San Francisco, CA

Mark Heimann

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Current Position

Computer Scientist — **Lawrence Livermore National Laboratory** — **2022-Present**
Center for Applied Scientific Computing — Livermore, CA

- Research in graph machine learning and foundation models, and applications to bioinformatics and software analysis.

Education

University of Michigan — **Ann Arbor, MI** — **2015-2020**

- Ph.D in Computer Science, focus in graph data mining.

Washington University in St. Louis — **St. Louis, MO** — **2011-2015**

- M.S. in Computer Science with a certificate in data mining and machine learning.
- A.B. in Economics and Mathematics *cum laude* with high distinction in economics.

Publications

- Akash Choudhuri, Yongjian Zhong, Mehrdad Moharrami, Christine Klymko, **Mark Heimann**, Jayaraman J. Thiagarajan, Bijaya Adhikari. "Conformal Edge-Weight Prediction in Latent Space." *SDM 2025*
- Konstantia Georgouli, Robert Stephany, Jeremy Tempkin; Claudio Santiago; Fikret Aydin, **Mark Heimann**, Loïc Pottier, Xiaohua Zhang, Timothy Carpenter, Tim Hsu, Dwight Nissley, Frederick Streitz, Felice Lightstone, Helgi Ingólfsson, Peer-Timo Bremer. "Generating Protein Structures for Pathway Discovery Using Deep Learning." *Journal of Chemical Theory and Computation 2024*.
- **Mark Heimann**, Christine Klymko, Jayaraman J. Thiagarajan. "Adapting Large Language Models to Predict Gene Interactions." *BioKDD @ KDD 2024.*
- Puja Trivedi, **Mark Heimann**, Rushil Anirudh, Danai Koutra, and Jayaraman Thiagarajan. "On Estimating the Epistemic Uncertainty of Graph Neural Networks using Stochastic Centering." *ICLR 2024.* **Also presented at DMLR @ ICML 2023, GLFrontiers @ NeurIPS 2023.**
- Donald Loveland, Jiong Zhu, **Mark Heimann**, Benjamin Fish, Michael T Schaub, and Danai Koutra. "On Performance Discrepancies Across Local Homophily Levels in Graph Neural Networks." LOG 2023.
- Samuel Leventhal, Attila Gyulassy, Valerio Pascucci, and **Mark Heimann**. "Modeling Hierarchical Topological Structure in Scientific Images with Graph Neural Networks." *ICIP 2023.* **Also presented at *GLFrontiers @ NeurIPS 2022.***
- Jiong Zhu, Yujun Yan, **Mark Heimann**, Lingxiao Zhao, Leman Akoglu, and Danai Koutra. "Heterophily and Graph Neural Networks: Past, Present, and Future." *Data Engineering Bulletin 2023*.
- Samuel Leventhal, Attila Gyulassy, **Mark Heimann**, and Valerio Pascucci. "Exploring Classification of Topological Priors with Machine Learning for Feature Extraction." *TVCG 2023*.
- Rakshith Subramanyam, **Mark Heimann**, Jayram Thathachar, Rushil Anirudh, and Jayaraman J. Thiagarajan. "Contrastive Knowledge-Augmented Meta-Learning for Few-Shot Classification." *WACV 2023.*
- Puja Trivedi, Ekdeep Singh Lubana, **Mark Heimann**, Danai Koutra, and Jayaraman Thiagarajan. "Analyzing Data-Centric Properties for Contrastive Learning on Graphs." *NeurIPS 2022.* **Also presented at GLB @ WebConf 2022, MLG @ KDD 2022.**
- Jing Zhu, Danai Koutra, and **Mark Heimann**. "CAPER: Coarsen, Align, Project, Refine – A General Multilevel Framework for Network Alignment." *CIKM 2022.* **Also presented at MLG @ KDD 2022**
- Donald Loveland, Jiong Zhu, **Mark Heimann**, Ben Fish, Michael Schaub, and Danai Koutra. "On Graph Neural Network Fairness in the Presence of Heterophilous Neighborhoods." *DLG @ KDD 2022.*

