# Charles C. Margossian

#### Education

- 2017–2022 Ph.D. Statistics, Columbia University, New York, NY.
  - Thesis: Modernizing Markov chains Monte Carlo for scientific and Bayesian modeling
  - o Advisor: Andrew Gelman
  - o Dissertation Committee: Aki Vehtari, Matthew Hoffman, Sumit Mukherjee, David Blei
- 2011–2015 **B.Sci. Physics**, Yale University, New Haven, CT.
- 2009–2011 Baccalauréat Scientifique, Ecole Jeannine Manuel (High school), Paris, France.

#### Research Interest

Bayesian modeling; Bayesian workflow; Hierarchical models; ODE-based models; Markov chain Monte Carlo; Variational Inference; Integrated Laplace approximations; Automatic differentiation; Pharmacometrics; Epidemiology; Statistical Physics; Probabilistic programming (Stan, Torsten, TensorFlow Probability)

### Appointments

- 2022—present **Research Fellow**, Flatiron Institute, Center for Computational Mathematics, Simons Foundation, New York, NY.
- Summer 2021 Research Intern, Google Research, Bayesflow team, New York, NY.
- Summer 2019 Visiting Doctoral Student, Aalto University, Department of Computer Science, Probabilistic Machine Learning group, Espoo, Finland.
  - 2015–2017 **Visiting Scientist**, Metrum Research Group LLC, Pharmacometrics, Tariffville, CT and Cambridge, MA.
  - 2013–2015 Research Assistant, Yale University, Department of Astronomy, New Haven, CT.
- Summer 2014 Patent Law, Technical Specialist, Leinweber & Zimmermann, Munich, Germany.

### Academic services

2023 - present Stan Governing Body.

2016 - present Core developer, Stan development team.

2019 - present **Reviewer**, Computational Statistics (2022), Nature (2021), AISTATS (2021), Methods in ecology (2021), Journal of data science (2021), NeurIPS (2020), Journal of pharmacokinetics and pharmacodynamics (2019).

### Skills

Progamming: R, Python, C++, Stan, TensorFlow Probability, LATEX, GitHub Languages: English, French, German

# Papers as project lead

This section includes papers, first-authored by myself or a student I directly supervised.
\*: Supervised student

- [1] Charles C Margossian and Lawrence K Saul. The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference. *Preprint.* arXiv:2302.09163, February 2023.
- [2] Charles C Margossian, Yi Zhang, and William R Gillespie. Flexible and efficient Bayesian pharmacometrics modeling using Stan and Torsten, Part I. CPT: Pharmacometrics & Systems Pharmacology, 11:1151 1169, April 2022.
- [3] Charles C Margossian, Matthew D Hoffman, Pavel Sountsov, Lionel Riou-Durand, Aki Vehtari, and Andrew Gelman. Nested  $\widehat{R}$ : Assessing the convergence of Markov chain Monte Carlo when running many short chains. *Preprint. arXiv:2110.13017.*, December 2022.
- [4] **Charles C Margossian** and Michael Betancourt. Efficient Automatic Differentiation of Implicit Functions. *Preprint. arXiv:2112.14217.*, March 2022.
- [5] **Charles C Margossian** and Sumit Mukherjee. Simulating Ising and Potts models at critical and cold temperatures using auxiliary Gaussian variables. *Preprint. arXiv:2110.10801.*, October 2021.
- [6] Léo Grinsztajn\*, Elizaveta Semenova, Charles C Margossian, and Julien Riou. Bayesian workflow for disease transmission modeling in Stan. Statistics in Medicine, 40:6209 – 6234, September 2021.
- [7] Charles C Margossian, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Hamiltonian Monte Carlo using an adjoint-differentiated Laplace approximation: Bayesian inference for latent Gaussian models and beyond. Advances in Neural Information Processing Systems (NeurIPS), 33:9086 9097, October 2020.
- [8] Charles C Margossian. A Review of automatic differentiation and its efficient implementation. Awarded "WIRES Top article in 2022", Wiley interdisciplinary reviews: data mining and knowledge discovery, 9, March 2019.

# Papers as contributor

- [1] Lionel Riou-Durand, Pavel Sountsov, Jure Vogrinc, **Charles C Margossian**, and Sam Power. Adaptive Tuning for Metropolis Adjusted Langevin Trajectories. *Proceedings of the 25th International Conference on Artificial Intelligence and Statistics (AISTATS)*, (to appear) 2023.
- [2] Philip Greengard, Jeremy Hoskins, **Charles C Margossian**, Jonah Gabry, Andrew Gelman, and Aki Vehtari. Fast methods for posterior inference of two-group normal-normal models. *Bayesian Analysis*, Advanced Publication:1 19, August 2022.

