CHAITANYA K. JOSHI Curriculum vitæ (19th March 2024)

Ph.D. Student Department of Computer Science & Technology Clare Hall College University of Cambridge, UK

\searrow	chaitanya.joshi@cl.cam.ac.uk
	chaitjo.com [™]
3	Chaitanya K. Joshi [®]
0	github.com/chaitjo [™]
in	linkedin.com/in/chaitjo/ [™]

Education

01/2022-present	University of Cambridge, UK , Ph.D. in Computer Science. <i>Geometric Deep Learning for Biomolecule Modelling & Design</i> ; 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. <i>Graph Neural Networks for the Travelling Salesman Problem</i> ; 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
07/2023-09/2023	Research Scientist Intern, Prescient Design Team [™] , Genentech, Roche, Basel, Switzerland. Geometric GNNs for protein design and molecular dynamics, with Dr. Andreas Loukas.
07/2020–12/2021	Research Engineer, Institute for Infocomm Research ^应 , A*STAR, Singapore. Resource-efficient GNNs, with Dr. Chuan Sheng Foo and Dr. Lin Jie.
07/2019-07/2020	Research Assistant, Graph Deep Learning Lab^E, NTU , Singapore. GNN architectures and applications to combinatorial optimisation, with Prof. Xavier Bresson.
01/2018–06/2018	Research Intern, SAP Machine Learning ^{L2} , Singapore. Deep Learning systems for <i>Cash Application</i> , 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	• Cambridge HPC Pioneer Project compute grant , for my project on <i>Geometric Deep Learning for RNA Design</i> , awarded to pilot <i>Dawn</i> , UK's new AI supercomputer based in Cambridge.
2022	• Top Reviewer Award, NeurIPS 2022 (top 10%).
	• Highlighted Reviewer Award, ICLR 2022 (top 10%).
2021	 National Science Scholarship, A*STAR, Singapore. Fully funded scholarship to pursue PhD studies at University of Cambridge, UK.
	Outstanding Reviewer Award, NeurIPS 2021 (top 10%).
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[™].

	 gRNAde: Geometric Deep Learning for 3D RNA Inverse Design.
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.
	On the Expressive Power of Geometric Graph Neural Networks.
01/2024	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.
1	Centre for Frontier AI Research, A'SIAK, Singapore, nost: Dr. Ivor Isang.
01/2023	Neur IDS 2022 Workshop on Summeters and Coometers Neur Orleans, USA, and presentation
12/2022	Department of Computer Science, NUS, Singapore, best, Brof, Bryan Hooi
10/2022	Institute for Infocomm Research, A*STAR, Singapore, host: Prof. Xiaoli Li.
	Benchmarking Graph Neural Networks
09/2020	Defense Science Organisation Laboratories, Singapore, host: Dr. Chieu Hai Leong.
	Graph Neural Networks for the Travelling Salesman Problem.
06/2021	Canadian Operations Research Society Conference, host: Dr. Maxime Gasse.
10/2019	INFORMS Annual Meeting, Seattle, USA, host: Prof. Quentin Cappart.
	Publications
	Equal first authorship/contribution is indicated using \dagger and highlighted works are indicated using \bigstar . Up
	to date publication list and citations can be found on my Google Scholar profile ¹² (1.8K+ citations).
	Preprints
	A Duvel [†] C V Methic [†] C V Jack ^{††} V Schmidt [†] C Minet E D Melliance T Cohen D Lie V Bengie and
2023	M. Bronstein: A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems, 2023. arXiv: 2312.07511
	2. C. K. Joshi, A. R. Jamasb, R. Viñas, C. Harris, S. Mathis, and P. Liò: <i>Multi-State RNA Design with Geomet-</i> <i>ric Multi-Graph Neural Networks</i> . ICML Workshop on Computational Biology, 2023. arXiv: 2305.14749 ^{L2}
	3. 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 ¹²
	CONFERENCE PUBLICATIONS
2024	4. 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. Interna-
	tional Conference on Learning Representations (ICLR) 2024 LIRI
	tional contentee on Learning representations (TCLR), 2024. ORL
2023	5. C. K. Joshi [†] , C. Bodnar [†] , S. V. Mathis, T. Cohen, and P. Liò: <i>On the Expressive Power of Geometric Graph</i>
2023	 C. K. Joshi[†], C. Bodnar[†], S. V. Mathis, T. Cohen, and P. Liò: <i>On the Expressive Power of Geometric Graph Neural Networks</i>. International Conference on Machine Learning (ICML), 2023. Also presented as an
2023	 5. 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^{L²}
2023 2022	 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^{L2} F. Liu, G. Lin, CS. Foo, C. K. Joshi, and J. Lin: Point Discriminative Learning for Unsupervised Repres-
2023 2022	 C. K. Joshi[†], C. Bodnar[†], S. V. Mathis, T. Cohen, and P. Liò: <i>On the Expressive Power of Geometric Graph Neural Networks</i>. International Conference on Machine Learning (ICML), 2023. Also presented as an oral at NeurIPS 2022 Workshop of Symmetry & Geometry. arXiv: 2301.09308^{L²} F. Liu, G. Lin, CS. Foo, C. K. Joshi, and J. Lin: <i>Point Discriminative Learning for Unsupervised Representation Learning on 3D Point Clouds</i>. International Conference on 3D Computer Vision (3DV), 2022.
2023 2022	 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^{L2} F. Liu, G. Lin, CS. 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^{L2}
2023 2022	 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^{L2} F. Liu, G. Lin, CS. 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^{L2} C. K. Joshi, O. Cappart, LM. Rousseau, and T. Laurent: Learning TSP Reauires Rethinking Generalization
2023 2022 2021	 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^{L2} F. Liu, G. Lin, CS. 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^{L2} C. K. Joshi, Q. Cappart, LM. Rousseau, and T. Laurent: Learning TSP Requires Rethinking Generalization. International Conference on Principles and Practice of Constraint Programming, 2021. arXiv: 2006.