- Konstantia Georgouli, Helgi I. Ingólfsson, Fikret Aydin, **Mark Heimann**, Felice Lightstone, Peer-Timo Bremer, Harsh Bhatia. "Emerging Patterns in the Continuum Representation of Protein-Lipid Fingerprints." *CompBio @ ICML 2022.*
- Junchen Jin, **Mark Heimann**, Di Jin, and Danai Koutra. "Understanding and Evaluating Structural Node Embeddings." *TKDD 2021.* **Contributed talk at MLG @ KDD 2020**
- **Mark Heimann**, Xiyuan Chen, Fatemeh Vahedian, and Danai Koutra. "Refining Network Alignment to Improve Matched Neighborhood Consistency." *SDM 2021.*
- Jing Zhu*, Xingyu Lu*, **Mark Heimann**, and Danai Koutra. "Node Proximity is All You Need: A Unified Framework for Proximity-Preserving and Structural Node and Graph Embedding." *SDM 2021.*
- Jiong Zhu, Yujun Yan, Lingxiao Zhao, **Mark Heimann**, Leman Akoglu, and Danai Koutra. "Beyond Homophily in Graph Neural Networks: Current Limitations and Effective Designs." *NeurIPS 2020.*
- **Mark Heimann**, Goran Murić, and Emilio Ferrara. "Structural Node Embedding in Signed Social Networks: Finding Online Misbehavior at Multiple Scales." *Complex Networks 2020*.
- Kai Qin, Flora D. Salim, Yongli Ren, Wei Shao, **Mark Heimann** and Danai Koutra. "G-CREWE: Graph CompREssion With Embedding for Network Alignment." *CIKM 2020.*
- Xiyuan Chen, **Mark Heimann**, Fatemeh Vahedian, and Danai Koutra. "CONE-Align: Consistent Network Alignment with Proximity-Preserving Node Embedding." *CIKM 2020.* **Also presented at MLG @ KDD 2020**
- **Mark Heimann**, Tara Safavi, and Danai Koutra. "Distribution of Node Embeddings as Multiresolution Features for Graphs." *ICDM 2019.* **Best Student Paper**
- Di Jin, **Mark Heimann**, Ryan Rossi, and Danai Koutra. "node2bits: Compact Time- and Attribute-aware Node Representations for User Stitching." *PKDD 2019.*
- Di Jin*, **Mark Heimann***, Tara Safavi, Mengdi Wang, Wei Lee, Lindsay Snider, and Danai Koutra. "Smart Roles: Inferring Professional Roles in Email Networks." *KDD 2019.*
- **Mark Heimann**, Haoming Shen, Tara Safavi, and Danai Koutra. "REGAL: Representation Learning-based Graph Alignment." *CIKM 2018.* **Taught in graduate classes at UMich, Purdue**
- **Mark Heimann***, Wei Lee*, Shengjie Pan, Kuan-Yu Chen, and Danai Koutra. "HashAlign: Hash-Based Alignment of Multiple Graphs." *PAKDD 2018.*
- Yujun Yan, **Mark Heimann**, Di Jin, and Danai Koutra. "Fast Flow-based Random Walk with Restart in a Multi-query Setting." *SDM 2018.*
- **Mark Heimann** and Danai Koutra. "On Generalizing Neural Node Embedding Methods to Multi-Network Problems." *MLG @ KDD, 2017*.

** equal contribution*

Teaching Experience

- Lawrence Livermore National Laboratory (2022): Mining and Learning with Graphs (short course for Data Science Summer Institute, ~30 students.)
- University of Michigan (2016-19): Foundations of Computer Science (EECS 376, ~500 students), Introduction to Artificial Intelligence (EECS 492/592, ~200 students), Advanced Data Mining (EECS 576, ~50 students)
- Washington University in St. Louis (2014-15): Introduction to Machine Learning (CSE 417A, ~100 students), Multi-Agent Systems (CSE 516A, ~30 students), Fair Division (CSE/Pol Sci 245A, ~50 students)

work Experience

Postdoctoral Researcher — **Lawrence Livermore National Laboratory** — **Sep 2020-Sep 2022**
Center for Applied Scientific Computing — Livermore, CA

- Foundational research in graph-based few-shot learning and self-supervised learning, and uncertainty quantification, as well as combining foundation models and graph neural networks.
- Applied research in computational biology and software analysis.

Visiting Research Assistant — **Information Sciences Institute** — **Jun 2019-Aug 2019**
Artificial Intelligence Group — Marina Del Rey, CA

- Used node embeddings to identify cyberbullying in social media sessions.

- Theoretically analyzed algorithmically fair node embedding methods and proposed new techniques.

Data Science Research Intern **Adobe Research** **Jan 2019-Apr 2019**
Big Data Experience Lab San Jose, CA
- Performed large-scale entity resolution on cross-device web log data with millions of users.

Graduate Research Intern **Oak Ridge National Laboratory** **Apr 2018-Aug 2018**
Computational Data Analytics Group Oak Ridge, TN
- Developed dimensionality reduction algorithm with applications to unmixing of hyperspectral image data.

Software Engineer Intern **Algorithmia** **Jun 2015-Aug 2015**
Algorithm Development Team Seattle, WA
- Made cutting edge machine learning algorithms easy to use through a standardized API, along with demos.

Researcher **Harvey Mudd College** **Jun 2014-Aug 2014**
NSF REU Program Claremont, CA
- Designed and implemented an algorithm to generate more harmonically structured jazz solos.

Researcher **University of North Carolina, Greensboro** **Jun 2013-Jul 2013**
NSF REU Program Greensboro, NC
- Resolved open mathematical questions with applications to computer science and biology.

Student Trainee **Washington University School of Medicine** **Jun 2012-Jul 2012**
NHLBI Summer Institute for Training in Biostatistics (SIBS) St. Louis, MO
- Studied biostatistics and analyzed biomedical datasets as part of an accompanying practicum.

