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Education

- 2022– Postdoc, UdeM; Mila – Quebec AI Institute. Supervisor: Yoshua Bengio.
- 2017–2021 Ph.D. in Computer Science, Yale University. Advisor: Smita Krishnaswamy.
Graph Priors, Optimal Transport, and Deep Learning in Biomedical Discovery
Thesis committee: Ronald Coifman, Guy Wolf, and James Aspnes.
- 2017–2020 M.Phil. & M.S. in Computer Science, Yale University.
- 2015–2017 M.S. in Computer Science, Tufts University. Advisor: Soha Hassoun.
- 2013–2017 B.S. in Computer Science, Tufts University. (*summa cum laude*).

Publications

* † Denote equal contribution.

Links to full publications available on my website: <https://alextong.net/publications>

- [1] Zapatero, M. R.^{*}, **Tong, A.**^{*}, Sufi, J., Vlckova, P., Rodriguez, F. C., Nattress, C., Qin, X., Hochhauser, D., Krishnaswamy, S.[†] & Tape, C. J.[†] *Trellis Single-Cell Screening Reveals Stromal Regulation of Patient-Derived Organoid Drug Responses*. **Cell** (2023).
- [2] Huguet, G.^{*}, **Tong, A.**^{*}, De Brouwer, E.^{*}, Zhang, Y., Wolf, G., Adelstein, I.[†] & Krishnaswamy, S.[†] *A Heat Diffusion Perspective on Geodesic Preserving Dimensionality Reduction*. Neural Information Processing Systems (NeurIPS) (2023).
Also presented at TAG ML Workshop @ ICML (2023).
- [3] Atanovick, L.^{*}, **Tong, A.**^{*}, Hartford, J., Lee L. J., Wang, Bo. & Bengio, Y. *DynGFN: Bayesian Dynamic Causal Discovery using Generative Flow Networks*. Neural Information Processing Systems (NeurIPS) (2023).
Also presented at A Causal View on Dynamical Systems Workshop @ NeurIPS (2022).
- [4] Perlmutter, M., **Tong, A.**, Gao, F., Wolf, G. & Hirn, M. *Understanding Graph Neural Networks with Generalized Geometric Scattering Transforms*. SIAM Journal on Mathematics of Data Science (SIMODS) (2023).
- [5] Huguet, G.^{*}, **Tong, A.**^{*}, Zapatero, M. R., Tape, C. J., Wolf, G. & Krishnaswamy, S. *Geodesic Sinkhorn: optimal transport for high-dimensional datasets*. IEEE Machine Learning and Signal Processing (MLSP) (2023).

