PINAR DEMETCI

□ pinardemetci.github.io ♦ \$ 857 · 919 · 2448 ♦ □ pinardemetci@gmail.com \$ https://tinyurl.com/DemetciScholar ♦ (Last Updated: 5 January 2024)

SUMMARY & INTERESTS

I am an applied ML/AI researcher in computational biology and biomedical informatics. My research interests revolve around developing probabilistic algorithms and machine learning models tailored to the challenges of biological data in order to facilitate the study of genomic regulatory mechanisms through integrated analysis of single-cell multi-omics, with applications in precision medicine. My long-term career goal is to establish myself as a effective interdisciplinary researcher and mentor at the intersection of biomedical data science and machine learning.

Methodological interests: representation learning, manifold learning, optimal transport, geometric deep learning, Bayesian nonparametrics, dynamic neural networks, Bayesian variable selection, interpretability in ML/DL.

Application domain interests: regulatory genomics, precision medicine, single-cell sequencing, multi-modal data integration, perturbation biology, drug discovery, cellular reprogramming, cancer, neurodenegerative diseases.

EDUCATION

Brown University

Providence, RI

Ph.D. Computer Science, Computational Biology—GPA: 3.90/4.00

2023

Dissertation: "Probabilistic algorithms for integrated analysis of single-cell multi-omic data"

Advisors: Ritambhara Singh, Ph.D. (primary), Sorin Istrail, Ph.D.

M.Sc. Computer Science — (Concurrent to PhD) GPA: 4.0/4.0

Thesis Project: "Statistical and combinatorial methods for predicting gene expression and identifying eQTLs from haplotype sequences"

Advisor: Sorin Istrail, Ph.D.

Olin College of Engineering

Needham, MA

B.Sc. Engineering (with concentration in Bioengineering) — GPA: 3.67/4.00

2017

RESEARCH EXPERIENCE

Broad Institute of MIT and Harvard

July 2023 - Present

Eric and Wendy Schmidt Center Postdoctoral Fellow

Cambridge, MA

· Received a postdoctoral fellowship (up to three years) to establish an independent research agenda at the intersection of computational and biomedical sciences. Primarly working under the advisement of Dr. Caroline Uhler.

Brown University

Sept 2018 - May 2023

Graduate Research Assistant

Providence, RI

- · Developed probabilistic algorithms (based on optimal transport, and graph neural networks) for integrated analysis of single-cell multi-modal data, with applications in regulatory genomics. [Publications #4,#6,#7,#8].
- · Worked on (1) neural network interpretability methods with Bayesian variable selection for applications to genomewide association studies [Publication #5], and (2) combinatorial algorithms for gene expression prediction from haplotypes [Publication #3].

Microsoft Research

June 2022 - September 2022

Research Intern

Redmond, WA & Cambridge, MA (remote)

· Developed a novel machine learning method based on optimal transport with metric learning through graph neural networks to predict mechanism of action of chemical perturbations from single-cell datasets.

Microsoft Research

June 2020 - September 2020

Research Intern

Redmond, WA (remote)

· Implemented a Bayesian inference and machine learning pipeline on Microsoft Azure for disease risk prediction and clinical and genomic marker identification.

Massachusetts Institute of Technology

June 2017 - August 2018

Research Support Associate (Full Time)

Cambridge, MA

· Served as the lab manager in Gene-Wei Li lab. Investigated bacterial regulatory network rewiring [Publication #2]. Contributed to various quantitative biology projects to assist graduate students in the lab.

Olin College of Engineering

Undergraduate Research Assistant

Sep 2015 - May 2017 Needham, MA

- · Worked with Drs. Jean Huang and John Geddes on Lotka-Volterra-based dynamic modeling for bacterial communities undergoing environmental perturbations.
- · Designed an assistive software for blind navigation in Olin College Crowdsourcing and Machine Learning (OCCaML) Lab with Dr. Paul Ruvolo.

Daktari Diagnostics Student Engineer

Jan 2016 - Dec 2016

Cambridge, MA

· Implemeted an image analysis software to automate diagnosis for a novel rapid sickle-cell diagnostic device. Worked as a technical lead in a team of five engineering students.

