Yunchao “Lance” Liu

CONTACT INFORMATION

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GitHub: https://github.com/LanceKnight
Google Scholar: http://scholar.google.com/citations?user=oFtlWfwAAAAJ&hl=en

EDUCATION

Vanderbilt University

- **Doctor of Philosophy (Ph.D.)** student in Computer Science — Aug 2018 – Present
- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- Cumulative GPA: 3.92 / 4.00

University of Texas at Dallas

- **Master of Science (M.S.)** in Computer Science — May 2015
- Cumulative GPA: 3.85 / 4.0

Beijing University of Posts and Telecommunications

- **Bachelor of Science (B.S.)** in Management — Sep 2013

RESEARCH EXPERIENCE

Meiler Lab, Vanderbilt University
PhD Student, Computer Science Department — Sep 2018 – Present

- Advisors: Dr. Jens Meiler, Dr. Tyler Derr, Dr. Bobby Bodenheimer
- Research Areas: Computer-Aided Drug Discovery, Geometric Deep Learning, Self-Supervised Learning

State Key Laboratory of Intelligent Technology and Systems, Tsinghua University
Research Assistant, Department of Computer Science and Technology — Jul 2012 – Mar 2013

- Advisor: Dr. Xiaolin Hu
- Research areas: Visual Saliency for Road Sign Detection

PUBLICATIONS

Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery. Preceedings of the 37th Association for the Advancement of Artificial Intelligence (AAAI), 2023.

Yunchao Liu, Rocco Moretti, Bobby Bodenheimer and Jens Meiler. Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists. Preceedings of the 13th Annual ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG), 2020.

HONORS & AWARDS

AAAI2023 student scholarship and volunteer program travel award — Dec 2022
Reviewer Award @ ICML-AI4Science — Jun 2022
Nvidia Hardware Grant (RTX A6000) — Mar 2022

PRESENTATIONS & POSTERS

Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery *Learning on Graphs Conference (LoG)*, Poster 2022.

Yunchao Liu, Yu Wang, Oanh Vu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler and Tyler Derr. Interpretable Chirality-Aware Graph Neural Network for Quantitative Structure Activity Relationship Modeling in Drug Discovery *Summer RosettaCon*, Poster 2022.

Yunchao Liu, Rocco Moretti, Bobby Bodenheimer, Jens Meiler. Foldit Drug Design Game Usability Study: Comparison of Citizen and Expert Scientists, *ACM SIGGRAPH Conference on Motion, Interaction and Games (MIG)*, Presentation, 2020.

SERVICES

Journel Reviewer

- Big Data Research 2022

Conference Reviewer

- Association for the Advancement of Artificial Intelligence (AAAI) 2023
- ACM International Conference on Web Search and Data Mining (WSDM) 2023
- Machine Learning on Graphs @ International Conference on Data Mining (ICDM) 2022
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2022
- AI4Science @ International Conference on Machine Learning (ICML) 2022
- Deep Generative Models for Highly Structured Data (DGM4HSD) @ International Conference on Learning Representations (ICLR) 2022
- Conference on Neural Information Processing Systems (NeurIPS) 2022
- Machine Learning on Graphs (MLoG) @ ACM International Conference on Web Search and Data Mining (WSDM) 2022
- The Web Conference (TheWebConf) 2022
- International Conference on Learning Representations (ICLR) 2022
- ACM International Conference on Web Search and Data Mining (WSDM) 2022
- ACM International Conference on Information and Knowledge Management (CIKM) 2021
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2021
- AI4Science @ Conference on Neural Information Processing Systems (NeurIPS) 2021

Volunteering

- Volunteer at International Conference on Learning Representations (ICLR) 2022
- Session Manager at ACM International Conference on Web Search and Data Mining (WSDM) 2022

OTHER WORK EXPERIENCE

American Wonder Porcelain LLC., Nashville, TN, USA
IT Specialist — Sep 2015 – Jan 2018

- Administrated IFS ERP system: user right control, workflow design and etc.
- Analyzed sales data with Power BI
- Planned internet layout
- Provided other technical support

Xtera Communicatons Inc., Allen, TX, USA
Software Engineer Intern — Jan 2015 – Jul 2015

- Developed visulization software for remotely monitoring optical signals

University of Texas at Dallas, Dallas, TX, USA
Website Developer Intern — Jun 2014 – Dec 2014

- Developed websites for the international center

PROJECTS

Foldit Drug Design (FolditDD) Usability Study 2020

- Used the think-aloud method to conduct a usability study on FolditDD
- Compared the expert scientists and citizen scientists for their scientific problem solving skill in a game setting

FolditDD Interface Revamp 2019

- Customized Foldit interface to meet the need for drug design
- Introduced a preset function to quickly set the interface to drug design settings

Geometric Objects Rendering with Ray Tracing Technique 2019

- Used C++ and OpenGL library to render objects using ray tracing technique
- Achieved optical effects including reflection, diffusion, (overlapping) shadows

Geographical Data Visualization for UFO reports 2018

- Visualized geographic data of USO reports in the USA
- Designed interactive UI with features including zooming/panning/subplot

Visualizing Protein Flexibility using the Visualization Toolkit (VTK) 2018

- Developed a C++ program using VTK library to show the distance of two conformations of a protein
- Designed visulization scheme to show color coded flexibility on different parts of the protein

IFS Enterprise Resource Planning (ERP) Deployment 2016– 2018

- Designed the workflows for purchase order, inventory management, sales order, invoice, shop order, work order in the IFS ERP system
- Extracted data using SQL and designed auto-generated financial reports including balance sheet, income statement, cost analysis etc.

Library Management System 2015

- Designed and developed a library management system uisng Java and SQL
- Features including book lookup, return, overdue fine calculation, fine payment etc.

Full-time Curricular Practical Training (CPT) calculator 2014

- Developed a web-based full-time CPT calculator at the international center at UT Dallas to help international students avoid overtime working

SKILLS

Proficient with: Python, LaTeX
Coded using: C, C++, C#, Java, Visual Basic, HTML, Javascript, MATLAB, R
Operating Systems: CentOS, Ubuntu, and Windows

PROFESSIONAL AFFILIATIONS & ACTIVITIES

Association for the Advancement of Artificial Intelligence (AAAI)
Member 2022
American Chemical Society's Division of Computers In Chemistry (ACS COMP)
Member 2022

LANGUAGES

English: Fluent (speaking, reading, writing).
Chinese: Native language.

REFERENCES

Available Upon Request

[*CV compiled on 2022-12-23*]