- [3] Anthony Hauser, Michel J Counotte, **Charles C Margossian**, Garyfallos Konstantinoudis, Nicola Low, Christian L Althaus, and Julien Riou. Estimation of SARS-CoV-2 mortality during the early stages of an epidemic: a modeling study in Hubei, China and six regions in Europe. *PLOS Medicine*, 17, July 2020.
- [4] Andrew Gelman, Aki Vehtari, Daniel Simpson, **Charles C Margossian**, Bob Carpenter, Yuling Yao, Lauren Kennedy, Jonah Gabry, Paul-Christian Bürkner, and Martin Modrák. Bayesian Workflow. *Preprint. arXiv:2011.01808*, October 2020.
- [5] Michael Betancourt, Charles C Margossian, and Vianey Leos-Barajas. The Discrete Adjoint Method: Efficient Derivatives for Functions of Discrete Sequences. Preprint. arXiv:2002.00326, February 2020.
- [6] Joseph R Schmitt, Eric Agol, Katherine M Deck, Leslie A Rogers, J Zachary Gazak, Debra A Fischer, Ji Wang, Matthew J Holman, Kian J Jek, Charles Margossian, Mark R Omohundor, Troy Winarski, John M Brewer, Matthew J Giguere, Chris Lintott, Stuart Lynn, Michael Parrish, Kevin Schawinski, Megan E Schwamb, Robert Simpson, and Arfon M Smith. Planet Hunters. VII. Discovery of a new low-mass, low-density planet (PH3 C) orbiting KEPLER-289 with mass measurements of two additional Planets (PH3 B and D). Astrophysical Journal, 795(2), October 2014.

# Conference notebooks and posters

- \*: Supervised student
- [1] **Charles C Margossian**, Matthew D Hoffman, Pavel Sountsov, Lionel Riou-Durand, Aki Vehtari, and Andrew Gelman. Assessing the convergence of Markov chains Monte Carlo when running many chains. In *BayesComp*, March 2023.
- [2] Stanislas du Ché\* and **Charles C Margossian**. Parallelization for Markov chains Monte Carlo with heterogeneous runtimes. In *BayesComp*, March 2023.
- [3] Charles C Margossian, Lu Zhang, Sebastian Weber, and Andrew Gelman. Solving ODEs in a Bayesian context: challenges and opportunities. In *Population Approach Group in Europe (PAGE)* 29, September 2021.
- [4] Aurélien Marc, Marion Kerioui, **Charles Margossian**, Julie Bertrand, Pauline Maisonnasse, Yoan Aldon, Rogier W Sanders, Marit Van Gils, Roger Le Grand, and Jérémie Guedj. Developping a model of SARS-CoV-2 viral dynamics under monoclonal antibody treatment. In *Population Approach Group in Europe (PAGE)* 29, September 2021.
- [5] Johann D Gaebler\* and **Charles C Margossian**. Propagating Derivatives through Implicit Functions in Reverse Mode Autodiff. In *Student Presentation*, *Stanford Institute for Computational & Mathematical Engineering*, May 2021.
- [6] **Charles C Margossian**, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Approximate Bayesian inference for latent Gaussian models in Stan. In *StanCon 2020*, August 2020.
- [7] **Charles C Margossian** and Andrew Gelman. Bayesian model of planetary motion: exploring ideas for a modeling workflow when dealing with ordinary differential equations and multimodality. In *Stan Case Studies*, volume 7, October 2020.

- [8] Charles C Margossian. Computing Steady States with Stan's Nonlinear Algebraic Solver. In StanCon 2018, January 2018.
- [9] Charles C Margossian and William R Gillespie. Gaining Efficiency by Combining Analytical and Numerical Methods to Solve ODEs: Implementation in Stan and Application to Bayesian PK/PD. *Journal of Pharmacokinetics and Pharmacodynamics*, 44, October 2017.
- [10] **Charles C Margossian** and William R Gillespie. Differential Equation Based Models in Stan. In *StanCon 2017*, January 2017.
- [11] Charles C Margossian and William R Gillespie. Stan Functions for Pharmacometrics Modeling. *Journal of Pharmacokinetics and Pharmacodynamics*, 43, October 2016.

#### Software

Core developer, Stan: a probabilistic programming language, mc-stan.org.

Co-creator, Torsten: an extension of Stan for Bayesian pharmacometrics modeling, GitHub link.

**Contributor**, mrgSolve: Simulation from ODE-Based Population PK/PD and System Pharmacology Models, GitHub link.

# Awards and recognitions

- 2022 WIRES Top Article, For A Review of Automatic Differentiation and its Efficient Implementation, which was amongst the top 10 most cited articles in the 2021 Journal Citation Report for WIRES, Data Mining and Knowledge Discovery.
- 2022 Minghui Yu Teaching Assistant Award, Department of Statistics, Columbia University, Awarded by the Director of Graduated Studies based on student feedback.
- 2022 **AISTATS Top Reviewer**, The top reviewers were selected based on the feedback received from the Area Chairs and comprise the top-10% of AISTATS reviewers.
- 2017 Dean's Fellowship, Department of Statistics, Columbia University, 5 years funding for PhD degree.
- 2010 Yale Book Award, For "character and intellectual promise".