AWARDS AND DISTINCTIONS

2023	Eric-Wendy Schmidt Postdoctoral Fellowship (Broad Institute of MIT and Harvard)
2023	Harvard/DFCI Data Science Postdoctoral Fellowship (turned down)
2022	Rising Stars in Electrical Engineering and Computer Science (by University of Texas at Austin)
2022	RECOMB Travel Fellowship
2020	Microsoft Research Ph.D. Fellowship Nominee (by Brown CCMB)
2020	ICML WCB Fellowship
2020	ICML WCB Best Poster Award
2018-2020	Brown Graduate Fellowship
2016	Meritorious Winner (Top 10%): COMAP MCM/ICM Contest in Mathematical Modeling
2015-2017	Olin Alumni Merit Scholarship (towards living expenses)
2013-2017	Sunlin Chou International Scholarship (50% tuition)
2013-2017	Olin Merit Scholarship (50% tuition)
2013	Honorable Mention, the 21^{st} Intl. Competition of First Step to Nobel Prize in Physics
	by the Polish Academy of Sciences
2013	First Place in Physics, the 22^{nd} MEF International Research Projects Contest (Turkiye)

PEER-REVIEWED PUBLICATIONS

- *Denotes equal contribution, <u>Mentees underlined</u>, [JP]: journal paper, [CP]: conference paper
 - 9. [CP] **P Demetci**, Q. H. Tran, I Redko, R Singh (2024). Breaking isometric ties and introducing priors in Gromov-Wasserstein distances. Proceedings of The 27th International Conference on Artificial Intelligence and Statistics (AISTATS 2024), to appear
 - Earlier formulation of this work appeared as extended abstracts under the title "Jointly aligning cells and features of single-cell multi-omics datasets with co-optimal transport." at:

 2022 NeurIPS Learning Meaningful Representations of Life (LMRL) Workshop and
 2022 Machine Learning in Computational Biology (MLCB) conference
 - 8. [CP] QH Tran, H Janati, N Courty, R Flamary, I Redko, P Demetci, R Singh. (2022). "Unbalanced CO-Optimal Transport". Proceedings of the AAAI Conference on Artificial Intelligence (AAAI 2023).
 - 7. [CP] P Demetci, R Santorella, B Sandstede, and R Singh (2022). "Unsupervised integration of single-cell multi-omics datasets with disparities in cell type representation". International Conference on Research in Computational Biology (RECOMB 2022). Springer Lecture Notes in Computer Science. 306:3-19.
 - Also appeared as an extended journal paper:
 [JP] P Demetci, R Santorella, M Chakravarthy, B Sandstede, W Stafford Noble, and R Singh (2022).
 "SCOTv2: Single-cell multi-omic alignment with disproportionate cell-type representation". Journal of Computational Biology. RECOMB 2022 issue.
 - 6. [CP] P Demetci*, R Santorella*, B Sandstede, W Stafford Noble, and R Singh (2021). "Gromov-Wasserstein optimal transport to align single-cell multi-omics data". International Conference on Research in Computational Molecular Biology (RECOMB 2021).
 - Also published as an extended journal paper: [JP] P Demetci, R Santorella, B Sandstede, W Stafford Noble, and R Singh (2021). "SCOT: Single-

- Cell multi-omic integration with Optimal Transport". Journal of Computational Biology. 29(1):3-18. RECOMB 2021 issue (extended paper)
- [WP] Also appeared as an extended abstract at the following workshop: the 37th International Comference on Machine Learning (ICML) Workshop on Computational Biology (2020).
- 5. [JP] P Demetci, W Cheng, G Darnell, X Zhou, S Ramachandran, and L Crawford (2021). Multi-scale genomic inference using biologically annotated neural networks PLOS Genetics. 17(8): e1009754.
- 4. [CP] R Singh, **P Demetci**, G Bonora, V Ramani, C Lee, H Fang, Z Duan, X Deng, J Shendure, C Disteche, and W Stafford Noble (2020). "Unsupervised manifold alignment for single-cell multi-omics data". ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (ACM-BCB 2020).
- 3. [JP] B Alpay*, **P Demetci***, S Istrail, and D Aguiar (2020). "Combinatorial and statistical prediction of gene expression from haplotype sequence". Bioinformatics. 36:Supplement-1: i194-i202.
- 2. [JP] D Parker*, **P Demetci***, G W Li (2019). "Rapid accumulation of motility-activating mutations in resting liquid culture of *Escherichia coli*". Journal of Bacteriology. 201(19):e00259-19.
- 1. [CP] P Demetci, C Nichols, Y V Zastavker, J D Stolk, A Dillon, M Gross (2016). "Externalization and internalization in the classroom: How do they emerge and why is it important?". IEEE Frontiers in Education Conference.

MANUSCRIPTS UNDER REVIEW

1. [JP] S Zeppilli, AO Gurrola, **P Demetci**, R Attey, N Nisim, T Kimchi, R Singh, MA Tosches, A Crombach, A Fleischmann. 2023. The mammalian olfactory cortex retains ancestral molecular signatures of cell type evolution. Under review at Nature Neuroscience.

