

CHAITANYA K. JOSHI

Curriculum vitæ (5th July 2024)

Ph.D. Student

Department of Computer Science & Technology
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University of Cambridge, UK

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EDUCATION

- 01/2022–present **University of Cambridge, UK**, Ph.D. in Computer Science.
Qualcomm Innovation Fellow, A*STAR National Science Scholar.
Geometric Deep Learning for Biomolecule Modelling & Design; supervisor: Prof. Pietro Liò.
- 07/2015–05/2019 **Nanyang Technological University, Singapore**, B.Eng. in Computer Science.
Valedictorian, Best Thesis Gold Medal, Best Internship Award, Dean's List ×2.
Graph Neural Networks for the Travelling Salesman Problem; supervisor: Prof. Xavier Bresson.
- 01/2017–07/2017 **École Polytechnique Fédérale de Lausanne, Switzerland**, Exchange Semester.
Personalisation in Goal-oriented Dialog Systems; supervisor: Prof. Boi Faltings.

WORK EXPERIENCE

- 07/2024–09/2024 **Research Scientist Intern, Chemistry Team**, Fundamental AI Research (FAIR), Meta, San Francisco, California, USA.
- 07/2023–09/2023 **Research Scientist Intern, Prescient Design**, Genentech, Roche, Basel, Switzerland.
Geometric Deep Learning for protein design and molecular dynamics, with Dr. Andreas Loukas.
- 07/2020–12/2021 **Research Engineer, Institute for Infocomm Research**, A*STAR, Singapore.
Resource-efficient Graph Neural Networks, with Dr. Chuan Sheng Foo and Dr. Lin Jie.
- 07/2019–07/2020 **Research Assistant, Graph Deep Learning Lab**, NTU, Singapore.
Graph Neural Networks and applications to combinatorial optimisation, with Prof. Xavier Bresson.
- 01/2018–06/2018 **Research Intern, SAP Machine Learning**, Singapore.
Deep Learning systems for *Cash Application*, SAP's flagship automated accounting product handling over 200M EUR in annual sales pipeline for global companies. Direct work led to 3 US patents.

HONOURS & AWARDS

- 2024
- **Qualcomm Innovation Fellowship**, for my proposal *Geometric Generative Models for 3D RNA Design*; value: 40K USD, top 5 PhD students across Europe.
 - **Cambridge HPC Pioneer Project grant**, for my project on *Geometric Deep Learning for RNA Design*, awarded to pilot *Dawn*, UK's new AI supercomputer.
- 2023
- **Accelerate Science & Cambridge Centre for Data-Driven Discovery grant**, to host the conference *Understanding Biology in the age of AI* held in Cambridge, UK in June 2023; value: 14K GBP.
- 2022
- **Top Reviewer Awards** at NeurIPS 2022, ICLR 2022, NeurIPS 2021.
- 2021
- **National Science Scholarship**, A*STAR, Singapore. Fully funded scholarship to pursue PhD studies at University of Cambridge, UK; value: >800K USD, 5 years of research funding.
- 2019
- **Valedictorian, School of Computer Science & Engineering**, NTU, Singapore.
Awarded for excellent academic performance, leadership qualities and public-speaking skills among the graduating cohort. Valedictory speaker for Class of 2019.
 - **Best Final Year Thesis Gold Medal**, NTU, Singapore, for B.Eng. thesis with Prof. Xavier Bresson.
- 2018
- **Best Professional Internship Award**, NTU, Singapore, for Research Internship at SAP.

PRESENTATIONS & INVITED TALKS

Most talks and slides are available via [my YouTube channel](#)[📄].

