

# Isaac Rankin

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## Research Interests

Variational Inference, Bayesian Optimization, Uncertainty Quantification, Ensemble Methods, Markov Chain Monte Carlo, Drug Discovery, Simulation-Based Inference, Bioinformatics, *In Silico* Pharmaceutical Development, Robust Statistics, Generative Models, Audio Generation, Design of Experiments

## Education

2025 – 2029

### **Ph.D. in Statistics, University of British Columbia**

Leadership: Co-President of the Statistics Graduate Student Association (SGSA)

Supervisor: Dr. Geoff Pleiss

2023 – 2024

### **M.Sc. in Statistical Sciences (Distinction), University of Oxford**

Dissertation: *Conditional Diffusion Models for Structure-Based Drug Design with Considerations for Physical Plausibility and a Celecoxib Rediscovery Case Study*

Key Achievement: improved the sensitivity and accuracy of the Python package Pose-Busters in detecting physically implausible molecules.

Leadership: Sports & Gym Officer, Green Templeton College. MSc cohort EDI Representative, Department of Statistics.

Supervisor: Dr. Garrett M. Morris

2018 – 2023

### **B.Sc. in Mathematics and Statistics (Distinction), University of Victoria**

97.52% overall course average, GPA: 9.00/9.00

Supervisor: Dr. Julie Zhou

## Honours and Awards

- 2025–2029 Four-Year Doctoral Fellowship (University of British Columbia) (\$72,800)
- 2025 Four-Year Fellowships Tuition Award (University of British Columbia) (\$3,750)
- 2025 President's Academic Excellence Initiative PhD Award (University of British Columbia) (\$840)
- 2025 Entrance Scholarship (University of British Columbia) (\$8,500)
- 2023 Third Prize, Undergraduate Poster Presentation Competition, 11th Annual Canadian Statistics Student Conference
- 2023 Undergraduate Student Research Award (Natural Sciences and Engineering Research Council of Canada administered at the University of Victoria) (\$6,000)
- 2023 Constance Van Eeden Scholarship (Declined) (University of British Columbia) (\$3,000)
- 2023 Departmental Entrance Scholarship (Declined) (University of British Columbia) (\$2,000)
- 2020–2023 Dean's List (University of Victoria)
- 2022 Leeder Family Memorial Award in Mathematics (University of Victoria) (\$3,461)
- 2022 Columbia Coast Mission Scholarship (University of Victoria) (\$1,166)
- 2022 Undergraduate Student Research Award (Natural Sciences and Engineering Research Council of Canada administered at the University of Victoria) (\$6,000)
- 2021 President's Scholarship (University of Victoria) (\$1,498)
- 2021 Leeder Family Memorial Award in Mathematics (University of Victoria) (\$2,502)
- 2020 Transfer Scholarship (University of Victoria) (\$2,500)
- 2018–2020 President's Honour Roll (Simon Fraser University)
- 2018–2020 Dean's Honour Roll (Simon Fraser University)
- 2020 Undergraduate Open Scholarship (Simon Fraser University) (\$2,500)
- 2020 Alumni Scholarship (Simon Fraser University) (\$1,250)
- 2019 Alumni Scholarship (Simon Fraser University) (\$1,250)
- 2015–2018 Celebration of Excellence in Mathematics (Mark R. Isfeld Secondary)
- 2016 Celebration of Excellence in Woodwork (Mark R. Isfeld)

## Publications and Works

- 2025 **RAD-Median and trimmed mean, new multivariate generalizations of the classical estimators**  
Rankin, I. and Zhou, J.  
*Communications in Statistics - Simulation and Computation, pp. 1–19.*
- 2024 **Conditional Diffusion Models for Structure-Based Drug Design with Considerations for Physical Plausibility and a Celecoxib Rediscovery Case Study**  
Rankin, I.  
*Master of Science in Statistical Science Dissertation, University of Oxford*
- 2023 **Conference Poster - Bayesian and maximin A-optimal designs for spline regression models with unknown knots**  
Rankin, I. and Zhou, J.  
*The Eleventh Annual Canadian Statistics Student Conference.*
- 2023 **Bayesian and maximin A-optimal designs for spline regression models with unknown knots**  
Rankin, I. and Zhou, J.  
*Statistical Papers, Volume 65, pp. 2011–2032.*

## Research Experience

- Summer 2024 **Oxford MSc Dissertation** – Oxford, UK  
Supervisors: Professor Garrett M. Morris, Doctoral Candidate Martin Buttenschoen.  
Worked with two conditional diffusion models for structure-based drug design. Improved the sensitivity of the Python package *PoseBusters* for detecting physically implausible molecules (*PoseBusters* was used in the *AlphaFold 3 Nature* manuscript).
- Summer 2023 **NSERC USRA administered by UVic (Researcher)** – Victoria, BC  
Supervisor: Professor Julie Zhou.  
Defined and named a novel robust multivariate estimator of central location, conducted simulations to assess various estimators, and wrote a research paper for publication. Researched advanced methods for multivariate time series analysis and forecasted real estate markets with high accuracy, leveraging data from multiple sources.
- Spring 2023 **University of Victoria (Research Assistant)** – Victoria, BC  
Supervisor: Professor Julie Zhou.  
Developed and implemented a novel clustering algorithm. Contributed to writing research papers and corresponding with peer-reviewers.