KEYNOTES, CONFERENCES AND INVITED TALKS

Acc.R: "Acceptance Rate" for conferences, where work is accepted after peer review (listed only if known)

Keynotes:

"Enabling integrated analysis of single-cell multi-omics data with optimal transport"

2020 NeurIPS Workshop on Optimal Transport in Machine Learning (OTML): Invited Keynote

Contributed Talks and Posters at Conferences:

"Unbalanced CO-Optimal Transport"

2023 The AAAI Conference on Artificial Intelligence (AAAI): Poster Presentation (Acc. R: 19.6%)

"Joint alignment of cells and genomic features of single-cell multi-omic datasets with co-optimal transport"

2022 Machine Learning in Computational Biology (MLCB): Contributed Talk & Poster (Acc. R: 17%)

2022 CSHL Biological Data Science Meeting: Poster Presentation

2022 NeurIPS Learning Meaningful Representations of Life: Contributed Talk & Poster

"Unsupervised integration of single-cell multi-omics datasets with disparities in cell-type representation"

2022 RECOMB Proceedings: Contributed Talk (Acc. R.: 20%)

RECOMB: International Conference on Research in Computational Molecular Biology

2021 Machine Learning in Computational Biology (MLCB): Contributed Talk (Acc. R.: 25%)

"Gromov-Wasserstein Optimal Transport to Align Single-cell Multi-omics Data"

2021 RECOMB Proceedings: Contributed Talk (Acc. R: 19%)

2021 Machine Learning in Computational Biology (MLCB): Contributed Talk (Acc. R.: 15%)

2020 ICML Workshop on Computational Biology: Spotlight Talk & Poster (Acc. Rate: 21%)

2020 Intelligent Systems in Molecular Biology (ISMB): Contributed Talk & Poster (Acc. rate: 25%)

Invited Talks & Panels:

Title: "Foundation Models in Genomics"

2023 Broad Institute/Helmholtz Munich - ML in Genomics Collaboration Kick-off: Invited Panelist

Title: "Breaking isometric ties and introducing feature priors in Gromov-Wasserstein distance"

2023 OSU Topology, Geometry, and Data Analysis Seminar: Invited Talk

2023 Models, Inference and Algorithms Seminar @ Broad Institute: Invited Talk

Title: "Enabling integrated analysis of single-cell multi-omics data with optimal transport"

2022 SigmaXi iFoRE Conference: Invited Talk

("The Convergence of Data, Geometry, and Biology: Insights from the 'shape' of biological data" session)

2021 University of Connecticut Bioinformatics Seminar: Invited Seminar Talk

Title: "Biologically Annotated Neural Networks for Multi-Scale Genomic Discovery in GWAS"

2022 Stanford University (Kundaje Lab): Invited Seminar Talk

2021 Translational Bioinformatics Seminar, Brown University: Invited Seminar Talk

2019 Brown Center for Computation & Visualization Conference – CCV-Con: Invited Talk

Title: "Gromov-Wasserstein Optimal Transport to Align Single-cell Multi-omics Data"

2020 Workshop on Optimal Control, Optimal Transport & Data Science: Invited Poster at University of Minnesota – Institute for Mathematics and Its Applications (IMA)

2020 Brown Unconference on Computational Intelligence and Applications: Invited Talk

TECHNICAL SKILLS

n. R. Java	C++. N	MATLAB.	SQL
]	n, R, Java	n, R, Java, C++, I	n, R, Java, C++, MATLAB,

Linux, UNIX, slurm, High Performance Computing, Google Cloud, Azure Environments

Frameworks &

Machine Learning: PyTorch, PyTorch-Geometric (PyG), Tensorflow, Pyro, DGL, CUDA,

Tools Python OT (POT), Sklearn, SkImage, Cython Data Visualization: ggplot, seaborn, Bokeh Data Processing: Numpy, Pandas, SciPy, HDF5, AnnData, openCV, Pillow Other: Docker Bioinformatics: ScanPy, Seurat, Signac, Bioconductor, VCFtools, BEDtools, SAMtools,

