Rui Wang

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EDUCATION

Michigan State University — East Lansing, MI
Ph.D., Department of Mathematics — September 2017 - August 2022
Michigan State University — East Lansing, MI
Exchange student, Department of Mathematics — January 2016 - May 2016
Xi'an Jiaotong University — Xi'an, China
B.Sc. School of Mathematics and Statistics — September 2013 - June 2017

RESEARCH EXPERIENCE

New York University — New York, NY
Postdoctoral Fellow at Simons Center for Computational Physical Chemistry — December 2023 - Present
Michigan State University — East Lansing, MI
Visiting Assistant Professor, Department of Mathematics — August 2022 - October 2023
Michigan State University — East Lansing, MI
Research Assistant, Department of Mathematics — January 2019 - August 2022

RESEARCH INTERESTS

- **Genomics**
  DNA sequencing; single-nucleotide polymorphism (SNP) calling; UMAP-assisted clustering of large SARS-CoV-2 mutation datasets
- **Mathematical Modeling of Infectious Disease**
  Algebraic topology model TopNetmAb for 1) predicting the transmission and evolution trajectory of SARS-CoV-2; 2) predicting the mutation-induced impact for the SARS-CoV-2 vaccines and antibody therapies
- **Machine Learning**
  Convolution neural network(CNN); U-Net; Long Short Term Memory network (LSTM); Gated Recurrent Units (GRU); Multitask learning; Transfer learning; AutoEncoder; Generative Adversarial Network (GAN); Clustering
- **Computational Topology and Graphs**
  Persistent spectral graph; Persistent Laplacian; Persistent Path Laplacian; Geometric Graph Learning
- **Drug Discovery**
  Statistical tool-assisted generative model for generating highly druggable compounds that target to multiple proteins

SKILLS

- **Data Analysis**
  Data Acqusition, Data Storage, Data Cleaning, Date Pre-processing, High Performance Computing
- **Programming Languages**
  Python, BASH, JavaScript, MATLAB, C++
- **Machine Learning Libraries**
  NumPy, Pandas, Scipy, Scikit-learn, Biopython, Pytorch, Tensorflow, Keras, Matplotlib, Seaborn, Plotly
- **Molecular Visualization and Computer Graphics Software**
  VMD, PyMOL, ChimeraX, Blender, Illustrator

AWARDS AND SCHOLARSHIPS

- **SIAM Conference on the Life Sciences (LS22) Travel Award** — July 2022
  For a presentation at SIAM LS22 Conference in Pittsburgh, Pennsylvania, U.S.
- **College of Natural Science Completion Fellowship** — May 2022 - August 2022
  Michigan State University
- **Dr. Paul and Wilma Dressel Endowed Scholarship** — April 2022
  Michigan State University
- **Herbert T. Graham Scholarship Award** — April 2020
  Department of Mathematics, Michigan State University
- **SCMLLS Travel Support Fund** — October 2019
  For presenting a poster at SCMLLS conference at Texas Tech University

- **College of Natural Science Continuation Fellowship** May 2019 - August 2019
  Michigan State University

SOFTWARE PACKAGES DEVELOPED

- **HERMES**
  A package for simultaneous topological data analysis (persistent Betti numbers) and geometric data analysis (persistent eigenvalues).

WEBSITE DEVELOPED

- **Mutation Tracker**
  An interactive website for tracking SARS-CoV-2 mutations.
- **Mutation Analyzer**
  An interactive website for analyzing Spike protein RBD mutations.

PUBLICATIONS

(* co-first author)

