

# Charles C. Margossian

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## Education

- 2017–2022 **Ph.D. Statistics**, *Columbia University*, New York, NY.  
◦ Thesis: *Modernizing Markov chains Monte Carlo for scientific and Bayesian modeling*  
◦ Advisor: Andrew Gelman  
◦ 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, Mention *très bien*.

## Research Interest

Markov chains Monte Carlo; Bayesian modeling; Bayesian workflow; Hierarchical models; ODE-based models; Approximate Bayesian computation; Integrated Laplace approximations; Automatic differentiation; Probabilistic programming; Pharmacometrics; Epidemiology; Statistical Physics.

## Experience

- 2022–present **Research Fellow**, *Flatiron Institute, Center for Computational Mathematics*, Simons Foundation, New York, NY.
- Summer 2021 **Research Intern**, *Google Research*, Bayesflow and TensorFlow Probability team, New York, NY.
- Summer 2019 **Visiting Doctoral Student**, *Aalto University, Department of Computer Science*, 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 2014 **Patent Law, Technical Specialist**, *Leinweber und Zimmermann*, Munich, Germany.

## Skills

**Programming:** R, Python, C++, Stan, TensorFlow Probability, L<sup>A</sup>T<sub>E</sub>X, GitHub  
**Languages:** English, French, German

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## Preprints

- [1] **Charles C Margossian**, Matthew D Hoffman, Pavel Sountsov, Lionel Riou-Durand, Aki Vehtari, and Andrew Gelman. Nested  $\hat{R}$ : Assessing the convergence of Markov chains Monte Carlo when running many short chains. *Preprint. arXiv:2110.13017.*, September 2022.
- [2] Lionel Riou-Durand, Pavel Sountsov, Jure Vogrinc, **Charles C Margossian**, and Sam Power. Adaptive Tuning for Metropolis Adjusted Langevin Trajectories. *Preprint. arXiv:2210.12200*, October 2022.
- [3] **Charles C Margossian** and Michael Betancourt. Efficient Automatic Differentiation of Implicit Functions. *Preprint. arXiv:2112.14217.*, March 2022.
- [4] **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.
- [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.

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## Publications

\*: Supervised student

- [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*, 11:1151 – 1169, April 2022.
- [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*, page (to appear), August 2022.
- [3] 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.
- [4] **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.

- [5] 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.
- [6] **Charles C Margossian**. A Review of automatic differentiation and its efficient implementation. *Wiley interdisciplinary reviews: data mining and knowledge discovery*, 9, March 2019.
- [7] 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.

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## 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 (Accepted; to appear)*, March 2023.
- [2] **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.
- [3] Aurélien Marc, Marion Keroui, **Charles Margossian**, Julie Bertrand, Pauline Maisonnasse, Yoan Aldon, Rogier W Sanders, Marit Van Gils, Roger Le Grand, and Jérémie Guedj. Developing a model of SARS-CoV-2 viral dynamics under monoclonal antibody treatment. In *Population Approach Group in Europe (PAGE) 29*, September 2021.
- [4] 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.
- [5] **Charles C Margossian**, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Approximate Bayesian inference for latent Gaussian models in Stan. In *StanCon 2020*, August 2020.
- [6] **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.
- [7] **Charles C Margossian**. Computing Steady States with Stan’s Nonlinear Algebraic Solver. In *StanCon 2018*, January 2018.
- [8] **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.

- [9] **Charles C Margossian** and William R Gillespie. Differential Equation Based Models in Stan. In *StanCon 2017*, January 2017.
- [10] **Charles C Margossian** and William R Gillespie. Stan Functions for Pharmacometrics Modeling. *Journal of Pharmacokinetics and Pharmacodynamics*, 43, October 2016.

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## Software

**Core developer**, *Stan: a probabilistic programming language*, [mc-stan.org](https://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](#).

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## 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”.

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## 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.

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## 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*

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## Teaching experience (selected)

- 2019 – 2022 **Lecturer**, *Probability and Bayes, lecture for PHC 506: Biometry in Pharmaceuticals*, University of Buffalo, School of Pharmacy, Buffalo, NY.
- 2019 – 2022 **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 2017 **Teacher Assistant**, *Stan for Physics*, Massachusetts Institute of Technology, Cambridge, MA.
- June 2017 **Teacher Assistant**, *Getting Started with Bayesian PKPD Modeling using Stan and Torsten*, Population Approach Group in Europe 26, Budapest, Hungary.

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## 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 2020 **Developing a Bayesian modeling workflow for population PBPK**, American Conference on Pharmacometrics, 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 2016 **Differential equations based models in Stan**, *Stan Meetup in Boston*, Harvard University, Cambridge, MA.
- February 2016 **Practice (and malpractices!) of Bayesian analysis**, *Metrum Journal Minute*, 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 October 2022*