HANNES STÄRK

MIT PhD Student in Electrical Engineering and Computer Science

hannes-stark.com | Google Scholar | GitHub | LinkedIn | hstark@mit.edu

EDUCATION

PhD in EECS | Machine Learning

Massachusetts Institute of Technology — June 2022 - June 2027

- Co-advised by Prof. Tommi Jaakkola and Prof. Regina Barzilay

M.Sc. Informatics | Machine Learning major

Technical University of Munich — Oct 2019 - Sept 2021

- "passed with high distinction" (1.2) - No corrections for thesis
- Learning theory, ML, DL, Quantum Computing, Protein Prediction, ...

Attending theoretical foundations of AI and protein prediction reading groups

B.Sc. Informatics | Mathematics track

Bundeswehr University Munich — Oct 2017 – Sept 2019

- Only student who completed the 3 year curriculum in 2 years

Built concept and started development of the app CoachPTBS

EXTRACURRICULAR TRAINING

Machine Learning Summer School: MLSS — Aug 2021

- Strong student award and nominated for best paper (selective admission)

Eastern European ML Summer School: EEML — Jul 2021

- 1 of 4 chosen students to present research (selective admission)

RESEARCH TRAJECTORY

ML for Free Energy Calculations and Molecular Simulation

In PhD: Tommi Jaakkola + Regina Barzilay, MIT

- Accelerating MD for sampling the Boltzmann distribution, transition path sampling, and protein-ligand free energy calculations

Molecular Docking with Generative models

In PhD: Tommi Jaakkola + Regina Barzilay, MIT

- Diffusion generative model over the Boltzmann distribution of a ligand and a protein to improve accuracy from 20 to 38%: DiffDock Paper

Geometric DL for Molecular Docking and Drug Discovery

Tommi Jaakkola + Regina Barzilay + Octavian Ganea, MIT

- SE(3)-invariant prediction of the bound ligand's 3D coordinates: Paper

Master's Thesis: Graph ML for 2D + 3D Molecular ML

Pietro Liò, University of Cambridge + Stephan Günnemann, TUM

- Use SSL to pre-train GNNs with 3D information of molecules leading to a 22% average improvement in prediction error: Paper

SELECTED PAPERS (find all here:)

- Gabriele Corso*, **Stärk Hannes*** et al. (2023) "DiffDock: Diffusion Steps, Twists, and Turns for Molecular Docking. In: ***ICLR 2023***. *Best paper at NeurIPS'22 Score-Based Methods Workshop*
- Stärk et al. (2022) "EquiBind: Geometric Deep Learning for Drug Binding Structure Prediction". In: ***ICML 2022***. *Also spotlight at ICLR'22 MLDD.*
- Stärk et al. (2021) "3D Infomax improves GNNs for Molecular Property Prediction". *In:* ***ICML 2022***. *Also at NeurIPS 2021 ML4PH, AI4S, SSL workshops and ELLIS ML4Molecules workshop.*
- Stärk et al. (2021) "Light Attention Predicts Protein Location from the Language of Life". In: ***OUP Bioinformatics Advances***. *Spotlight at ICLR'21 MLPCP. Poster + talks at MLCSB 2021 and WCB ICML 2021.*

SUMMARY

I am a first-year PhD student at MIT CSAIL co-advised by Tommi Jaakkola and Regina Barzilay. I work on geometric deep learning and generative models for ***molecular simulation and biochemistry****. I aim to use ML to model complex systems that cannot be captured by simple equations. This is with the purpose of improving our understanding of the world and helping tackle impactful* ***real-world problems****.*

NEWS

MIT News featured DiffDock — Mar 2023

MIT News featured EquiBind — Jul 2022

SKILLS

Python ●●●●●
Main language in projects and personal use

Java + Scala ●●●○○
Two years of backend development and main language during studies

Other Languages: HTML, CSS, JavaScript (proficient) R, C++, SQL, ARM assembly, Swift, MATLAB (used occasionally)

PyTorch ●●●●○
Self-Supervised learning, Transformers for proteins, Differentiable rendering, Reinforcement learning, WaveNet for denoising audio, Enzyme prediction + projects done as coursework and exercises created for courses

