

Spencer Krieger

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POSITIONS HELD

August 2022 – present

Lane Fellow

Carnegie Mellon University, Computational Biology
Research Advisor: Jian Ma

June 2016 – July 2022

Research Associate

University of Arizona, Computer Science
Research Advisor: John Kececioglu

January 2014 – April 2016

Research Assistant

Brigham Young University, Chemistry and Biochemistry
Research Advisor: Roger Harrison

EDUCATION

July 2022

PhD in Computer Science

University of Arizona

May 2020

MS in Computer Science

University of Arizona

April 2016

BS in Biochemistry

Brigham Young University
Computer Science minor

RESEARCH INTERESTS

Algorithms in bioinformatics; in systems biology, pathway inference in cell-signaling and metabolic networks; in structural bioinformatics, protein structure prediction; in personalized medicine, drug design.

RESEARCH PROJECTS

Pathway inference in cell-signaling and metabolic networks (2017 – 2022, University of Arizona, Department of Computer Science) Modeling cell-signaling networks as directed hypergraphs, we find the shortest-hyperpath or factory with fewest hyperedges from a set of receptors to a set of transcription factors to assist biologists in researching disease pathways. Comprehensive experiments on over 5,000 instances from standard reaction network databases showed our shortest hyperpath heuristic found an optimal hyperpath on 99.5% of all instances. Our practical mixed-integer linear programming approach for finding optimal minimum-hyperedge factories incorporates negative regulation into pathway inference for the first time, and runs in a few seconds.

Protein structure prediction (2016 – 2022, University of Arizona, Department of Computer Science) Our fast and accurate protein secondary structure predictor computes maximum-likelihood physically-valid structure predictions and uses a variant of nearest-neighbor classification, which avoids using an expensive sequence-database homology search. We developed several novel ensemble approaches and our highest-accuracy hybrid approach that combines our method with an alternate method is over 8% more accurate than state-of-the-art tools on benchmark datasets and runs in half the time.

Approximation algorithms for Steiner tree variants (2018 – 2019, University of Arizona, Department of Computer Science) The vertex-weighted grade-of-service Steiner tree problem (VGSST) generalizes the vertex-weighted Steiner tree problem (VST). VST with T terminals is inapproximable within $2 \ln |T|$. Surprisingly, we developed an approximation algorithm for the seemingly harder VGSST with the same approximation factor ($2 \ln |T|$).

Target preconcentration and separation by ion chromatography (2014 – 2016, Brigham Young University, Department of Chemistry and Biochemistry) Using large macrocyclic molecules, we separated perhenate, a safe analog of pertechnetate, a common ingredient in cancer treatments, from ionic solutions.

CONFERENCE PAPERS

Spencer Krieger and John Kececioglu, "Computing optimal factories in metabolic networks with negative regulation." Proceedings of the 28th International Conference on *Intelligent Systems for Molecular Biology* (ISMB), *Bioinformatics* 38, 2022. doi.org/10.1093/bioinformatics/btac231

Spencer Krieger and John Kececioglu, "Fast approximate shortest hyperpaths for inferring pathways in cell signaling hypergraphs." Proceedings of the 21st International Workshop on *Algorithms in Bioinformatics* (WABI), 20, 1-20, 2021. doi.org/10.4230/LIPIcs.WABI.2021.20

Spencer Krieger and John Kececioglu, "Predicting protein secondary structure by an ensemble through feature-based accuracy estimation." Proceedings of the 11th ACM Conference on *Bioinformatics, Computational Biology, and Health Informatics* (ACM-BCB), 29, 1-10, 2020. doi.org/10.1145/3388440.3412425

Spencer Krieger and John Kececioglu, "Boosting the accuracy of protein secondary structure prediction through nearest neighbor search and method hybridization." Proceedings of the 28th International Conference on *Intelligent Systems for Molecular Biology* (ISMB), *Bioinformatics* 36, i317-i325, 2020. doi.org/10.1093/bioinformatics/btaa336

JOURNAL PAPERS

Spencer Krieger and John Kececioglu, "Heuristic shortest hyperpaths in cell signaling hypergraphs." *BMC Algorithms for Molecular Biology* 17, 12, 2022. doi.org/10.1186/s13015-022-00217-9

Wai Ning Chan, Jacob Warren, Spencer Krieger, Benjamin Vestal and Roger Harrison, "Separation and preconcentration of perrhenate from ionic solutions by ion exchange chromatography." *Journal of Chromatography A* 1631, 461588, 2020. doi.org/10.1016/j.chroma.2020.461588

OTHER PUBLICATIONS

Wim Cuypers, Handan Melike Dönertaş, Jasleen Grewal, Chase Donnelly, Arvind Singh Mer, Spencer Krieger and Bart Cuypers, "Highlights from the 16th International Society for Computational Biology Student Council Symposium 2020." *F1000Research*, 10(ISCB Comm J): 443, 2021. doi.org/10.12688/f1000research.53408.1

Faryad Darabi Sahneh, Alon Efrat, Stephen Kobourov, Spencer Krieger and Richard Spence, "Approximation algorithms for the vertex-weighted grade-of-service Steiner tree problem." 2018. arxiv.org/abs/1811.11700

PAPERS IN PREPARATION

Spencer Krieger and John Kececioglu, "Ensemble prediction of protein secondary structure through feature-based accuracy estimation." In preparation for submission to *PLOS Computational Biology*, 2022.

Spencer Krieger and John Kececioglu, "Inferring pathways in cell signaling networks via shortest hyperpaths in directed hypergraphs." In preparation, 2022.