Summer 2022 **NSERC USRA administered by UVic (Researcher)** – Victoria, BC  
Supervisor: Professor Julie Zhou.  
Researched optimal experimental designs for spline regression models. Implemented an optimization algorithm in MATLAB. Wrote and published a research paper on the results which led to an award-winning poster at the Canadian Statistics Student Conference.

## Teaching experience

Fall 2025 **Teaching assistant, STAT 251: Elementary Statistics (University of British Columbia)** – Vancouver, BC  
Taught a weekly lab of 41 students. Responsibilities include marking, monitoring the discussion board Piazza, exam invigilation, and holding office hours. Course topics include probability, discrete and continuous random variables, joint probability distributions, estimation, hypothesis testing, regression, and analysis of variance.

## Industry experience

November 2024 – Present **ALVITUR Analytics and Data Solutions (Founder)** – Remote  
Providing client-tailored statistical consulting and data solutions.  
FFAW-Unifor: Developed mapping software, designed a quota allocation algorithm for the snow crab fishery, automated reporting pipelines, analyzed a bycatch mitigation experiment, and analyzed vessel satellite data to investigate the Atlantic cod collapse. Created a novel light-intensity proxy for redfish catch. This work is leading to three co-authored manuscripts (cod collapse, bycatch mitigation, and redfish proxy) and shows how insights from data can help shape policy on sustainable fishing practices.

Devinci Cycles: Web-scraped inventory data of retailers and competitor brands to improve cash flow by predicting the optimal arrival and quantity of SKUs.

Chinook Business Advisory: Building a suite of computational tools to automate company valuations and feasibility analyses, streamlining mergers and acquisitions processes.

Fall 2024 **Outlier AI (Freelance AI Mathematics Domain Expertise Developer)** – Remote  
Applied various forms of supervised and reinforcement learning to improve AI models in mathematics, increasing model accuracy across analytic tasks.

June 2024 **Lightricity Ltd. (Technology Prototype Development Intern)** – Oxford, UK  
Developed Python algorithms to optimize photovoltaic cell test equipment. Delivered user-friendly analytic tools for cross-functional teams, accelerating product development and improving decision-making efficiency. Achieved a 43% improvement in light uniformity by reducing variance in the illumination distribution, guiding the development of next-generation products.

2014 – 2023 **Mountain City Cycle (Service and Operations Associate)** – Courtenay, BC  
Led store operations and supervised a team of 10 during periods of vacation coverage. Improved operational efficiencies by managing inventory and reducing overhead expenses. Delivered expert customer service by handling sales, providing repair quotes, and performing bicycle maintenance as a certified mechanic.

## Professional memberships

- 2025–Present **Vector Institute**  
As a PhD student of Dr. Geoff Pleiss, who holds a cross-appointment at the Vector Institute as a Faculty Member, the Vector Institute has invited me to join their machine learning community.
- 2023 **Statistical Society of Canada**  
Attended the Canadian Statistics Conference and the Canadian Statistics Student Conference at Carleton University in May 2023.

## Volunteer activities

- Summer 2025 **Statistician (Cancer Exercise & Physiotherapy Lab – UBC)**  
Contributed to the ACE, BE-FIT, and ECHO studies by cleaning clinical trial data, constructing tables, performing a social network analysis, modelling patient outcomes, and interpreting model results. These analyses support the studies to develop cancer rehabilitation programs, ultimately to improve the well-being of cancer survivors. Though less important than contributing to life-altering programs, research-wise, these analyses will result in two co-authorships (ACE and ECHO) and one acknowledgment (BE-FIT).
- Spring 2025 **Statistician (Raincoast Conservation Foundation)**  
Investigated eye patch ratio as a biomarker of orca whale health and analyzed maternal and grand-maternal effects on survival in the northern resident population. This project will contribute to a better understanding of the effects that impact orca survival and will help shape conservation policy. This study is in the works and will result in a co-authored publication.
- Spring 2025 **Ride Leader (Mark R. Isfeld Secondary)**  
Mentored high school athletes on the mountain bike team, coaching leadership, discipline, and teamwork while preparing for the provincial championships.
- 2012–Present **Trail Maintenance and Event Volunteer (United Riders of Cumberland)**  
Contribute regularly to trail maintenance days. Volunteer for course marshalling and timing for community bike races.

## Technical skills

### **Programming:**

R, Python, MATLAB, Stan, SQL, Excel, Linux OS

### **Machine Learning and Data Analysis:**

Tidyverse, PyTorch, TensorFlow, Keras, scikit-learn, XGBoost

### **Other:**

LaTeX, Git, French (12 years of immersion; Dual Dogwood Diploma)

## Other interests

Road Cycling, Gravel Riding, Mountain Biking, Vintage Car Restoration, Disc Golf, Surfing, Cross Country Skiing, Artisan Coffee, Baking, Snowboarding