

Gabriele Corso

MIT PHD STUDENT

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Education

Massachusetts Institute of Technology

Cambridge, US

PH.D. IN COMPUTER SCIENCE

Sep. 2021 - present

- Working in Tommi Jaakkola and Regina Barzilay's labs.
- My research focuses on *geometric deep learning* and *generative models* and their application to structural biology and drug discovery.
- Published several research papers at NeurIPS, ICLR, ICML, and other venues. Models from my research, such as DiffDock, are now regularly used by several pharmaceutical, tech and biotech companies and they are key components in cloud platforms such as [BioNeMo](#) from NVIDIA.
- Robert J. Shillman fellow (2021-2022).

M.S. IN COMPUTER SCIENCE

Sep. 2021 - Feb. 2023

- Thesis "Modeling Molecular Structures with Intrinsic Diffusion Models" under the supervision of T. Jaakkola and R. Barzilay. 5.0/5.0 GPA

University of Cambridge

Cambridge, UK

B.A. HONS IN COMPUTER SCIENCE

Sep. 2018 - Jun. 2021

- *1st Class Honours with Distinction*, recognition only given, on average, to one student per year in the department.
- *Ranked 2nd* in the whole Computer Science class (>130 students) in exams.
- *Highly Commended Dissertation prize* for thesis under the supervision of Pietro Lió, Jure Leskovec and Rex Ying.
- Research in Professor Lió's group resulted in two publications at *NeurIPS* (as first author) and one oral at *ICML*.

Publications

CONFERENCES

* indicates equal contribution

1. **Deep Confident Steps to New Pockets: Strategies for Docking Generalization.** [G. Corso*](#), A. Deng*, B. Fry, N. Polizzi, R. Barzilay, T. Jaakkola. **ICLR 2024**.
2. **Particle Guidance: non-I.I.D. Diverse Sampling with Diffusion Models.** [G. Corso](#), Y. Xu, V. de Bortoli, R. Barzilay, T. Jaakkola. **ICLR 2024**.
3. **DiffDock: Diffusion Steps, Twists, and Turns for Molecular Docking.** [G. Corso*](#), H. Stärk*, B. Jing*, R. Barzilay, T. Jaakkola. **ICLR 2023** and **Best Student Paper Award** at the NeurIPS 2022 Score-Based Modeling workshop.
4. **Torsional Diffusion for Molecular Conformer Generation.** B. Jing*, [G. Corso*](#), J. Chang, R. Barzilay, T. Jaakkola. **NeurIPS 2022 (oral)**.
5. **Subspace Diffusion Generative Models.** B. Jing*, [G. Corso*](#), R. Berlinghieri, T. Jaakkola. **ECCV 2022**.
6. **3D Infomax improves GNNs for Molecular Property Prediction.** H. Stärk, D. Beaini, [G. Corso](#), P. Tossou, C. Dallago, S. Günemann, P. Liò. **ICML 2022**.
7. **Learning Graph Search Heuristics.** M. Pándy, W. Qiu, [G. Corso](#), P. Veličković, Z. Ying, J. Leskovec, P. Liò. **LoG 2022**.
8. **Neural Distance Embeddings for Biological Sequences.** [G. Corso](#), R. Ying, M. Pándy, P. Veličković, J. Leskovec, P. Liò. **NeurIPS 2021**.
9. **Directional Graph Networks.** D. Beaini, S. Passaro, V. Létourneau, W. L. Hamilton, [G. Corso](#), P. Liò. **ICML 2021 (oral)**.
10. **Principal Neighbourhood Aggregation for Graph Nets.** [G. Corso*](#), L. Cavalleri*, D. Beaini, P. Liò, P. Veličković. **NeurIPS 2020**.

JOURNALS

1. **Graph neural networks.** [G. Corso*](#), H. Stark*, S. Jegelka, T. Jaakkola, R. Barzilay. **Nature Reviews Methods Primers**, 2024.
2. **Diffusion Models in Protein Structure and Docking** J. Yim, H. Stark, [G. Corso](#), B. Jing, T. Jaakkola. **WIREs Computational Molecular Science**, 2024.

