low-dimensional relation embeddings using shared block settings and regularization-based method to integrate human logic rules.
- **Project 2: Motif-based Graph Representation Learning on Molecules** *[Paper][Code]*
  - Designed a novel convolution module for graph representational learning on molecules with an efficient pretraining strategy, enabling the capture of local structural and semantic information from graph motifs.
  - Demonstrated the superiority of the proposed model in molecular learning across multiple dimensions: (1) better results in various molecular property prediction tasks, (2) more stable training, and (3) improved interpretability.
- **Project 3: Explainable Contrastive Multimodal Learning on Molecules** *[Paper][Code]*
  - Proposed Asymmetric Contrastive Multimodal Learning, an effective and training-efficient framework tailored for molecules, promoting cross-modality understanding between the molecular graph and other chemical modalities.
  - Demonstrated the effectiveness and interpretability of the proposed framework in various key tasks: (1) large-scale cross-modality retrieval, (2) isomer discrimination, and (3) molecular property prediction.
- **Project 4: Controllable Molecule Generation by Diffusion Language Model** *[Code]*
  - Proposed a molecule generation framework inspired by the diffusion language model in controllable text generation, showing it superiority in discovering novel and diverse drug molecules.
  - Implemented a light-weight and modular plug-and-play approach to control the generation process, enabling the generation of molecules with optimized chemical properties and controlled substructures.

View B: Fairness and Bias.

- **Project 5: Exploring and Mitigating Bias in Graph Connections** *[Paper]*
  - Investigated the disparity of graph embedding for link prediction bridging on intra- and inter-sensitive groups. Proposed a chain of theoretical analyses on how graph connections could affect dyadic fairness.
  - Accordingly introduced an algorithm for fair link prediction by adjusting the adjacency weight matrix to address the fairness-utility trade-off.
- **Project 6: Unveiling Systematic Differences in Group Fairness Evaluation in Medical Contexts** *[Paper][Code]*
  - Explored the influence of systematic differences and confounding effects on group fairness estimation and proposed a counterpart-based fairness (CFair) index to improve fairness estimation by mitigating these influences.
  - Studied long-term mortality prediction of patients with chronic diseases, utilizing CFair to assess racial disparities in model predictions and offering insights into the influence of racial bias on model performance.

SKILLS

- **Programming Languages:** Python (familiar with most deep learning packages and platforms such as Sklearn, Pytorch, Pytorch Geometric, Diffusion, Transformers, Peft, HuggingFace, etc.), MATLAB, R.
- **Languages:** English (proficient), Chinese (native).
- **Research Skills:** Algorithm Development, Theoretical Proof, Quantitative Analysis, Experiment Design, Interdisciplinary collaboration, Presentation, Writing and Communication.
- **Soft Skills:** Time Management, Problem Solving, Project Management, Collaboration, Mentorship.

SERVICES

- **Reviewer:** NeurIPS, ICLR, ICML, COLING, KDD Workshop, AMIA Annual Symposium, International Journal of Medical Informatics.
- **Teaching Assistant:** Computation Theory, Spring 2024 & Statistical Machine Learning, Fall 2020, 2021, 2022.
- **Undergraduate Thesis Advisor:** Supervised a thesis that earned the Kukin Moskowitz Prize for Excellence 2024.