AWARDS

- **Best Program Committee Member, WebConf 2021 & 2024**: For high-quality reviewing service.
- **Best Student Paper, ICDM 2019**: Best paper whose first author was a full-time student.
- **Travel grants (KDD 2017,2019,2020; CIKM 2018; SDM 2019; ICDM 2019):** Attend and present work.
- **Adam Smith Prize for Excellence in Economics (2015):** For writing an outstanding senior thesis.
- **Arnold J. Lien Scholarship (2011):** Four-year full-tuition merit scholarship.

MENTORING

- Akash Choudhuri (PhD, SU2023). Work in progress on uncertainty estimation for link prediction with graph neural networks. **Current:** PhD at University of Iowa CS.
- Yongjian Zhong (PhD, SU2023). Work in progress on calibrated graph neural networks. **Current:** PhD at University of Iowa CS.
- Samuel Leventhal (PhD, SP2021-present). Paper in submission on topological analysis of scientific image data with graph neural networks. Second paper in preparation. **Current**: PhD at University of Utah CS.
- Rakshith Subramanyam (PhD, SU2021-present). Paper in submission on designing hierarchical knowledge graph structures for few-shot learning. **Current**: PhD at Arizona State University CS.
- Puja Trivedi (PhD, SU2021-present). Paper in submission on self-supervised learning on graphs. **Current**: PhD at University of Michigan CSE.
- Jing Zhu (UG & PhD, SU2020-present). Published two lead-author papers: on node and graph embeddings, and multilevel network alignment. Work in progress on using biomedical knowledge graphs for gene interaction prediction. **Next**: PhD at University of Michigan CSE.
- Xingyu Lu (UG, SU2020). Published lead-author paper on node and graph embedding. **Next**: MS at Columbia Data Science Institute.
- Xiyuan Chen (UG, FL2019-WN2020)**.** Wrote senior thesis and published two papers on network alignment, one as lead author. **Next**: MS at Stanford CS.
- Junchen Jin (UG, WN2019-WN2020)**.** Published journal paper and contributed to a conference tutorial on evaluating structural node embeddings. **Next**: MS at Northwestern Data Science.
- Haoming Shen (MS, SU17-SU18). Published paper on network alignment. **Next**: PhD at UMich IOE.

Reviewing

- **Program Committee:** AAAI 2022-2025, GLFrontiers @ NeurIPS 2023, WebConf 2021-2025, WSDM 2023-2024, LOG 2022-2024, SDM 2022-2025, KDD 2021-2022, IEEE BigData 2024, SDM 2021-2025, CIKM 2021-2023, Complex Networks 2020-2022, WebConf GLB Workshop 2022, CIKM Demos 2019-2020, PKDD GEM Workshop 2019-2021, ICANN 2019, ICDM Demos 2019
- **Reviewer:** WACV 2023, WebConf GLB Workshop 2021, AAAI 2021, DAMI, KnoSys, TSIPN, Trans. on Computers, Trans. on Cybernetics, TKDE, KAIS, Neural Computation, SNAM

tutorials & symposia

- Konstantia Georgouli, **Mark Heimann**, Harsh Bhatia, Timothy S. Carpenter, Felice C. Lightstone, Helgi I. Ingólfsson, Peer-Timo Bremer. "Generating Protein Structures for Pathway Discovery Using Deep Learning." AAAI Symposium on Computational Approaches to Scientific Discovery. March 2023.
- **Mark Heimann**, Junchen Jin, and Danai Koutra. "Network Embedding for Role Discovery: Concepts, Tools, and Applications." SIAM International Conference on Data Mining. April 2022.
- Thomas Blum*, Srinivas Eswar*, Jeffrey Graves*, **Mark Heimann***, and Ramakrishnan Kannan. "Machine Learning in Materials Science: An Introduction through Python." Center for Nanophase Materials Science User Meeting, Oak Ridge National Laboratory. August 2018.

Invited talks and lectures

- *Embedding-based Role Discovery.* Guest lecture, Department of Computer Science, Vanderbilt University, Nashville, TN (virtual). December 2021.
- *Refining Network Alignment to Achieve Matched Neighborhood Consistency.* SPIRAL Seminar, Northeastern University, Boston, MA (virtual). April 2021.
- *Introduction to Machine Learning.* Guest lecture, Department of Information Systems, Carnegie Mellon University, Pittsburgh, PA (virtual). October 2020.
- *Node Embedding on Multiple Networks.* 5th International Summer School on Data Science, Split, Croatia (virtual). September 2020.
- *REGAL: Representation Learning-based Graph Alignment.* NABD Conference, Criteo Labs, Ann Arbor, MI. May 2019.

other activities

- **Chess:** Hold the title of Grandmaster, the highest title in the game. Active in professional tournaments, as well as teaching and lecturing.
- **Powerlifting:** USA Powerlifting national-level athlete (top ~2% of competitive lifters in 2022) and referee.