JOURNAL PUBLICATIONS

2023

2022

2021

2020

2023

2022

2020

2019

2017

1. R. Viñas, C. K. Joshi, D. Georgiev, B. Dumitr	ascu, 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^{L2}
- 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^E. arXiv: 2111.04964^E
 - 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^{L²}. arXiv: 2006.07054^{L²}
- 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^{L2}. arXiv: 1912.11258^{L2}

Patents

- S. Saito, T. V. Le, C. K. Joshi, and R. Shanmugamani: Representing Sets of Entitites for Matching Problems. US Patent App. 16/208,681²⁷.
 - S. Saito, C. K. Joshi, R. Shanmugamani, T. V. Le, and R. Arumugam: Utilizing Embeddings for Efficient Matching of Entities. US Patent App. 16/217,148th.
 - 8. T. V. Le, S. Saito, C. K. Joshi, and R. Shanmugamani: *Graphical Approach to Multi-Matching*. US Patent App. 16/210,070^{E*}.

WORKSHOP PAPERS AND INFORMAL PUBLICATIONS

- 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^{L²}
 - 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^E
- 11. C. K. Joshi and R. Anand: *Recent Advances in Deep Learning for Routing Problems*. Blog Track, International Conference on Learning Representations, 2022. URL².
- 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^E. 2020.
- 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^{L2}
- 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^{E²}
- 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: 1905.03092¹²
- 16. **C. K. Joshi**, F. Mi, and B. Faltings: *Personalization in Goal-oriented Dialog*. NeurIPS Workshop on Conversational AI, 2017. arXiv: 1706.07503^{L2}