28. **Wang, R.**, Feng, H., Wei, G., ChatGPT in Drug Discovery: A Case Study on Anticocaine Addiction Drug Development with Chatbots, *Journal of Chemical Information and Modeling*, (2023)
27. Cottrell, S., **Wang, R.**, Wei, G., PLPCA: Persistent Laplacian-Enhanced PCA for Microarray Data Analysis, *Journal of Chemical Information and Modeling*, (2023)
26. Feng, H., **Wang, R.**, Zhan, C., Wei, G., Multi-objective Molecular Optimization for Opioid Use Disorder Treatment Using Generative Network Complex, *Journal of Medicinal Chemistry*, (2023)
25. Hayat, H., **Wang, R.**, Sun, A., Mallett, C., Nigam, S., Bunn, D., Gjelaj, E., Talebloo, N., Alessio, A., Moore, A., Zinn, K., Wei, G., Fan, J., Wang, P., Automated segmentation and quantification of simultaneous PET/MRI for monitoring cell transplantation with Deep Learning, *iScience*, (2023)
24. Chen, J., Qiu, Y., **Wang, R.**, Wei, G., Persistent Laplacian projected Omicron BA. 4 and BA. 5 to become new dominating variants, *Computers in Biology and Medicine*, (2022)
23. **Wang, R.**, Wei, G., Persistent Path Laplacian, *Foundations of Data Science*, (2022)
22. Gao, K.*, **Wang, R.***, Chen, J., Cheng, L., Frishcosy, J., Huzumi, Y., Qiu, Y., Schluckbier, T., Wei, X., and Wei, G., Methodology-centered review of molecular modeling, simulation, and prediction of SARS-CoV-2, *Chemical Reviews*, 122(13), 11287-11368 (2022).
21. **Wang, R.**, Chen, J;, Hozumi, Y;, Yin, C;, and Wei, G., Emerging vaccine-breakthrough SARS-CoV-2 variants, *ACS Infectious Diseases*, 8(3), 546-556, (2022).
20. Chen, J., **Wang, R.**, Gilby, N.B., and Wei, G., Omicron (B.1.1.529): Infectivity, vaccine breakthrough, and antibody resistance, *Journal of Chemical Information and Modeling*, 62(2), 412-422, (2022).
19. **Wang, R.**, Chen, J., and Wei, G., Mechanisms of SARS-CoV-2 evolution revealing vaccine-resistant mutations in Europe and America, *The Journal of Physical Chemistry Letters*, 12, 11850-11857, (2021)
18. Chen, J., Gao, K., **Wang, R.**, and Wei, G., Revealing the threat of emerging SARS-CoV-2 mutations to antibody therapies, *Journal of Molecular Biology*, 433(18), (2021)
17. Gao, K., **Wang, R.**, Chen, J., Huang, F., and Wei, G., Perspectives on SARS-CoV-2 Main Protease Inhibitors, *Journal of Medicinal Chemistry*, 64(23), 16922-16955, (2021).
16. **Wang, R.**, Gao, K., Chen, J., and Wei, G., Vaccine-escape and fast-growing mutations in the United Kingdom, the United States, Singapore, Spain, South Africa, and other COVID-19-devastated countries, *Genomics*, 113(4), 2158-2170, (2021).
15. Chen, J.*, Gao, K.*, **Wang, R.***, and Wei, G., Prediction and mitigation of mutation threats to COVID-19 vaccines and antibody therapies, *Chemical Science*, 10.1039/D1SC01203G, (2021).
14. **Wang, R.**, Zhao, R., Ribando-Gros, Emily., Chen, J., Tong, Y., and Wei, G., HERMES: Persistent spectral graph software, *Foundations of Data Science*, 3(1), 67-97, (2021).
13. Jiang, J., **Wang, R.**, and Wei, G., GGL-Tox: Geometric graph learning for toxicity prediction, *Journal of Chemical Information and Modeling*, 61(4), (2021).
12. Hozumi, Y., **Wang, R.**, Yin, C., and Wei, G., UMAP-assisted K-means clustering of large-scale SARS-CoV-2 mutation datasets, *Computers in Biology and Medicine*, 131, p.104264, (2021).
11. Chen, J.*, Gao, K.*, **Wang, R.**, Duc Nguyen, and Wei, G., Review of COVID-19 antibody therapies, *Annual Review of Biophysics*, 50, 1-30 (2021). doi.org/10.1146/annurev-biophys-062920-063711
10. **Wang, R.**, Chen, J., Gao, K., Hozumi, Y., Yin, C., and Wei, G., Analysis of SARS-CoV-2 mutations in the United States suggests presence of four substrains and novel variants, *Communications Biology*, 4,228 (2021).
9. Chen, J., **Wang, R.**, and Wei, G., SARS-CoV-2 becoming more infectious as revealed by algebraic topology and deep learning. *Communications in Information and Systems* 21(1), 31-36 (2021).
8. **Wang, R.**, Chen, J., Hozumi, Y., Yin, C., and Wei, G., Decoding Asymptomatic COVID-19 infection and transmission, *The Journal of Physical Chemistry Letters*, 11, 10007-10015 (2020).