UNDER REVIEW AND WORKSHOPS

1. **DisCo-Diff: Enhancing Continuous Diffusion Models with Discrete Latents.** Y. Xu, [G. Corso](#), T. Jaakkola, A. Vahdat, K. Kreis. Under review.
2. **Dirichlet Flow Matching with Applications to DNA Sequence Design.** H. Stark, B. Jing, C. Wang, [G. Corso](#), B. Berger, R. Barzilay, T. Jaakkola. Under review and Spotlight at ICLR 2024 ML for Genomics Explorations Workshop.
3. **EigenFold: Generative Protein Structure Prediction with Diffusion Models.** B. Jing, E. Erives, P. Pao-Huang, [G. Corso](#), B. Berger, T. Jaakkola. ICLR 2023 Machine Learning and Drug Discovery Workshop.

Work Experience

Twitter

London, UK

MACHINE LEARNING RESEARCH INTERN

Jun. 2021 - Aug. 2021

- Worked in the Learning Methods team under the supervision of Professor Michael Bronstein extending message passing beyond discrete graphs to continuous Riemannian spaces.

D.E. Shaw

New York, US

QUANTITATIVE RESEARCH INTERN

Jun. 2020 - Sep. 2020

- Worked in the Futures team on financial time-series forecasting using various statistical and machine learning techniques.

Alchera Technologies

Cambridge, UK

MACHINE LEARNING R&D INTERN

Jun. 2019 - Sep. 2019

- Developed original spatio-temporal graph neural network model which improves achieving state-of-the-art performances on traffic prediction benchmark datasets.
- Deployed model to production on AWS integrating it with existing APIs for live predictions.

IBM

Hursley, UK

SOFTWARE ENGINEERING INTERN

July 2018

- Developed a conversation assistant to voice-enable the IoT laboratory, allowing natural language interaction and the control of IoT devices.

Honors & Awards

2022	Best Student Paper Award , NeurIPS 2022 Score-Based Modeling workshop	New Orleans, US
2021-22	Robert J. Shillman fellow , MIT, value >\$90,000	Cambridge, US
2021	Highly Commended Dissertation , University of Cambridge, Computer Science Department	Cambridge, UK
2019-21	Trinity College Senior Scholarship , Trinity College, University of Cambridge	Cambridge, UK
2018	Bronze Medal , Central European Olympiad in Informatics	Warsaw, Poland
2017	Silver Medal in Mathematics , International Olympiad of Metropolises	Moscow, Russia
2017	Gold Medal , Italian Olympiad in Informatics (4th place)	Trento, Italy
2017	Gold Medal , Italian Mathematical Olympiad	Cesenatico, Italy
2017	Bank of Italy prize in Mathematics and Informatics , Bank of Italy	Rome, Italy

Program Committees and Volunteering

2023	Program Chair and Organizer , NeurIPS Machine Learning for Structural Biology Workshop	New Orleans
	<ul style="list-style-type: none">• NeurIPS workshop with more than 300 attendees and more than 100 paper submissions.	
2022-23	Organizer , Molecular Machine Learning (MoML) Conference	MIT
	<ul style="list-style-type: none">• In-person conference with more than 300 attendees every year.	
2022	Organizer , 1st Learning on Graphs (LoG) Conference	Online
	<ul style="list-style-type: none">• Online conference with 266 paper submissions, 372 reviewers, 83 accepted papers with proceedings in PMLR, 3000 registered attendees and \$35k funding.	
2024	Reviewer , ICML 2024	
2023	Reviewer , NeurIPS 2023	
2023	Reviewer , Nature Communications	
2023	Reviewer , IEEE Transactions on Pattern Analysis and Machine Intelligence	
2022-23	Reviewer , ACS Journal of Chemical Information and Modeling (JCIM)	
2018-now	Core Team Member , LeadTheFuture	Italy
	<ul style="list-style-type: none">• Non-profit association providing mentorship and community support for outstanding Italian students.• Joined the core team a couple of months after the founding (only 3 people at the time)• We now have more than 600 mentees, students from universities in Italy and abroad (<25% acceptance rate), and 200 selected mentors, professionals from top academic and industrial institutions.	
2021-22	Mentor , Graduate Application Assistance Program (GAAP)	MIT