- 04/2024 • **gRNade: Geometric Deep Learning for 3D RNA Inverse Design.**
 Department of Computer Science, NUS, Singapore, host: Prof. Yang Zhang.
 Genome Institute of Singapore, A*STAR, host: Dr. Yue Wan.
 Institute of Molecular and Cell Biology, A*STAR, Singapore, host: Dr. Sherry Aw.
- 03/2024 Roche, Advanced Analytics Network Conference, Basel, Switzerland, host: Dr. Igor Kulev.
- 01/2024 CASP RNA Special Interest Group, host: Dr. Marcin Magnus (Harvard), Rachael Kretsch (Stanford).
- 11/2023 NUS Yong Loo Lin School of Medicine, Singapore, host: Prof. Roger Foo.
- 10/2023 MRC Laboratory of Molecular Biology, host: Dr. Phil Holliger.

- 01/2024 • **On the Expressive Power of Geometric Graph Neural Networks.**
 Department of Computer Science, IIT Delhi, India, host: Prof. Sayan Ranu.
- 05/2023 Mathematical Institute, University of Oxford, UK, host: Prof. Xiaowen Dong.
- 02/2023 Department of Computer Science, Texas A&M University, USA, host: Prof. Shuiwang Ji.
 Centre for Frontier AI Research, A*STAR, Singapore, host: Dr. Ivor Tsang, Prof. Ong Yew-Soon.
- 01/2023 Prescient Design, Genentech, Roche, Switzerland/USA, host: Dr. Andreas Loukas.
- 12/2022 NeurIPS 2022 Workshop on Symmetry and Geometry, New Orleans, USA, oral presentation.
- 10/2022 Department of Computer Science, NUS, Singapore, host: Prof. Bryan Hooi.
 Institute for Infocomm Research, A*STAR, Singapore, host: Prof. Xiaoli Li.

PUBLICATIONS

Equal first authorship/contribution is indicated using †, and highlighted works are indicated using ★.
 Latest publication list and citations can be found on my [Google Scholar profile](#)[📄] (2K+ citations).

PREPRINTS

- 2024 1. R. Anand[†], **C. K. Joshi[†]**, A. Morehead, A. R. Jamasb, C. Harris, S. Mathis, K. Didi, B. Hooi, and P. Liò: *RNA-FrameFlow: Flow Matching for de novo 3D RNA backbone design*, 2024. To be presented as an **Oral** at ICML 2024 Structured Probabilistic Inference Generative Modeling Workshop, and a **Spotlight** at ICML 2024 AI4Science Workshop. arXiv: [2406.13839](#)[📄] ★
- 2023 2. **C. K. Joshi**, A. R. Jamasb, R. Viñas, C. Harris, S. Mathis, A. Morehead, R. Anand, and P. Liò: *gRNade: Geometric Deep Learning for 3D RNA inverse design*. Invited book chapter, Springer Methods in Molecular Biology (forthcoming). ICML Workshop on Computational Biology, 2023. arXiv: [2305.14749](#)[📄] ★
- 3. A. Duval[†], S. V. Mathis[†], **C. K. Joshi[†]**, V. Schmidt[†], S. Miret, F. D. Malliaros, T. Cohen, P. Lio, Y. Bengio, and M. Bronstein: *A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems*, 2023. arXiv: [2312.07511](#)[📄] ★
- 4. X. Zhang, L. Wang, J. Helwig, Y. Luo, C. Fu, Y. Xie, M. Liu, Y. Lin, Z. Xu, K. Yan, et al.: *Artificial intelligence for science in quantum, atomistic, and continuum systems*. Preprint, 2023. (62 authors, 263 pages survey on AI4Science led by Prof. Shuiwang Ji). arXiv: [2307.08423](#)[📄]