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- [6] Leone, S., Venkat, A., Huguet, G., **Tong, A.**, Wolf, G. & Krishnaswamy, S. *Graph Fourier MMD for Signals on Graphs*. SAMPTA: Sampling Theory and Applications (2023).
 - [7] Fasina, O.^{*}, Huguet, G.^{*}, **Tong, A.**, Zhang, Y., Wolf, G., Nickel, M., Adelstein, I.[†] & Krishnaswamy, S.[†] *Neural FIM for learning Fisher information metrics from point cloud data*. International Conference on Machine Learning (ICML) (2023).
 - [8] Huguet G.^{*}, **Tong A.**^{*}, Rieck B.^{*}, Huang J.^{*}, Kuchroo M., Hirn M.[†], Wolf G.[†], & Krishnaswamy S.[†] *Time-inhomogenous diffusion geometry and topology*. SIAM Journal of Mathematical Data Science (SIMODS) (2023).
 - [9] Kuchroo, M., DiStasio, M., Song, E., Calapkulu, E., Zhang, L., Ige, M., Sheth, A. H., Majdoubi, A., Menon, M., **Tong, A.**, Godavarthi, A., Xing, Y., Gigante, S., Steach, H., Huang, J., Huguet, G., Narain, J., You, K., Mourgos, G., Dhodapkar, R. M., Hirn, M. J., Rieck, B., Wolf, G., Krishnaswamy, S. & Hafler, B. P. *Single-cell analysis reveals inflammatory interactions driving macular degeneration*. Nature Communications (2023).
 - [10] Huguet G.^{*}, Magruder DS.^{*}, **Tong A.**^{*}, Fasina O., Kuchroo M., Wolf G.[†], & Krishnaswamy S.[†] *Manifold Interpolating Optimal-Transport Flows for Trajectory Inference*. Neural Information Processing Systems (NeurIPS) (2022).
 - [11] Perdigoto, A. L., Deng, S., Du, K. C., Kuchroo, M., Burkhardt, D. B., **Tong, A.**, Israel, G., Robert, M. E., Weisberg, S. P., Kirkiles-Smith, N., Stamatouli, A. M., Kluger, H. M., Quandt, Z., Young, A., Yang, M.-L., Mamula, M. J., Pober, J. S., Anderson, M. S., Krishnaswamy, S. & Herold, K. C. *Immune cells and their inflammatory mediators modify beta cells and cause checkpoint inhibitor-induced diabetes*. JCI Insight (2022).
 - [12] Hafler, B. P., Kuchroo, M., DiStasio, M., Song, E., Zhang, L., Ige, M., Sheth, A., Menon, M., **Tong, A.**, Xing, Y., Gigante, S., Huang, J., Mourgos, G., Krishnaswamy, S., Dhodapkar, R. & Wolf, G. *Topological analysis of single-cell hierarchy reveals inflammatory glial landscape of macular degeneration*. Investigative Ophthalmology & Visual Science (2022).
 - [13] **Tong A.**^{*}, Huguet G.^{*}, Shung D.^{*}, Natic A., Kuchroo M., Lajoie G., Wolf G.[†], Krishnaswamy S.[†]. *Embedding Signals on Knowledge Graphs with Unbalanced Diffusion Earth Mover's Distance*. International Conference on Acoustics, Speech, and Signal Processing (ICASSP) (2022).
 - [14] Kuchroo, M.^{*}, Huang, J.^{*}, Wong, P.^{*}, Grenier, J.-C., Shung, D., **Tong, A.**, Lucas, C., Klein, J., Burkhardt, D., Gigante, S., Godavarthi, A., Israelow, B., Oh, J. E., Silva, J., Takahashi, T., Odio, C. D., Fournier, J., Cruz, D., Ko, A. I., Wilson, F. P., Hussin, J., Wolf, G. & Krishnaswamy, S. *Multiscale PHATE Exploration of SARS-CoV-2 Data Reveals Multimodal Signatures of Disease*. Nature Biotechnology (2022).
 - [15] Gerasimiuk, M.^{*}, Shung, D.^{*}, **Tong, A.**, Stanley, A., Schultz, M., Ngu, J., Laine, L., Wolf, G.[†] & Krishnaswamy, S.[†] *MURAL: An unsupervised random forest-based embedding for electronic health record data*. IEEE International Conference on Big Data (2021).
 - [16] **Tong, A.**, Wolf, G. & Krishnaswamy, S. *Fixing Bias in Reconstruction-based Anomaly Detection with Lipschitz Discriminators*. Journal of Signal Processing Systems (2021).
 - [17] Luecken, M. D.^{*}, Burkhardt, D. B.^{*}, Cannoodt, R.^{*}, Lance, C.^{*}, Agrawal, A., Aliee, H., Chen, A. T., Deconinck, L., Detweiler, A. M., Granados, A., Huynh, S., Isacco, L., Kim, Y. J., Kuppasani, S., Lickert, H., McGeever, A., Mekonen, H., Caceres, J., Morri, M., Mueller,