PLINK, Cromwell, GATK, Picard PyMOL, Cell Profiler, Cytoscape, QIIME, VAMPS

PROFESSIONAL COMMUNITY SERVICE & MEMBERSHIPS

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2023		(Grants) External reviewer for European Commission SEP Grants
2023		(Journals) Reviewer for Journal of Machine Learning Research (JMLR), Bioinformatics, and
		PLOS Computational Biology journals
2023		(Conferences) Reviewer for Artificial Intelligence and Statistics (AISTATS) conference,
		NeurIPS Workshop on Optimal Transport in Machine Learning (NeurIPS-OTML), and
		Intelligent Systems in Molecular Biology (ISMB) conference
2020	- 2023	Program Committee member and reviewer for the Machine Learning in Computational Biology
		(MLCR 2020 2023) conformers

(MLCB 2020-2023) conferences

2020 - 2023 Sub-reviewer for ICML, NeurIPS, RECOMB conferences (on behalf of Dr. Ritambhara Singh)

Leadership:

Dec 2023 - Present Co-chair at Models, Inference and Algorithms Group (at Broad Institute)

Sep 2023 - Present Steering Committee Member at Models, Inference and Algorithms Group (at Broad Institute)

Mentorship Programs:

2022 - Present Alumnus	Mentor	for the	"Olin	College	Banter	Program"
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2020 - 2021 Mentor for the "Application Feedback Program for Under-represented Applicants"

2020 - 2023 Peer Mentor for International Graduate Students at Brown University

in the Computer Science Department at Brown University

Admissions:

2020 - 2021 Brown U. Computational Biology Ph.D. Program admissions committee member

Memberships:

2020 - Present Student Member at Society for Industrial and Applied Mathematics (SIAM)

AnitaB.org, and New England Statistical Society (NESS).

2018 - Present Student Member at International Society for Computational Biology (ISCB)

2018 - 2023 Member at Graduate Women in Science and Engineering (GWiSE) at Brown U.

TEACHING EXPERIENCE

Instructor at Brown University

• (Workshop) Introduction to High Performance and Parallel Computing (Fall 2022)

Organized and led a hands-on workshop series for training first year graduate students and T32 trainees on high performance and parallel computing.

Graduate Teaching Assistant at Brown University

• CSCI2820 Advanced Algorithms in Comp. Bio. & Medical Bioinformatics (Spring 2019 & 2021)

Guest-lectured a few times, held recitation sessions and office hours, wrote and graded assignments <u>Instructor</u>: Sorin Istrail, Ph.D.

Undergraduate Teaching Assistant at Olin College of Engineering

• SCI1240: Designing Better Drugs, with Laboratory (Fall 2015)

Assisted in the classroom and laboratory, graded assignments

Instructor: Joanne Pratt, Ph.D.

RESEARCH MENTORSHIP

Project: "Interpretable graph neural networks for cell-type prediction using single-cell multi-omic data" Mentees:

- Hossam Zaki (Class of 2022, Brown University, Senior Honors Thesis) → now MD-PhD student at Brown
- Ananya Pavuluri (Ph.D. student in Computational Biology, Brown University)
- Momoka Kobayashi (Brown University, Class of 2023, Biomedical Engineering and Computer Science)
- Chris Chae (Brown U. Class of 2023, Computer Science)

Project: "Optimal transport for identify cell-type similarities across mammalian and reptilian brain cortices" **Mentees:**

- Samantha Hong (Brown U. Class of 2023, Computational Biology)
- Manay Chakrayarthy (Brown U. Class of 2024, Computer Science and Economics)

Project: "Optimal transport applications in single-cell multi-omic analyses"

Mentees:

• Tuan M. Pham (Ph.D. student in Computational Biology, Brown University)

SOFTWARE

- AGW: <u>A</u>ugemented <u>G</u>romov <u>W</u>asserstein Optimal Transport (link: <u>github.com/pinardemetci/AGW</u>)

 Alternating optimization procedure for aligning both cells and features of unpaired single-cell multi-omic datasets
- SCOT: Single-Cell Optimal Transport (link: github.com/rsinghlab/SCOT)

 Multi-marginal Gromov-Wasserstein optimal transport for aligning unpaired single-cell multi-omic datasets
- SCOOTR: Single-cell CO-Optimal TRansport (link: github.com/rsinghlab/SCOOTR)

 Alternating optimization procedure for aligning both cells and features of unpaired single-cell multi-omic datasets
- BANN: Biologically Annotated Neural Networks (link: github.com/lcrawlab/BANNs)

 Three-layered feed-forward neural networks with spike-and-slab variables (for variable selection through sparsity)
 for SNP- and gene-level association finding with traits
- **HAPLEXD:** <u>HAPL</u>otype <u>EX</u>pression- <u>D</u>iscrete (link: github.com/pinardemetci/HAPLEX) Regularized suffix trees with spectral clustering for gene expression prediction from haplotype sequences