CONFERENCE PUBLICATIONS

- 2024 5. A. R. Jamasb[†], A. Morehead[†], **C. K. Joshi[†]**, Z. Zhang[†], K. Didi, S. V. Mathis, C. Harris, J. Tang, J. Cheng, P. Liò, and T. L. Blundell: *Evaluating Representation Learning on the Protein Structure Universe*. International Conference on Learning Representations (ICLR), 2024. [URL](#)[📄].
- 2023 6. **C. K. Joshi[†]**, C. Bodnar[†], S. V. Mathis, T. Cohen, and P. Liò: *On the Expressive Power of Geometric Graph Neural Networks*. International Conference on Machine Learning (ICML), 2023. Also presented as an **oral** at NeurIPS 2022 Workshop of Symmetry & Geometry. arXiv: [2301.09308](#)[📄] ★
- 2022 7. F. Liu, G. Lin, C.-S. Foo, **C. K. Joshi**, and J. Lin: *Point Discriminative Learning for Unsupervised Representation Learning on 3D Point Clouds*. International Conference on 3D Computer Vision (3DV), 2022. arXiv: [2108.0210](#)[📄]

- 2021 8. **C. K. Joshi**, Q. Cappart, L.-M. Rousseau, and T. Laurent: *Learning TSP Requires Rethinking Generalization*. International Conference on Principles and Practice of Constraint Programming, 2021. arXiv: [2006.07054](#)[📄]

JOURNAL PUBLICATIONS

- 2023 1. R. Viñas, **C. K. Joshi**, D. Georgiev, B. Dumitrascu, E. R. Gamazon, and P. Liò: *Hypergraph Factorisation for Multi-tissue Gene Expression Imputation*. Nature Machine Intelligence 5:7, pp. 739–753, 2023. **Cover article**. DOI: [10.1038/s42256-023-00684-8](#)[📄] ★
2. V. P. Dwivedi, **C. K. Joshi**, T. Laurent, Y. Bengio, and X. Bresson: *Benchmarking Graph Neural Networks*. Journal of Machine Learning Research 24:43, pp. 1–48, 2023. arXiv: [2003.00982](#)[📄]
- 2022 3. **C. K. Joshi**, F. Liu, X. Xun, J. Lin, and C.-S. Foo: *On Representation Knowledge Distillation for Graph Neural Networks*. IEEE Transactions of Neural Networks and Learning Systems, 2022. DOI: [10.1109/TNNLS.2022.3223018](#)[📄]. arXiv: [2111.04964](#)[📄]
4. **C. K. Joshi**, Q. Cappart, L.-M. Rousseau, and T. Laurent: *Learning the Travelling Salesperson Problem Requires Rethinking Generalization*. Constraints, pp. 1–29, 2022. **Invited article**. DOI: [10.1007/s10601-022-09327-y](#)[📄]. arXiv: [2006.07054](#)[📄]
- 2021 5. P. Xu, **C. K. Joshi**, and X. Bresson: *Multi-Graph Transformer for Free-Hand Sketch Recognition*. IEEE Transactions of Neural Networks and Learning Systems, 2021. DOI: [10.1109/TNNLS.2021.3069230](#)[📄]. arXiv: [1912.11258](#)[📄]

PATENTS

- 2020 6. S. Saito, T. V. Le, **C. K. Joshi**, and R. Shanmugamani: *Representing Sets of Entities for Matching Problems*. US Patent App. [16/208,681](#)[📄].
7. S. Saito, **C. K. Joshi**, R. Shanmugamani, T. V. Le, and R. Arumugam: *Utilizing Embeddings for Efficient Matching of Entities*. US Patent App. [16/217,148](#)[📄].
8. T. V. Le, S. Saito, **C. K. Joshi**, and R. Shanmugamani: *Graphical Approach to Multi-Matching*. US Patent App. [16/210,070](#)[📄].

