# Rui Wang

(517)-348-5702 | wangru25@msu.edu | East Lansing, MI | Google Scholar

#### **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 - July 2017

#### **WORK EXPERIENCE**

Michigan State University East Lansing, MI Research Associate, Department of Mathematics August 2022 - Present Michigan State University East Lansing, MI Research Assistant, Department of Mathematics January 2019 - August 2022 **Michigan State University** East Lansing, MI Teaching Assistant, Department of Mathematics August 2017 - December 2018

#### **RESEARCH INTERESTS**

• Computational Topology and Graphs

Persistent spectral graph; Persistent Laplacian; Geometric Graph Learning

• 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

Genomics

DNA sequencing; single-nucleotide polymorphism (SNP) calling; UMAP-assisted clustering of large-scale SARS-CoV-2 mutation datasets

• 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); Reinforcement learning; Clustering

## AWARDS AND SCHOLARSHIPS

• SIAM Conference on the Life Sciences (LS22) Travel Award (\$650)

July 2022

For a presentation at SIAM LS22 Conference on July 11 - 14, 2022 in Pittsburgh, Pennsylvania, U.S.

• College of Natural Science Completion Fellowship (\$10,000) Michigan State University

May 2022 - August 2022

• Dr. Paul and Wilma Dressel Endowed Scholarship (\$1,975) Michigan State University

April 2022

• Herbert T. Graham Scholarship Award (\$2,000)

April 2020

Department of Mathematics, Michigan State University

October 2019

• SCMLLS Travel Support Fund (\$350)

For presenting a poster at Scientific Computing meets Machine Learning and Life Sciences conference at Texas Tech University

• College of Natural Science Continuation Fellowship (\$6,000) May 2019 - August 2019 Michigan State University

## **SOFTWARE PACKAGES DEVELOPED**

# HEMERS

A software 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.

#### **PROGRAMMING LANGUAGES**

• Python, BASH, JavaScript, MATLAB, C++, MATHEMATICS

#### MOLECULAR VISUALIZATION and COMPUTER GRAPHICS SOFTWARES

• VMD, PyMOL, ChimeraX, Blender, Illustrator

#### **PUBLICATIONS**

(\* co-first author)

- 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*, in press, (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)

- 6. 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, (2022)
- 5. Hozumi, Y., Wang, R., Wei, G., CCP: Correlated Clustering and Projection for Dimensionality Reduction, arXiv, (2022)
- 4. Wang, R., Wei, G., Persistent Path Laplacian, arXiv, (2022)
- 3. Chen, J., Qiu, Y., Wang, R., Wei, G., Persistent Laplacian projected Omicron BA. 4 and BA. 5 to become new dominating variants, arXiv, (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., 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 (Talk)
- Wang, R., 2022 SIAM Conference on the Life Sciences (LS22), David L. Lawrence Convention Center, July 11th 14th, 2022 (Talk)
- Wang, R., Evolution mechanism of SARS-CoV-2 evolution, Mathematical Molecular Bioscience and Biophysics (MMBB), webinar, October 25, 2021 (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

# • Graduate Teaching Assistant

- MTH 994, Machine Learning and Deep Learning Teaching Assistant
- MTH 309, Linear Algebra *Grader*
- Math Learning Center (MLC)

### • Undergraduate Research Mentoring

- Ms. Rana Elladki(Undergraduate Student, MSU)
- Ms. Jaclyn Frishcosy (Professorial Assistantship (PA) Program, MSU)
- Mr. Tom Schluckbier (Professorial Assistantship (PA) Program, MSU)
- Mr. Neel Sandeep Modi (Mathematics Exchange Program, MSU)
- Mr. Billy Pan (Mathematics Exchange Program, MSU)
- Mr. Che Yang (Mathematics Exchange Program, XJTU)

# PROFESSIONAL SERVICES

#### **Journal Reviewer**

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

MAJOR MEDIA COVERAGE

Michigan State University September 2019 - present Michigan State University September 2018 - December 2018 Michigan State University September 2017 - December 2018

> January 2022 - May 2022 September 2019 - May 2021 September 2019 - May 2021 January 2019 - May 2019 January 2019 - May 2019 January 2019 - May 2019

- 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.