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- M., Neff, N. F., Paul, S., Schneider, K., Steelman, S., Sterr, M., Treacy, D. J., **Tong, A.**, Villani, A.-C., Wang, G., Yan, J., Zhang, C., Pisco, A. O., Theis, F. J. & Bloom, J. M. *A sandbox for prediction and integration of DNA, RNA, and protein data in single cells*. NeurIPS Datasets and Benchmarks Track (2021).
- [18] **Tong, A.**^{*}, Wenkel, F.^{*}, MacDonald, K. Krishnaswamy S.[†] & Wolf, G.[†] *Data-driven Learning of Geometric Scattering Modules for GNNs*. IEEE Machine Learning and Signal Processing (MLSP) (2021).
Also presented at Machine Learning for Molecules Workshop @ NeurIPS (2020).
- [19] Kuchroo, M.^{*}, Godavarthi A.^{*}, **Tong, A.** Wolf, G.[†], & Krishnaswamy S.[†]. *Multimodal data visualization and denoising with integrated diffusion*. IEEE Machine Learning and Signal Processing (MLSP) (2021).
Also presented at ICML: Workshop on Computational Biology (2021)
- [20] **Tong, A.**^{*}, Huguet, G.^{*}, Natick, A.^{*}, MacDonald, K., Kuchroo, M., Coifman, R., Wolf, G.[†] & Krishnaswamy, S.[†] *Diffusion Earth Mover's Distance and Distribution Embeddings*. International Conference on Machine Learning (ICML) (2021).
An earlier version of this work presented in LMRL Workshop @ NeurIPS (2020).
- [21] Flamary, R., Courty, N., Gramfort, A., Alaya, M. Z., Boissunon, A., Chambon, S., Chapel, L., Corenflos, A., Fatras, K., Fournier, N., Gautheron, L., Gayraud, N. T. H., Janati, H., Rakotomamonjy, A., Redko, I., Rolet, A., Schutz, A., Seguy, V., Sutherland, D. J., Tavenard, R., **Tong, A.** & Vayer, T. *POT: Python Optimal Transport*. Journal of Machine Learning Research (JMLR) (2021).
- [22] Burkhardt, D. B.^{*}, Stanley, J. S.^{*}, **Tong, A.**, Perdigoto, A. L., Gigante, S. A., Herold, K. C., Wolf, G., Giraldez, A. J.[†], van Dijk, D.[†], & Krishnaswamy, S.[†] *Quantifying the Effect of Experimental Perturbations in Single-Cell RNA-Sequencing Data Using Graph Signal Processing*. Nature Biotechnology (2021).
- [23] Castro, E., Benz, A., **Tong, A.**, Wolf, G.[†], & Krishnaswamy, S.[†] *Uncovering the Folding Landscape of RNA Secondary Structure with Deep Graph Embeddings*. IEEE International Conference on Big Data (2020).
Also presented at the Graph Representation Learning and Beyond Workshop @ ICML (2020)
- [24] **Tong, A.**, Huang, J., Wolf, G.[†], van Dijk, D.[†] & Krishnaswamy, S.[†] *TrajectoryNet: A Dynamic Optimal Transport Network for Modeling Cellular Dynamics*. ICML (2020).
Also Presented at the LMRL Workshop @ NeurIPS (2019). (Spotlight).
- [25] **Tong, A.**, Wolf, G. & Krishnaswamy, S. *Fixing Bias in Reconstruction-based Anomaly Detection with Lipschitz Discriminators*. IEEE Machine Learning and Signal Processing (MLSP) (2020).
Best Student Paper Award
- [26] **Tong, A.**^{*}, van Dijk, D.^{*}, Stanley III, J. S., Amodio, M., Yim, K., Muhle, R., Noonan, J., Wolf, G.[†] & Krishnaswamy, S.[†] *Interpretable Neuron Structuring with Graph Spectral Regularization*. Advances in Intelligent Data Analysis (IDA) (2020).
An earlier version of this work appeared at the Workshop on Representation Learning on Graphs and Manifolds @ ICLR (2019).

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- [27] van Dijk, D.^{*}, Burkhardt, D. B.^{*}, Amodio, M., **Tong, A.**, Wolf, G.[†] & Krishnaswamy, S.[†] *Finding Archetypal Spaces Using Neural Networks*. IEEE International Conference on Big Data (2019).
 - [28] Aspnes, J., Haeupler, B., **Tong, A.** & Woelfel, P. *Allocate-On-Use Space Complexity of Shared-Memory Algorithms*. International Symposium on Distributed Computing (DISC) (2018). (Note: authors ordered alphabetically)