WORKSHOP PAPERS AND INFORMAL PUBLICATIONS

- 2023 9. C. Harris, K. Didi, A. R. Jamasb, **C. K. Joshi**, S. V. Mathis, P. Lio, and T. Blundell: *PoseCheck: Generative Models for 3D Structure-based Drug Design Produce Unrealistic Poses*. NeurIPS Workshop on Machine Learning for Structural Biology, 2023. arXiv: [2308.07413](#)[📄]
10. K. Bujel[†], Y. Gideoni[†], **C. K. Joshi**, and P. Liò: *Group Invariant Global Pooling*. ICML Workshop on Topology, Algebra, & Geometry, 2023. arXiv: [2305.19207](#)[📄]
- 2022 11. **C. K. Joshi** and R. Anand: *Recent Advances in Deep Learning for Routing Problems*. Blog Track, International Conference on Learning Representations, 2022. [URL](#)[📄].
- 2020 12. **C. K. Joshi**: *Transformers are Graph Neural Networks*. The Gradient. **Read 80,000+ times**, featured in *Probabilistic ML textbook* by Kevin Murphy, taught in courses at Stanford (CS224W), Cambridge (L45), and Oxford. [URL](#)[📄]. 2020. ★
- 2019 13. **C. K. Joshi**, T. Laurent, and X. Bresson: *On Learning Paradigms for the Travelling Salesman Problem*. NeurIPS Graph Representation Learning Workshop, 2019. arXiv: [1910.07210](#)[📄]
14. **C. K. Joshi**, T. Laurent, and X. Bresson: *An Efficient Graph Convolutional Network Technique for the Travelling Salesman Problem*. INFORMS Annual Meeting, Session on Boosting Combinatorial Optimization using Machine Learning, 2019. arXiv: [1906.01227](#)[📄]
15. K. Joshi and **C. K. Joshi**: *Working women and caste in India: A study of social disadvantage using feature attribution*. ICLR Workshop on AI for Social Good, 2019. arXiv: [1905.03092](#)[📄]
- 2017 16. **C. K. Joshi**, F. Mi, and B. Faltings: *Personalization in Goal-oriented Dialog*. NeurIPS Workshop on Conversational AI, 2017. arXiv: [1706.07503](#)[📄]

OPEN SOURCE SOFTWARE

All my code is available via [GitHub](#) (over 4.5K total stars).

100+ stars

- **Geometric RNA Design (gRNAd)**: A toolkit for 3D RNA inverse design.

150+ stars

- **ProteinWorkshop**: A benchmarking framework for deep learning on 3D protein structure (ICLR 2024).

400+ stars

- **Geometric GNN Dojo**: Pedagogical implementations and experiments on 3D GNNs (ICML 2023).

2,500+ stars

- **Benchmarking GNNs**: A benchmarking framework for Graph Neural Networks (JMLR 2023).

TEACHING EXPERIENCE

I have served as a teaching assistant/supervisor for the following courses.

2022, 2023, 2024

- **Representation Learning on Graphs**, M.Phil. in Advanced Computer Science, University of Cambridge, UK; instructors: Prof. Pietro Liò, Dr. Petar Veličković (Google DeepMind).
Creation & grading of practical sessions on *Geometric Graph Neural Networks* (100+ students), mini-project supervision (17 students), guest lectures on *Introduction to Graph Generative Models* (2023) and *Geometric Graph Neural Networks* (2024).

2022, 2023

- **Introduction to Artificial Intelligence**, Part IB in Computer Science, University of Cambridge, UK; instructor: Prof. Sean Holden.
Creation & grading of personalised supervision sessions for 12 undergraduate students.

MENTORSHIP

2024

- Batu El, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
Term project: *Mechanistic Interpretability of Graph Neural Networks*.
Next: Ph.D. Student, Stanford University, USA. **Knight-Hennessey Scholar**.
- Deepro Chaudhury, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
Term project: *Mechanistic Interpretability of Graph Neural Networks*.
Next: Ph.D. Student, University of Oxford, UK.
- Rishabh Anand, B.Sc. in Computer Science, National University of Singapore.
Bachelor's thesis: *Generative Modelling for 3D RNA Structure Design*.
Outstanding Undergraduate Researcher Award, Best Poster Award.
Next: M.Sc. Student, Yale University, USA.

