# Charles Margossian

### Education

2017–2022 Ph.D. Statistics, Columbia University, New York, NY.

Advisor: Andrew Gelman

Dissertation Committee: Aki Vehtari, Matthew Hoffman, Sumit Mukherjee, David Blei Thesis: Modernizing Markov chains Monte Carlo for scientific and Bayesian modeling

2011–2015 **B.Sci. Physics**, Yale University, New Haven, CT.

2009–2011 **Baccalauréat Scientifique**, Ecole Jeannine Manuel (High school), Paris, France, Mention très bien.

### Research Interest

I work on the development of statistical methods for problems that integrate scientific and probabilistic modeling. My primary focus is on Bayesian inference, in particular Markov chains Monte Carlo algorithms and approximate Bayesian computation. My work has been applied to various fields, most recently Pharmacometrics and Epidemiology.

# Experience

2022—present **Research Fellow**, Flatiron Institute, Center for Computational Mathematics, Simons Foundation, New York, NY.

Summer Research Intern, Google Research, Bayesflow and TensorFlow Probability team,

2021 New York, NY.

Summer Visiting Doctoral Student, Aalto University, Department of Computer Science,

2019 Probabilistic Machine Learning group, Espoo, Finland.

2016–2017 Visiting Scientist, Metrum Research Group LLC, Cambridge, MA.

2015–2016 Pharmacometrics Bootcamp, Metrum Research Group LLC, Tariffville, CT.

2013–2015 Researcher, Yale Department of Astronomy, New Haven, CT.

Summer Patent Law, Technical Specialist, Leinweber und Zimmermann, Munich,

2014 Germany.

#### Skills

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

### **Preprints**

- [1] **Charles C Margossian** and Michael Betancourt. Efficient Automatic Differentiation of Implicit Functions. *Preprint. arXiv:2112.14217.*, March 2022.
- [2] **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.
- [3] Charles C Margossian, Matthew D Hoffman, and Pavel Sountsov. Nested  $\hat{R}$ : assessing convergence for Markov chains Monte Carlo when using many short chains. *Preprint.* arXiv:2110.13017., October 2021.
- [4] Philip Greengard, Jeremy Hoskins, **Charles C Margossian**, Andrew Gelman, and Aki Vehtari. Fast methods for posterior inference of two-group normal-normal models. *Preprint.* arXiv:2110.03055., October 2021.
- [5] 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.
- [6] 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.

### Publications

- [1] **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*, page (to appear), April 2022.
- [2] 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.
- [3] 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.
- [4] 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.
- [5] Charles C Margossian. A Review of automatic differentiation and its efficient implementation. Wiley interdisciplinary reviews: data mining and knowledge discovery, 9, March 2019.
- [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

- [1] 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.
- [2] 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.
- [3] 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.
- [4] Charles C Margossian, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Approximate Bayesian inference for latent Gaussian models in Stan. In StanCon 2020, August 2020.
- [5] **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.
- [6] Charles C Margossian. Computing Steady States with Stan's Nonlinear Algebraic Solver. In StanCon 2018, January 2018.
- [7] 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.
- [8] Charles C Margossian and William R Gillespie. Differential Equation Based Models in Stan. In StanCon 2017, January 2017.
- [9] 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

- 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".

### Academic service

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).

2019 - 2020 Student representative, PhD program in statistics at Columbia University.

# Supervised research projects

- 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

### Teaching experience (selected)

- 2019, 2020, Lecturer, Probability and Bayes, lecture for PHC 506: Biometry in Pharmaceutics,
  - 2021 University of Buffalo, School of Pharmacy, Buffalo, NY.
- 2019, 2020, Instructor, Building, fitting, and criticizing Bayesian PK/PD models, (one day 2021 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.
- Spring 2021 **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, 2017 Cambridge, MA.
- June 2017 **Teacher Assistant**, Getting Started with Bayesian PKPD Modeling using Stan and Torsten, Population Approach Group in Europe 26, Budapest, Hungary.

#### Presentations

- October 2021 Nested  $\hat{R}$ : Assessing convergence for Markov chains Monte Carlo when running many short chains, Bayesian Computation Journal Club, Flatiron Institute Simons Foundation, New York, NY.
  - 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, Amer-2020 ican Conference 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, 2016 Harvard University, Cambridge, MA.
  - February Practice (and malpractices!) of Bayesian analysis, Metrum Journal Minute, 2016 Tariffville, 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 May 2022