Preprints

- [1] **Tong, A.**^{*}, Kuchroo, M.^{*}, Gupta, S., Venkat, A., San Juan, B. P., Rangel, L., Zhu, B., Lock, J. G., Chaffer, C. L.[†] & Krishnaswamy, S.[†] *Learning transcriptional and regulatory dynamics driving cancer cell plasticity using neural ODE-based optimal transport*. Under Review at **Nature** (2023).
Presented at American Association of Cancer Research (AACR) (2021).
- [2] Nguyen, T., **Tong, A.**, Madan, K., Bengio, Y. & Liu, D. *Causal inference in gene regulatory networks with GFlowNet: Towards scalability in large systems*. ArXiv (2023).
Presented at GenBio Workshop @ NeurIPS (2023)
- [3] Bose, A. J.^{*}, Akhound-Sadegh, T.^{*}, Fatras, K., Huguet, G., Rector-Brooks, J., Liu, C.-H., Nica, A. C., Korablyov, M., Bronstein, M. & **Tong, A.** *SE(3)-Stochastic Flow Matching for Protein Backbone Generation*. ArXiv (2023).
Presented in MoML (2023)
- [4] Neklyudov, K.^{*}, Brekelmans, R.^{*}, **Tong, A.**, Atanackovic, L., Liu, Q. & Makhzani, A. A *Computational Framework for Solving Wasserstein Lagrangian Flows* ArXiv (2023).
Presented at OTML Workshop @ NeurIPS (2023)
- [5] **Tong, A.**, Malkin, N., Fatras, K., Atanackovic, L., Zhang, Y., Huguet, G., Wolf, G. & Bengio, Y. *Simulation-free Schrödinger bridges via score and flow matching*. ArXiv (2023).
Presented in Frontiers4LCD Workshop @ ICML (2023)
- [6] **Tong, A.**, Malkin, N., Huguet, G., Zhang, Y., Rector-Brooks, J., Fatras, K., Wolf, G. & Bengio, Y. *Conditional Flow Matching: Simulation-Free Dynamic Optimal Transport*. ArXiv (2023).
Presented in Frontiers4LCD Workshop @ ICML (2023)
- [7] **Tong, A.**^{*}, Wenkel, F.^{*}, Bhaskar, D., Macdonald, K., Grady, J., Perlmutter, M., Krishnaswamy, S. & Wolf, G. *Learnable Filters for Geometric Scattering Modules*. ArXiv (2022).

Non-archival work

- [1] Venkat, A., Miyagishima, D., **Tong, A.**, Günel, M., Krishnaswamy, S. *Manifold-based gene density estimates reveal immune signaling in meningioma tumors*. 29th Conference on Intelligent Systems for Molecular Biology (ISMB). (2021).
- [2] **Tong, A.** & Krishnaswamy, S. *Interpolating optimal transport barycenters of patient manifolds*. 28th Conference on Intelligent Systems for Molecular Biology (ISMB). (2020).

Experience

Dreamfold, Montreal, QC, CA

Cofounder and CTO, 2022—

- Dreamfold is a protein design company using generative modeling techniques employing 10+ scientists and engineers.
- Cofounded with Maksym Korablyov, Chenghao Liu, Jarrod Rector-Brooks, Michael Bronstein.
- Investors: IQ Capital, Panache Ventures, and Techhammer.

MoirAI Biosciences, New Haven, CT, USA

Cofounder, 2022—

- MoirAI Biosciences is a startup applying our work on dynamics and causality in single cell for target discovery
- Cofounded with Manik Kuchroo, Smita Krishnaswamy, and Christine Chaffer.
- Winner of CT Innovation Fund, Blavatnick Fund, and Robert's Innovation Fund competitions.

Mila—Quebec AI Institute, Montreal, QC, CA

Visiting Researcher, (virtual Fall 2020), Fall 2021

- Collaboration with Guy Wolf on geometric scattering
- Collaboration with Yoshua Bengio on causal single-cell dynamics

Artificial Intelligence Laboratory, Xevo Inc., Bellevue, WA, USA

AI Research Intern, Summer 2017

- Productized object detection algorithms for use in automotive computer vision systems
- Improved embedded high-performance, low-power machine learning framework

Ab Initio, Lexington, MA, USA

Software Engineering Intern, Summer 2016

- Integrated statistics tracking into Hadoop Map-reduce multi-process environment
- Worked on meta-programming system to cross compile on multiple architectures

Amazon Robotics (formerly Kiva Systems), North Reading, MA, USA

Software Engineering Intern, Summer 2015

- Developed a visual localization system to augment personnel tracking system
- Simultaneous Localization and Mapping (SLAM) system presented to CEO

Surround.io, Seattle, WA, USA

Software Engineering Intern, Summer 2014

- Implemented Raspberry Pi based Hadoop Map-reduce cluster
- First intern in early stage startup with four senior software engineers

