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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] 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.* To appear in ICLR (Spotlight) (2024).
Presented in MoML (2023)

[2] **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.* To appear in AISTATS (2024).
Presented in Frontiers4LCD Workshop @ ICML (2023)

[3] Ramos Zapatero, M.*, **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).

[4] 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).

[5] 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).

[6] 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).

[7] 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).

[8] 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).

[9] 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).

[10] 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).

[11] 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., Mourgkos, 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).

[12] 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).

[13] 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).

[14] 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., Mourgkos, 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).

[15] **Tong A.**[*], Huguet G.[*], Shung D.[*], Natik 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).

[16] 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).

[17] 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).

[18] **Tong, A.**, Wolf, G. & Krishnaswamy, S. *Fixing Bias in Reconstruction-based Anomaly Detection with Lipschitz Discriminators.* Journal of Signal Processing Systems (2021).

[19] 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, 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).

[20] **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).

[21] 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)

[22] **Tong, A.**[*], Huguet, G.[*], Natik, 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).

[23] Flamary, R., Courty, N., Gramfort, A., Alaya, M. Z., Boisbunon, 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).

[24] 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).

[25] 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)

[26] **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).

[27] **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

[28] **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).

[29] 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).

[30] 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] 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)

[4] **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)

[5] **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, Jarrid Rector-Brooks, Michael Bronstein.

- Investors: IQ Capital, Panache Ventures, and Techammer.

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)
  Co-supervised internship under Yoshua Bengio.
  Resulting in NeurIPS 2023 publication. — 2022—

- Katherine Du (Now M.D. student at University of Pittsburgh)
  Co-supervised senior thesis under Smita Krishnaswamy.
  Publication in JCI Insight. — 2021—2022

- 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 Worshop   2023
- NeurIPS: ML4M Workshop   2022
- NeurIPS: Causal Discovery Workshop 2022   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