7. Nguyen, D. D., Gao, K., Chen, J., **Wang, R.**, and Wei, G., Unveiling the molecular mechanism of SARS-CoV-2 main protease inhibition from 137 crystal structures using algebraic topology and deep learning, *Chemical Sciences*, 11, 12036 - 12046 (2020).
6. **Wang, R.**, Hozumi, Y., Zheng, Y., Yin, C., and Wei, G., Host immune response driving SARS-CoV-2 evolution, *Viruses*, 12, 1095 (2020).
5. **Wang, R.**, Hozumi, Y., Yin, C., Wei, G., Mutations on COVID-19 diagnostic targets, *Genomics*, 112, 5204-5213 (2020).
4. Chen, J., **Wang, R.**, Wang, M., and Wei, G., Mutations strengthened SARS-CoV-2 infectivity, *Journal of Molecular Biology*, 432, 5212-5226 (2020).
3. **Wang, R.**, Hozumi, Y., Yin, C., and Wei, G., Decoding SARS-CoV-2 transmission, evolution and ramification on COVID-19 diagnosis, vaccine, and medicine, *Journal of Chemical Information and Modeling*, 60, 5853-5865 (2020).
2. Jiang, J., **Wang, R.**, Menglun Wang, Gao, K., Nguyen, D. D., and Wei, G., Boosting tree-assisted multitask deep learning for small scientific datasets. *Journal of Chemical Information and Modeling*, 60 (3), 1235-1244 (2020).
1. **Wang, R.**, Duc D Nguyen and Wei, G., Persistent spectral graph, *International Journal for Numerical Methods in Biomedical Engineering*, 36(9), e3376 (2020).

PREPRINTS

(* co-first author)

3. Hozumi, Y., **Wang, R.**, Wei, G., CCP: Correlated Clustering and Projection for Dimensionality Reduction, in revision, (2022)
2. Ribando, Emily., **Wang, R.**, Chen, J., Tong, Y., Wei, G., Graph and Hodge Laplacians: Similarity and Difference, arXiv, (2022)
1. Chen, J., **Wang, R.**, and Wei, G., Review of the mechanisms of SARS-CoV-2 evolution and transmission, (2021).

CONFERENCES AND PRESENTATIONS

- **Wang, R.**, Applications of Persistent Spectral Graphs in COVID-19, Applied Math Seminar at the George Washington University, Dec 09, 2022 (Invited Talk)
- **Wang, R.**, Applications of Persistent Spectral Graphs in COVID-19, Women in Scientific Computing on Complex Physical and Biological Systems at University of Florida, Oct 24 - Oct 26, 2022 (Invited Talk)
- **Wang, R.**, 2022 SIAM Great Lakes Section Annual Meeting (GLSIAM), Mini-Symposium titled "Mathematical Analysis of Bio-molecular Data", Sep 24, 2022 (Organizer)
- **Wang, R.**, 2022 Applied Topology in Frontier Sciences on Applied, Combinatorial and Toric Topology, Insititute for Mathematical Science (IMS), National University of Singapore, July 18th - 22th, 2022 (Invited Talk)
- **Wang, R.**, 2022 SIAM Conference on the Life Sciences (LS22), David L. Lawrence Convention Center, July 11th - 14th, 2022 (Invited Talk)
- **Wang, R.**, Evolution mechanism of SARS-CoV-2 evolution, Mathematical Molecular Bioscience and Biophysics (MMBB), webinar, October 25, 2021 (Invited Talk)
- **Wang, R.**, Emerging vaccine-breakthrough SARS-CoV-2 variants, Computational Biology Forum, Michigan State University, September 8, 2021 (Talk)
- **Wang, R.**, Persistent spectral graphs, Second Graduate Student Conference: Geometry and Topology meet Data Analysis and Machine Learning (GTDAML2021), July 31 - August 1, 2021 (Talk)
- **Wang, R.**, Persistent spectral graphs and COVID-19 related research, Computational Topology/Graph/Geometry Seminar, webinar, 2021 (Talk)
- **Wang, R.**, Persistent spectral graphs, Topological Data Analysis seminar, Michigan State University, 2021 (Talk)
- Roy, D.P., Martins, V.S., Huang, H., Egorov, A., Wei, G., **Wang, R.**, Machine learning PLANET high resolution training data for medium resolution land cover & disturbance mapping, NASA Earth Science Data System Working Group (ESDSWG) Meeting, Online, February 10 – 12, 2021
- **Wang, R.**, Graph neural network for protein-ligand predictions, Scientific Computing meets Machine Learning and Life Sciences Seminar, October 7 - 9, 2021 (Poster)