3/5

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. Creation & grading of practical sessions on <i>Geometric Graph Neural Networks</i> (100+ students), miniproject supervision (17 students), guest lectures on <i>Introduction to Graph Generative Models</i> (2023) and <i>Geometric Graph Neural Networks</i> (2024).
2022, 2023	• Introduction to Artificial Intelligence, Part IB in Computer Science, University of Cambridge, UK; in- structor: Prof. Sean Holden. Creation & grading of personalised supervision sessions for 12 undergraduate students.
	Mentorship & Thesis co-supervision
	I have had the pleasure of (co-)supervising the following students, jointly with Prof. Pietro Liò.
2023	 Teodora Reu, M.Phil. in Advanced Computer Science, University of Cambridge, UK. MPhil thesis: <i>Reimagining Graph Topology: Exploring Variational and Attentional Approaches</i>. Next: Ph.D. Student, University of Oxford; supervisor: Prof. Michael Bronstein.
	 Kamil Bujel, M.Phil. in Advanced Computer Science, University of Cambridge, UK. MPhil thesis: <i>Learning and Breaking Symmetries in Geometric Deep Learning</i>. Next: Quant Researcher, Jump Trading, London, UK.
	 Yonatan Gideoni, M.Phil. in Advanced Computer Science, University of Cambridge, UK. Term project: <i>Group Invariant Global Pooling</i> (ICML 2023 Workshop). Next: Ph.D. Student, University of Oxford; supervisor: Prof. Yarin Gal, Prof. Michael Bronstein. Rhodes Scholar.
	• Binjie (Anya) Chen, M.Phil. in Advanced Computer Science, University of Cambridge, UK. Term project: <i>Long-range and Hierarchical Interactions in Geometric Graph Neural Networks</i> . Next: Research Assistant, Computer Laboratory, University of Cambridge, UK.
	 Harry Shaw, Part III in Physics, Unversity of Cambridge, UK. MPhil thesis: <i>Expressive Equivariant Graph Neural Networks with Higher Rank Cartesian Tensors</i>. Next: Quant Researcher, Citadel, London, UK.
	Rishabh Anand, B.Sc. in Computer Science, National University of Singapore.
2022	 Peter Ralbovsky, M.Phil. in Advanced Computer Science, University of Cambridge, UK. Term project: <i>Geometrically Equivariant GNNs for Travelling Salesman Problem</i>. Next: Software Engineer, Google, Zurich, Switzerland.
	• Victor Zhao, M.Phil. in Advanced Computer Science, University of Cambridge, UK. Term project: <i>Improving Graph Generative Models via Expressive Graph Neural Networks</i> (LoG 2023). Next: Ph.D. Student, Imperial College London; supervisor: Prof. Aaron Zhao.
	Academic Service
	Organisation
2022, 2023, 2025	• Organiser, Learning on Graphs Conference ^{EZ} LoG is a new annual research conference for machine learning on graphs and geometry founded by pro- fessors, 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 ^{E7} Conference in Cambridge exploring AI in biology from three perspectives: <i>theory, science</i> , and <i>philosophy</i> . Awarded 14K GBP grant from Accelerate Science and Cambridge Centre for Data-Driven Discovery.

Reviewing

• Conferences

International Conference on Machine Learning (ICML) Advances in Neural Information Processing Systems (NeurIPS) International Conference on Learning Representations (ICLR)	2022–2024 2021–2023 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^{L²} sharing research in graph machine learning (over 6K subscribers).
- Twitter account² 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

03/2024	• "The rise of Dawn: How the UK's fastest AI supercomputer is supporting goals in clean energy, person- alised medicine and climate." ²⁷ , University of Cambridge covering the launch of selected pilot projects for <i>Dawn</i> , the UK's new AI supercomputer based in Cambridge, including my work on <i>Geometric Deep</i> <i>Learning for RNA Design</i> .
08/2023	• "New computational method can integrate gene expression across multiple tissue types" ² , Department of Computer Science, University of Cambridge announcing our cover article in <i>Nature Machine Intelligence</i> .
11/2022	• "Clare Hall students win prestigious 14K GBP grant" ² , Clare Hall, University of Cambridge announcing our grant to organise a conference titled <i>Understanding Biology in the Age of AI</i> .
03/2021	• "Stars in the making" ² , A*STAR Research Magazine.
03/2020	• "Yoshua Bengio and team introduce GNN benchmarking framework", Synced Review Magazine.
08/2019	• "The path behind, the road ahead" ^E , NTU Class of 2019 Valedictorians, NTULink Alumni Magazine.