SOFTWARE RELEASED

Mmunin: Integer-linear-programming-based cutting-plane algorithm for shortest source-sink hyperpaths, version 0.1, 2022. <http://mmunin.cs.arizona.edu>

Odinn: Optimal minimum-hyperedge factories in metabolic networks, version 0.1, 2022. <http://odinn.cs.arizona.edu>

Hhugin: Hyperpath heuristic for general shortest source-sink hyperpaths, version 1.0, 2022. <http://hhugin.cs.arizona.edu>

Nnessy: Nearest-neighbor-based prediction of protein secondary structure without searching for homology, version 1.0, 2020.

<http://nessy.cs.arizona.edu>

Ssylla: Protein secondary structure prediction by an ensemble leveraging accuracy estimation, version 0.1, 2020.

<http://ssylla.cs.arizona.edu>

INVITED TALKS

"Algorithmic inference of protein secondary structure and cell-signaling/metabolic pathways", Computational Biology Department, Carnegie Mellon University, Pittsburgh, May, 2022.

"Algorithmic inference of protein secondary structure and cell-signaling/metabolic pathways", University of California - San Diego, La Jolla, April, 2022.

"Algorithmic inference of protein secondary structure and cell-signaling/metabolic pathways", National Cancer Institute, NIH, Bethesda, April, 2022.

"Algorithms for pathway inference and protein secondary structure prediction", The Pennsylvania State University, State College, March, 2022.

"Shortest hyperpaths and their applications in cell-signaling networks", Department of Computer Science Colloquium, University of Montana, Missoula, February, 2022.

"Boosting the accuracy of protein secondary structure prediction through nearest neighbor search and method hybridization", Highlights talk in the 11th ACM Conference on *Bioinformatics, Computational Biology, and Health Informatics* (ACM-BCB), September, 2020.

CONFERENCE TALKS

"Computing optimal factories in metabolic networks with negative regulation", Proceedings talk in the 30th International Conference on *Intelligent Systems for Molecular Biology* (ISMB), July, 2022.

"Computing optimal factories in metabolic networks with negative regulation", Proceedings talk in the 18th *ISCB Student Council Symposium* (SCS), July, 2022.

"Fast approximate shortest hyperpaths for inferring pathways in cell signaling hypergraphs", Proceedings talk in the 21st International *Workshop on Algorithms in Bioinformatics* (WABI), August, 2021.

"Fast approximate shortest hyperpaths for inferring pathways in cell signaling hypergraphs", Proceedings talk in the 17th *ISCB Student Council Symposium* (SCS), July, 2021.

"Predicting protein secondary structure by an ensemble through feature-based accuracy estimation", Proceedings talk in the 11th ACM Conference on *Bioinformatics, Computational Biology, and Health Informatics* (ACM-BCB), September, 2020.

"Boosting the accuracy of protein secondary structure prediction through nearest neighbor search and method hybridization", Proceedings talk in the 28th International Conference on *Intelligent Systems for Molecular Biology* (ISMB), July, 2020.

"Predicting protein secondary structure through nearest neighbor search and method hybridization", Proceedings talk in the 16th *ISCB Student Council Symposium* (SCS), July, 2020. (*Best talk award*)

"Separation of pertechnetate from nuclear waste", *Spring Research Conference*, Brigham Young University, March, 2016.

"Selective preconcentration of perrhenate using ion chromatography", *Spring Research Conference*, Brigham Young University, March, 2015.

POSTERS

"Boosting the accuracy of protein secondary structure prediction through nearest neighbor search and method hybridization", The 28th International Conference on *Intelligent Systems for Molecular Biology* (ISMB), July, 2020

"Predicting protein secondary structure through nearest neighbor search and method hybridization", The 16th *ISCB Student Council Symposium* (SCS), July, 2020

"Separation of pertechnetate from nuclear waste", *Spring Research Conference*, Brigham Young University, March, 2016

"Selective preconcentration of perrhenate using ion chromatography", *Spring Research Conference*, Brigham Young University, March, 2015

AWARDS

Graduate Student Research Award, Department of Computer Science, University of Arizona, February 2022

Department Fellowship Award, Department of Computer Science, University of Arizona, May 2021

Galileo Circle Scholar, College of Science, University of Arizona, August 2020 – May 2021

Best talk for "Predicting protein secondary structure through nearest neighbor search and method hybridization", SCS 2020, July 10, 2020

Graduate Student Service Award, Department of Computer Science, University of Arizona, April, 2020

Galileo Circle Scholar, College of Science, University of Arizona, August 2018 – May 2019

Undergraduate Research Award, College of Physical and Mathematical Sciences, Brigham Young University, April 2014 – April 2016

PROFESSIONAL SERVICE

Web Committee Chair, Student Council, International Society for Computational Biology (ISCB), 2018 – Present

Web Chair, *ISCB Student Council Symposium* (SCS), International Society for Computational Biology (ISCB), 2020

Web Committee Member, Student Council, International Society for Computational Biology (ISCB), 2017 – 2018

DEPARTMENT AND UNIVERSITY SERVICE

Vice President (and Cofounder), Graduate Student Council, Department of Computer Science, University of Arizona, 2018 – 2020

Graduate Affairs Committee Member, Department of Computer Science, University of Arizona, 2018 – 2020

Faculty Recruiting Committee Graduate Student Liaison, Department of Computer Science, University of Arizona, 2019 – 2020

HOBBIES

I love playing board games (own over 250 board games, played over 450 games last year, on the board of local board game convention (Rincon)), racquet sports (undefeated 4.0 mixed pickleball league team, intramural doubles racquetball runner-up), and travelling (have been to 6 continents, 42 countries, always looking forward to the next adventure)