# Supervised research projects

- Stanislas Du Ché (master student), Spring 2022
   Project: Parallelization for Markov chains Monte Carlo with heterogeneous runtimes
- Johann Gaebler (PhD student), Fall 2020
   Project: Propagating Derivatives through implicit functions in reverse mode automatic differentiation
- Léo Grinsztajn (master student), Summer 2020
   Project: Bayesian Workflow for disease transmission models
- Hyunjee Moon (undergraduate student), Summer 2020
   Project: Simulation-based Calibration for the embedded Laplace approximation

# Teaching experience (selected)

- 2019 2023 **Lecturer**, Probability and Bayes, lecture for PHC 506: Biometry in Pharmaceutics, University of Buffalo, School of Pharmacy, Buffalo, NY.
- 2019 2023 **Instructor**, Building, fitting, and criticizing Bayesian PK/PD models, (one day workshop), University of Buffalo, School of Pharmacy, Buffalo, NY.
- 2019, 2020 **Instructor**, Stan for the people: two days introductory workshop on Bayesian modeling, (two days workshop), McGill University, Montreal, Canada.
- August 2019 **Co-instructor**, Population and ODE-based models using Stan and Torsten, (two days workshop), Stan Conference 2019, Cambridge, UK.
- January 2018 Instructor, How to Develop for the Stan C++ Core Language, Stan Conference 2018, Pacific Grove, CA.
  - April 2017 **Invited Lecturer**, Introduction to Bayesian Data Analysis with Stan, Harvard University, STAT 220: Bayesian Statistics, Cambridge, MA.
  - 2021, 2022 **Teacher Assistant**, Applied Statistics II, STAT 6102 (PhD level), Columbia University, New York, NY.
  - 2019, 2020 **Teacher Assistant**, Foundation of Graphical Models, STAT 6701 (PhD level), Columbia University, New York, NY.
  - Spring 2019 **Teacher Assistant**, Statistical inference, STAT 5204 (Master level), Columbia University. New York, NY
    - Fall 2018 **Teacher Assistant**, Statistical Computing and Introduction to Data Science (Undergrad level), STAT 4206, Columbia University.

      New York, NY
  - September Teacher Assistant, Stan for Physics, Massachusetts Institute of Technology, Cambridge, 2017 MA
  - June 2017 **Teacher Assistant**, Getting Started with Bayesian PKPD Modeling using Stan and Torsten, Population Approach Group in Europe 26, Budapest, Hungary.

# Presentations (selected)

- October 2022 Solving ODEs in a Bayesian model, Flatiron-Wide Algorithms and Mathematics  $(F_{\omega}(\alpha + m)!)$ , New York, NY.
  - July 2022 Nested  $\hat{R}$ : Assessing convergence for Markov chains Monte Carlo when running many short chains, Center for Research in Economics and Statistics (CREST), Institut Polytechnique de Paris.
  - March 2021 Bayesian inference for latent Gaussian models: MCMC, approximate methods, and hybrids, Minghui Yu memorial conference, Columbia University.
  - November Developing a Bayesian modeling workflow for population PBPK, American Con-2020 ference on Pharmacomertrics, virtual.
- August 2020 Approximate Bayesian inference for latent Gaussian models in Stan, Stan Conference 2020, virtual.
  - June 2020 **Developing a Bayesian workflow to model the Covid-19 outbreak**, 12<sup>th</sup> Covid-19 symposium, Columbia University, New York, NY.

- April 2020 Laplace approximation for speeding up the computation of multilevel models, MRP conference, Columbia University, New York, NY.
- March 2020 Building a probabilistic programming language to diagnose our inference, Special seminar, University of Buffalo, School of Pharmacy.
  - July 2018 Understanding automatic differentiation to improve performance, Stan for Pharmacometrics Day 2018, Université Paris Diderot, School of Medicine, Paris, France.
- January 2018 Computing steady states with Stan's nonlinear algebraic solver, Stan Conference 2018, Pacific Grove, CA.
  - June 2017 **L'Avenir de Stan en pharmacométrie**, Université Paris Diderot, School of Medicine, Paris, France.
- January 2017 **Differential equations based models in Stan**, Stan Conference, Columbia University, New York, NY.
  - November Differential equations based models in Stan, Stan Meetup in Boston, Harvard Uni-2016 versity, Cambridge, MA.
  - February Practice (and malpractices!) of Bayesian analysis, Metrum Journal Minute, Tarif-2016 fville, CT.
  - March 2015 How stars and planets Interact: testing the effects of close-in giant planets on stellar magnetic activity, Davenport Mellon Forum, Yale University, New Haven, CT.

    Modified March 2023