TEACHING EXPERIENCES AND MENTEES

- **Instructor**
  - MTH 234, Multivariable Calculus — Michigan State University
    Lecture Instructor — January 2023 - May 2023
  - MTH 234, Multivariable Calculus — Michigan State University
    Recitation Instructor — August 2022 - December 2022
- **Graduate Teaching Assistant**
  - MTH 994, Machine Learning and Deep Learning — Michigan State University
    Teaching Assistant — September 2019 - December 2021

- MTH 309, Linear Algebra — Michigan State University
  Grader — September 2018 - December 2018
- Math Learning Center (MLC) — Michigan State University
  Tutor — September 2017 - December 2018

- **Undergraduate Research Mentoring**
  - Mr. Sean Cottrell (Undergradute Student, MSU) — October 2022 - Present
  - Mr. Alexander Ma (High School Student) — February 2022 - October 2022
  - Mr. Te'Ahrian Z., Tyler (Undergraduate Student, Virginia Commonwealth University) — July 2022 - August 2022
  - Ms. Rana Elladki (Undergraduate Student, MSU) — January 2022 - May 2022
  - Ms. Jaclyn Frishcosy (Professorial Assistantship (PA) Program, MSU) — September 2019 - May 2021
  - Mr. Tom Schluckbier (Professorial Assistantship (PA) Program, MSU) — September 2019 - May 2021
  - Mr. Neel Sandeep Modi (Mathematics Exchange Program, MSU) — January 2019 - May 2019
  - Mr. Billy Pan (Mathematics Exchange Program, MSU) — January 2019 - May 2019
  - Mr. Che Yang (Mathematics Exchange Program, XJTU) — January 2019 - May 2019

PROFESSIONAL SERVICES

- **Journal Reviewer**
  - Journal of Chemical Information and Modeling
  - Computational and Mathematical Biophysics
  - International Journal for Numerical Methods in Biomedical Engineering

- **Reviewer Editor**
  - Frontiers in Molecular Biosciences
  - Frontiers in Applied Mathematics and Statistics
  - Frontiers in Endocrinology
  - Frontiers in Public Health
  - Frontiers in Neuroscience
  - Frontiers in Nutrition

MAJOR MEDIA COVERAGE

- Matt Davenport, MSU researchers use AI to stay ahead of COVID-19 and other diseases, MSUTODAY, 27 June 2022.
- Kim Ward, Using AI to fight Coronavirus, MSUTODAY, 15 Feb 2022.
- Susha Cheriyedath, SARS-CoV-2 Mutations Strengthen RBD-ACE2 Binding, Making the Virus More Infectious, News-Medical.Net, 23 May 2021.
- Sally Robertson, A Host of Mutations Could Compromise COVID-19 Vaccines and Antibody Therapies, News-Medical.Net, 14 Apr 2021.
- Merogenomics,Vaccines and virus evolution - COVID-19 mRNA vaccines update 25, Third party YouTube video about our work on SARS-CoV-2, 01 Jan 2021
- Matt Davenport, "Machine learning helps hunt for COVID-19 therapies", MSUTODAY, 27 Oct 2020.
- Molly Glick, "How COVID-19 Variants Could Outsmart Vaccines", Discovery Magazine, 29 Sep 2021.
- Adrian de Novato, Machine learning model finds SARS-CoV-2 growing more infectious, MSUTODAY, 19 Aug 2020.
- Sara Tidwell, MSU researchers find COVID growing more infectious, Michigan at high-risk, The State News, 10 July 2020.
- Duc D. Nguyen and Guo-Wei Wei, Math and AI-based Repositioning of Existing Drugs for COVID-19, SIAM NEWS, 01 May 2020.