Zhongyuan Zhao

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Education

Binghamton University(SUNY), Department of Mathematics and Statistics

Binghamton University(SUNY), Department of Mathematics and Statistics

Ph.D. Candidate in Mathematics and Statistics

Aug 2021 - Present

Binghamton, NY

Binghamton, NY

Aug 2021 – May 2023

Jilin, China

Sep 2016 - Jun 2020

Jilin University, School of Mathematics

Master of Arts in Mathematics

Bachelor of Science in Mathematics and Applied Mathematics

Technical Skills

Programming: Python, R, MATLAB

ML/DL Frameworks: PyTorch, scikit-learn, TensorFlow, Hugging Face Transformers

Publication & Poster Presentation Publication

- 1. B. Yi, S. Chen, M. A. Rahman, S. H. Bea, M. Bashar, Z. Zhao, T. Zhang, "A PBPK Model for Prediction of Apixaban and Rivaroxaban Secretion into Milk" (Submitted)
- 2. Z. Zhao, P. Zou, Y. Fang, T. Si, B. Yi, T. Zhang, "Machine Learning Approaches for Assessing Medication Transfer to Human Breast Milk: Estimating Milk/Plasma Drug Ratios" (Under review: Journal of Pharmacokinetics and Pharmacodynamics)
- 3. A. Stratigakis, D. Paty, P. Zou, Z. Zhao, Y. Li, and T. Zhang, "A regression approach for assessing large molecular drug concentration in breast milk," Reproduction and Breeding, vol. 3, no. 4, pp. 199-207, 2023.

Poster Presentation

1. "Machine Learning Approaches for Assessing Medication Transfer to Human Breast Milk: Estimating Milk/Plasma Drug Ratios", AAPS 2024 PharmSci 360, Salt Lake City, UT, Oct 2024

Research Experience

Fake News Detection Using BERT (In Progress)

07/2025 - Now

- Currently fine-tuning a BERT model (bert-base-uncased) on around 40k news headlines
- Task: binary classification (FAKE vs REAL) using Hugging Face Trainer API
- Focused on optimizing F1-score and integrating model explainability
- Tools Used: Python, Hugging Face Transformers, PyTorch

Predicting Human Bioavailability of Monoclonal Antibodies from Antibody Sequences

05/2025 - Now

- Planning to develop machine learning models (CNN, Transformer-based methods) to predict human bioavailability and pharmacokinetic parameters of subcutaneously administered monoclonal antibodies directly from antibody sequences
- Aim to computationally extract sequence-derived physicochemical and biophysical features (isoelectric point, hydrophobicity, aggregation propensity) for predictive modeling
- Will integrate non-human primate pharmacokinetic data to improve prediction accuracy
- · Tools to be used: Python, PyTorch, Biopython

Research On Qusi-Stationarity of the Shiryaev Recurrence in Exponential Case (Ph.D. Dissertation)

05/2023 - Now

- Find tight bounds for the quasi-stationary function and ADD(Average Delay of Detection) in Shiryaev Robert change point detection method which corresponds to the accuracy of change point detection
- Find the boundary for the control parameter in Shiryaev Robert change point detection
- Prove the optimality of the Shiryaev-Robert Procedure
- Do simulation of quasi-stationary function, ADD, and control parameter
- · Tools Used: Matlab, Python

· Paper under prepare

Build a PBPK Model for Prediction of Apixaban and Rivaroxaban Secretion into Milk

05/2023 - 10/2024

- Led statistical modeling and data analysis for a whole-body PBPK lactation model to predict drug secretion of apixaban and rivaroxaban into breast milk
- Validated model predictions using clinical concentration—time profiles and calculated accuracy metrics (Tmax, Cmax, AUC, M/P ratio), achieving <10% prediction error
- · Tools Used: R
- · Paper [1] Submitted

ML Model to Predict Drug Secretion Ratios (M/P) using Clinical Features

08/2023 - 08/2024

- Using PCA to visualize the data focus on MP ratio distribution(Milk/Plasma) behavior
- Build KNN(K-Nearest Neighborhood), SVM(Support Vector Machine), RF(Random Forest), and NN(Neural Network) models to do classification for MP ratio
- Using a grid search combined with cross-validation to find the best tuning parameters for each method, combine with different attempts like normalizing the data, improve the average accuracy by around 20%
- Visualize machine learning models and compare by accuracy
- Tools Used: Python
- · Paper [2] under review

Multivariate Regression for Large Molecule Drug Modeling

05/2023 - 10/2023

- Developed a multivariate regression model to predict milk-to-plasma (M/P) drug concentration ratios of monoclonal antibodies (mAbs) using physicochemical and pharmacokinetic properties
- Conducted data curation from DrugBank, PubMed, and Antibody Society databases for 11 mAbs with clinical milk concentration data
- Applied the final model to predict M/P ratios for 79 approved therapeutic antibodies, supporting risk assessment of biologic drugs during lactation
- · Tools Used: R
- · Paper [3] published

Implementation of improved Fused Lasso Image Denoising

08/2022 - 12/2022

- Implemented the 2D Fused Lasso algorithm for grayscale image denoising via coordinate descent and group fusion strategy
- · Designed and optimized a custom objective function including MSE, L1, and total variation penalties
- Simulated and tested on various noise patterns (Gaussian, uniform, structured) to evaluate denoising performance
- Tool Used: R

Work Experience

Research Assistant, Binghamton University - Binghamton, NY

05/2023 - Now

- Research on machine learning and AI algorithms combined with clinical data from breast milk to predict PK parameters
- · Building PBPK model through Python and R
- · Data visualization and analysis to support other projects

Calculus Instructor & Statistics TA, Binghamton University - Binghamton, NY

08/2023 - Now

- Instructor of calculus(Math 224, 225, 226, 227) and teaching assistant of Elementary Statistics(Math 147)
- · Holding office hours

Research Assistant, Nankai University - Tianjin, China

06/2019 - 08/2019

- Research on Low-level Vision denoising Problems using Dual Convolutional Neural Networks
- Using MATLAB to apply Dual Convolutional Neural Networks to do image deraining