TensorFlow, Keras ●○○○○
Variational Autoencoder for aerial images

Other: Spectral Methods for Graphs, Computer Vision, Git, Unix systems, Shell, Docker, Cloudfoundry, Jenkins, Unittesting, Jupyter, LaTeX, **clean code**, AWS, Google Cloud Platform

Languages:

German ●●●●●
Native Speaker

English ●●●●●
Professional Proficiency | 96% in TOEFL test

French ●○○○○
Secondary language at school and from friends

LEISURE

Gymnastics, Philosophy, Acrobatics, Watching online lectures, Chess , Paper discussions

AWARDS

Highest prize money award at WCB ICML'21

Strong student award at MLSS

WORK EXPERIENCE

ML Research Intern

Valence Discovery

March 2022 - May 2022 | remote | Part-time

Graph ML for drug-target binding affinity prediction

Mathematics Instructor

BIB Augsburg gGmbH

Feb 2020 - Nov 2021 | Augsburg, DE | Part-time

4h per week: teaching linear algebra, analysis, and statistics

- Online lectures and weekly individual lessons

Student Assistant

Institute of Mathematics and OR, Bundeswehr University Munich

Sept 2018 – July 2019 | Munich, DE | Part-time

10h workweek: causal inference + structure learning in Bayesian networks

- Implemented and evaluated methods for regression on time-series data

Dual Study Program

Allianz Deutschland AG

Sept 2017 – Sept 2019 | Munich, DE | Part-time

38h workweek: web-development and digital infrastructure maintenance in an agile development team, technical training in computer science

- Designed and Developed an app for organizing large software releases
- Provided web-applications for customer interaction and deployment pipelines

Java (Spring Boot), HTML, CSS, TypeScript (Angular), Git, Jenkins, software engineering best practices, clean and fast programming

TEACHING

Operations Research

Technical University of Munich, Decision Sciences

April 2021 – Sept 2021 | Remote | Part-time

- Taught two recitations per week for 40 students, helped in online forum

Deep Learning

Technical University of Munich, CV & AI Niessnerlab

Nov 2020 – April 2021 | Remote | Part-time

- Held weekly office hours, created exercises and learning material like jupyter notebooks, answered questions in an online forum

VOLUNTEERING

Co-organizer of ML on Graphs Workshop @ WSDM 2022

ICLR 2021 and ICML 2021 Volunteer

- Help presenters and host talks including keynotes

Gymnastics and Acrobatics Trainer

VfL Buchloe

Sept 2015 – May 2022 | Buchloe, DE

- Started acrobatics show group Akrobatik Astral
- Training gymnastics and acrobatics groups for competitions and shows
- Choreograph acrobatics shows and participate in them

TALKS (find all here:)

American Chemical Society — Aug 2023
Invited talk at Skolnik Award Symposium

Mila - Quebec AI Institute — Jan 2022
Molecular Modelling. Host: Dr. Prudencio Tossou

Twitter Research — Jan 2022
Host: Prof. Michael Bronstein and Fabrizio Frasca

Technical University of Munich — Nov 2021
Two **guest lectures** about protein prediction for biology and CS students. Host: Prof. Burkhard Rost

University of Cambridge — Oct 2021
AI Research seminar. Host: Prof. Mateja Jamnik

Valence Discovery — Oct 2021
Invited talk. Host: Daniel Cohen

ISMB/ECCB 2021 — July 2021
Chosen for "Long Talk" on representation learning

RESEARCH OUTREACH

My Reading Group: LoGG

since Aug 2021 | virtual

- I am organizing the Learning on Graphs and Geometry reading group where paper authors present their work in an open discussion on Zoom
- >75 weekly attendees
- Community of over 2000 researchers
- sponsored by Valence Discovery

Co-founder and Organizer of the Learning on Graphs Conference

since Dec 2022 | virtual

- founded the LoG Conference with Petar Veličković and Yuanqi Du
- innovate reviewing process with financial incentives for reviewers and quality control
- decentralized meetups, free registration, and fully openly accessible

REVIEWING

- NeurIPS 2023 (3-4)
- ICML 2023 Frontiers in Learning, Control, and Dynamical Systems Workshop (3)
- ICML 2023 Synergy of Scientific and Machine Learning Modelling Workshop (1)
- IEEE Transactions on Pattern Analysis and Machine Intelligence (1)
- Bioinformatics (1)
- 2021 Machine Learning for Health Symposium (4)