2023

- Teodora Reu, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
MPhil thesis: *Reimagining Graph Topology: Exploring Variational and Attentional Approaches*.
Next: Ph.D. Student, University of Oxford, UK; supervisor: Prof. Michael Bronstein.
- Kamil Bujel, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
MPhil thesis: *Learning and Breaking Symmetries in Geometric Deep Learning*.
Next: Quant Researcher, Jump Trading, London, UK.
- Yonatan Gideoni, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
Term project: *Group Invariant Global Pooling*.
Next: Ph.D. Student, University of Oxford, UK; supervisors: Prof. Yarin Gal, Prof. Michael Bronstein.
Rhodes Scholar.
- Harry Shaw, Part III in Physics, University of Cambridge, UK.
MPhil thesis: *Expressive Equivariant Graph Neural Networks with Higher Rank Cartesian Tensors*.
Next: Quant Researcher, Citadel, London, UK.

2022

- Peter Ralbovsky, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
Term project: *Geometrically Equivariant GNNs for Travelling Salesman Problem*.
Next: Software Engineer, Google, Zurich, Switzerland.
- Victor Zhao, M.Phil. in Advanced Computer Science, University of Cambridge, UK.
Term project: *Improving Graph Generative Models via Expressive Graph Neural Networks*.
Next: Ph.D. Student, Imperial College London, UK; supervisor: Prof. Aaron Zhao.

ACADEMIC SERVICE

ORGANISATION

- 2022, 2023, 2024
- **Organiser, Learning on Graphs Conference**^ℒ
LoG is a new annual research conference for machine learning on graphs and geometry founded by professors, scientists, and PhD students from Cambridge, Oxford, Stanford, MIT, DeepMind, Google, and other top institutions. In its first year, LoG received over 250 submissions, 36K USD in sponsorship.
- 06/2023
- **Organiser, Understanding Biology in the age of Artificial Intelligence**^ℒ
Conference in Cambridge exploring AI in biology from three perspectives: *theory*, *science*, and *philosophy*. Awarded 14K GBP grant from Accelerate Science and Cambridge Centre for Data-Driven Discovery.

REVIEWING

- *Conferences*

International Conference on Machine Learning (ICML)	2022–2024
Advances in Neural Information Processing Systems (NeurIPS)	2021–2023
International Conference on Learning Representations (ICLR)	2022–2023
- *Journals*

IEEE Transactions on Pattern Analysis & Machine Intelligence (TPAMI)	2022
IEEE Transactions on Neural Networks & Learning Systems (TNNLS)	2022
Distill	2021

OUTREACH

- **GraphML Telegram channel**^ℒ sharing research in graph machine learning (over 6K subscribers).
- **Twitter account**^ℒ sharing research in graph machine learning (over 6K followers)
- Postgraduate Student Representative and Organiser of Friday Socials (formerly Happy Hours, a decades long department tradition) for students and staff at the Department of Computer Science & Technology, University of Cambridge, UK.

PRESS COVERAGE

- 07/2024
- **“Qualcomm Innovation Fellowship Europe Rewards Excellent Research in the Field of AI and Cybersecurity”**^ℒ, Qualcomm.
- 03/2024
- **“The rise of Dawn: How the UK’s fastest AI supercomputer is supporting goals in clean energy, personalised medicine and climate.”**^ℒ, University of Cambridge covering the launch of selected pilot projects for *Dawn*, the UK’s new AI supercomputer based in Cambridge, including my work on *Geometric Deep Learning for RNA Design*.
- 08/2023
- **“New computational method can integrate gene expression across multiple tissue types”**^ℒ, Department of Computer Science, University of Cambridge announcing our cover article in *Nature Machine Intelligence*.
- 11/2022
- **“Clare Hall students win prestigious 14K GBP grant”**^ℒ, Clare Hall, University of Cambridge announcing our grant to organise a conference titled *Understanding Biology in the Age of AI*.
- 03/2021
- **“Stars in the making”**^ℒ, A*STAR Research Magazine.
- 03/2020
- **“Yoshua Bengio and team introduce GNN benchmarking framework”**^ℒ, Synced Review Magazine.
- 08/2019
- **“The path behind, the road ahead”**^ℒ, NTU Class of 2019 Valedictorians, NTULink Alumni Magazine.