Charles C. Margossian

cmargossian@flatironinstitute.org • charlesm93.github.io • New York, NY

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.

Appointments

2022– **Postdoctoral Research Fellow**, *Flatiron Institute*, Center for Computational Mathematics, New York, NY.

Sum. 2021 **Research Intern**, *Google Research*, Bayesflow team, New York, NY.

Sum. 2019 **Visiting Doctoral Student**, *Aalto University*, Department of Computer Science, Espoo, Finland.

2015–2017 **Visiting Scientist**, *Metrum Research Group*, Tariffville, CT and Cambridge, MA.

2013–2015 **Research Assistant**, *Yale University*, Department of Astronomy, New Haven, CT.

Sum. 2014 **Patent Law Intern**, *Leinweber & Zimmermann*, Munich, Germany.

Academic service

Reviewer, *PeerJ, Journal of Machine Learning Research (2023 (2)), Journal of Pharmacokinetics and Pharmacodynamics (2023, 2019), Computational Statistics (2022), Nature Geoscience (2021), Artificial Intelligence and Statistics (2023, Top Reviewer 2021), Methods in ecology (2021), Journal of data science (2021), Neural Information Processing Systems (2020).*

2016– **Core developer**, *Stan: a probabilistic programming language*, mc-stan.org.

2022– **Elected Member**, *Stan Governing Body*, 2 year term.

Skills

Progamming: Python, R, C++, Stan, LaTeX, GitHub
Languages: English, French, German

Google Scholar: https://scholar.google.com/citations?user=nPtLsvIAAAAJ&hl=en

Preprints

[1] Charles C Margossian, Loucas Pillaud-Vivien, and Lawrence K Saul. An Ordering of Divergences for Variational Inference with Factorized Gaussian Approximations. *arxiv:2403.13748*, 2024.

[2] 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. *arXiv:2110.13017*, 2024.

[3] David Heurtel-Depeiges, Charles C Margossian, Ruben Ohana, and Bruno Régaldo-Saint Blancard. Listening to the noise: Blind Denoising with Gibbs Diffusion. *arXiv:2402.19455*, 2024.

[4] Diana Cai, Chirag Modi, Loucas Pillaud-Vivien, Charles C Margossian, Robert M Gower, David M Blei, and Lawrence K Saul. Batch and match: black-box variational inference with a score-based divergence. *arXiv:2402.14758*, 2024.

[5] Charles C Margossian. General adjoint-differentiated Laplace approximation. *arXiv:2306.14976*, 2023.

[6] Charles C Margossian and Michael Betancourt. Efficient Automatic Differentiation of Implicit Functions. *arXiv:2112.14217*, 2022.

[7] Charles C Margossian and Sumit Mukherjee. Simulating Ising and Potts models at critical and cold temperatures using auxiliary Gaussian variables. *arXiv:2110.10801*, 2021.

[8] 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. *arXiv:2011.01808*, 2020.

[9] Michael Betancourt, Charles C Margossian, and Vianey Leos-Barajas. The Discrete Adjoint Method: Efficient Derivatives for Functions of Discrete Sequences. *arXiv:2002.00326*, 2020.

Publications

*: Supervised student

[1] Charles C Margossian and Andrew Gelman. For how many iterations should we run Markov chain Monte Carlo? In *Handbook of Markov chain Monte Carlo*. Chapman & Hall/CRC, (upcoming) 2nd edition, 2024.

[2] Charles C Margossian and David M Blei. Amortized Variational Inference: When and Why? *Uncertainty in Artificial Intelligence*, PMLR (accepted), 2024.

[3] Charles C Margossian and Lawrence K Saul. The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference. *Selected for Oral Presentation, Uncertainty in Artificial Intelligence*, PMLR 216:1358–1367, 2023.

[4] Lionel Riou-Durand, Pavel Sountsov, Jure Vogrinc, Charles C Margossian, and Sam Power. Adaptive Tuning for Metropolis Adjusted Langevin Trajectories. *Artificial Intelligence and Statistics*, PMLR 206:8102–8116, 2023.

[5] Chirag Modi, Charles C Margossian, Yuling Yao, Robert Gower, David Blei, and Lawrence Saul. Variational Inference with Gaussian Score Matching. *Advances in Neural Information Processing Systems*, 37, 2023.

[6] 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(9):1151–1169, 2022.

[7] 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*, 18(3):889–907, 2022.

[8] Léo Grinsztajn*, Elizaveta Semenova, Charles C Margossian, and Julien Riou. Bayesian workflow for disease transmission modeling in Stan. *Statistics in Medicine*, 40(27):6209–6234, 2021.

[9] 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*, 34, 2020.

[10] 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(7), 2020.

[11] Charles C Margossian. A Review of automatic differentiation and its efficient implementation. *Awarded "Top WIRES articles in 2022", WIRES: Data Mining and Knowledge Discovery*, 9(4), 2019.

[12] 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), 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. *BayesComp*, 2023.

[2] Stanislas du Ché* and Charles C Margossian. Parallelization for Markov chains Monte Carlo with heterogeneous runtimes. *BayesComp*, 2023.

[3] Charles C Margossian, Lu Zhang, Sebastian Weber, and Andrew Gelman. Solving ODEs in a Bayesian context: challenges and opportunities. *Population Approach Group in Europe*, 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. *Population Approach Group in Europe*, 2021.