Invited Talks

- “Improving and Generalizing Flow-Based Generative Models with Mini-batch Optimal Transport”. Learning on Graphs and Geometry Reading Group. Online. 8/2023
- “Learning Continuous Dynamics from Time-lapsed Single-cell Data”. Human Cell Atlas General Meeting. Toronto, Canada. 7/2023
- “Simulation-free dynamic optimal transport and applications to cell dynamics”. Institute of Computational Biology Seminar. Munich, Germany. 6/2023
- “Learning Continuous Dynamics from Time-lapsed Single-cell data”. Helmholtz AI Conference. Hamburg, Germany. 6/2023
- “High Resolution Analysis of Single-cell Data with Manifold Optimal Transport Methods”. Yee Lab. Houston, USA. 3/2023
- “Bayesian Causal Discovery for Continuous-time Dynamical Systems”. Helmholtz-Mila Symposium. Montreal, Canada. 10/2022
- “Multiscale Earth Mover’s Distances”. Banff International Research Station: Deep Exploration of non-Euclidean Data with Geometric and Topological Representation Learning. 7/2022
- “Single-Cell Screening Reveals Stromal Regulation of Patient-Derived Organoid Drug Responses”. BD Life Sciences. 7/2022
- “Learning Continuous-Time Gene Regulatory Structure from time-lapsed Single-cell Experiments”. Broad Institute Single-cell Seminar. 3/2022

Teaching

- Graduate Teaching Fellow. CPSC 465/565, Theory of Distributed Systems. Yale University Spring 2019
- Graduate Teaching Fellow. CPSC 468/568, Computational Complexity. Yale University Fall 2018
- Teaching Assistant. COMP 165, Cryptography. Tufts University Fall 2016
- Teaching Assistant. COMP 160, Algorithms. Tufts University Fall 2015
- Teaching Assistant. COMP 160, Algorithms. Tufts University Spring 2015
- Teaching Assistant. COMP 40, Machine Architecture. Tufts University Fall 2014

Student Mentoring

- Lazar Atanackovic (Now Ph.D. student at Vector Institute) 2022—
Co-supervised internship under Yoshua Bengio.
Resulting in NeurIPS 2023 publication.
- Katherine Du (Now M.D. student at University of Pittsburgh) 2021—2022
Co-supervised senior thesis under Smita Krishnaswamy.
Publication in JCI Insight.

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- Andrew Benz (Now ML Scientist at Cellarity) 2020—2021
Co-supervised undergraduate research under Smita Krishnaswamy.
 - Abhinav Godavarthi 2020—2022
Co-supervised undergraduate research under Smita Krishnaswamy.
Resulted in IEEE MLSP co-authorship.
 - Kincaid MacDonald 2020—2021
Co-supervised undergraduate research under Smita Krishnaswamy.
Resulted in IEEE MLSP co-authorship.
 - Brandon Zhu 2020—2021
Co-supervised undergraduate research under Smita Krishnaswamy.

Honors

- Best Student Paper IEEE Machine Learning and Signal Processing 2020
- Qualified with distinction 2019
- Tau Beta Pi Honor Society 2016
- 3x Academic All-American Intercollegiate Sailing Association 2014-2017

Reviewing

- International Conference on Learning Representations (ICLR) 2022—
- International Conference on Machine Learning (ICML) 2021—
- Neural Information Processing Systems (NeurIPS) 2021—
- ICML: New Frontiers in Learning, Control, and Dynamical Systems Workshop 2023
- ICML: Topology, Algebra, and Geometry in Data Science Workshop 2023
- ICLR: Tiny Papers Workshop 2023
- NeurIPS: ML4M Workshop 2022
- NeurIPS: Causal Discovery Workshop 2022
- Microsoft Climate AI Grants 2021; 2023
- Learning on Graphs Conference 2022—
- Transactions of Machine Learning Research (TMLR) 2021—
- ACM Transactions on Computational Biology and Bioinformatics 2022—
- Yale Undergraduate Research Journal (YURJ) 2021—
- Cell Patterns 2020

Other Professional Activities

- BIRS Workshop Co-organizer “Deep Exploration of non-Euclidean Data with Geometric and Topological Representation Learning” July 2022
- Moderator of “Bridging the gap from theory to practice” at the Geometric and Topological Representation Learning Workshop at ICLR 2022
- Co-organizer of NeurIPS 2021 Competition on Multi-Modal Single-cell Data Integration
- Member of Yale Computer Science Diversity Equity and Inclusion Committee 2020-2021