[5] Johann D Gaebler* and Charles C Margossian. Propagating Derivatives through Implicit Functions in Reverse Mode Autodiff. *Stanford Institute for Computational & Mathematical Engineering*, 2021.

[6] Charles C Margossian, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Approximate Bayesian inference for latent Gaussian models in Stan. *StanCon*, 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, 2020.

[8] Charles C Margossian. Computing Steady States with Stan's Nonlinear Algebraic Solver. *StanCon*, 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. *American Conference on Pharmacometrics*, 2017.

[10] Charles C Margossian and William R Gillespie. Differential Equation Based Models in Stan. *StanCon*, 2017.

[11] Charles C Margossian and William R Gillespie. Stan Functions for Pharmacometrics Modeling. *American Conference on Pharmacometrics*, 2016.

Software

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

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

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

Contributor, *bayesplot: Plotting for Bayesian Models in R*, Cran.

Awards and recognitions

2023 **UAI Oral presentation**, For *The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference*, top ∼15% articles accepted at the conference on Uncertainty in Artificial Intelligence.

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 students

2023 **Manny Mokel (undergraduate student)**, *Nested $\widehat{R}$: pooled sampling and variance approximation*, Flatiron Institute, New York, NY.

2022 **Stanislas Du Ché (master student)**, *Parallelization for Markov chain Monte Carlo with heterogeneous runtimes*, Columbia University, New York, NY.

2020 **Johann Gaebker (PhD student)**, *Propagating Derivatives through implicit functions in reverse mode automatic differentiation*, Columbia University, New York, NY.

2020 **Léo Grinsztajn (master student)**, *Bayesian Workflow for disease transmission models*, Columbia University, New York, NY.

2020 **Hyunjee Moon (undergraduate student)**, *Simulation-based Calibration for the embedded Laplace approximation*, Columbia University, New York, NY.

Teaching

2023 **Instructor**, *Bayesian Workflow for hierarchical and ODE-based models*, Three day workshop, Summer School on Advanced Bayesian Methods, Leuven, Belgium.

2023 **Instructor**, *Fundamentals of Stan*, Half-day workshop, StanCon 2023, Washington University in St Louis, St Louis, MO.

2019–2023 **Instructor**, *Building, fitting, and criticizing Bayesian PK/PD models*, One day workshop, University of Buffalo, Buffalo, NY.

2019–2023 **Guest lecturer**, *Probability and Bayes*, Lecture for PHC 506: Biometry in Pharmaceutics, University of Buffalo, Buffalo, NY.

2019, 2020 **Instructor**, *Stan for the people: an introductory workshop to Bayesian modeling*, Two day workshop, McGill University, Montreal, Canada.

2019 **Instructor**, *Population and ODE-based models using Stan and Torsten*, Two day workshop, StanCon 2019, Cambridge University, Cambridge, UK.

2017 **Guest Lecturer**, *Introduction to Bayesian Data Analysis with Stan*, Lecture for STAT 2020: Bayesian Statistics, Harvard University, Cambridge, MA.

2017–2022 **Teaching Assistant**, *Recipient of the Minghui Yu Teaching Assistant Award*, Courses at all levels (undergrad, masters and PhD), Columbia University, New York, NY.

2013–2015 **Peer Tutor**, *Science, Technology, and Research Scholars (STARS) program*, Yale University, New Haven, CT.

Presentations (selected)

2023 **The Wisdom of Automatic Differentiation**, *Applied and Computational Math Group Meeting*, Courant Institute, New York University, New York, NY.

2023 **The Shrinkage-Delinkage Trade-off: An Analysis of Factorized Gaussian Approximations for Variational Inference**, Conference on Uncertainty in Artificial Intelligence, Pittsburgh, PA.

2023 **Amortized Variational Inference: when and why?**, Flatiron-wide Meeting on Machine Learning, Flatiron Institute, New York, NY.

2022 **Solving ODEs in a Bayesian model**, Flatiron-Wide Algorithms and Mathematics ($F_\omega(\alpha + m)$!), Flatiron Institute, New York, NY.

2022 **Nested $\hat{R}$: Assessing convergence for Markov chains Monte Carlo when running many short chains**, Center for Research in Economics and Statistics (CREST), École Polytechnique, Paris, France.

2021 **Bayesian inference for latent Gaussian models: MCMC, approximate methods, and hybrids**, Minghui Yu memorial conference, Columbia University, New York, NY.

2020 **Developing a Bayesian modeling workflow for population PBPK**, American Conference on Pharmacomertrics.

2020 **Approximate Bayesian inference for latent Gaussian models in Stan**, StanCon.

2020 **Developing a Bayesian workflow to model the Covid-19 outbreak**, 12th Covid-19 symposium, Columbia University, New York, NY.

2018 **Computing steady states with Stan's nonlinear algebraic solver**, *StanCon*, Pacific Grove, CA.

2017 **Differential equations based models in Stan**, *StanCon*, Columbia University, New York, NY.

November 2016 **Differential equations based models in Stan**, *Stan Meetup in Boston*, Harvard University, Cambridge, MA.

2016 **Practice (and malpractices!) of Bayesian analysis**, *Metrum Journal Minute*, Tariffville, CT.

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 April 2024