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

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

Appointments

2022– **Research Fellow**, *Flatiron Institute*, Center for Computational Mathematics, New York, NY.
- Independent research in computational mathematics, 3 years funding
- Computational Statistics and Machine Learning groups

Sum. 2021 **Research Intern**, *Google Research*, New York, NY.
- TensorFlow Probability team
- Hosts: Matt Hoffman and Pavel Sountsov

Sum. 2019 **Visiting Doctoral Student**, *Aalto University*, Department of Computer Science, Espoo, Finland.
- Probabilistic machine learning group
- Advisor: Aki Vehtari

2015–2017 **Visiting Scientist**, *Metrum Research Group*, Tariffville, CT and Cambridge, MA.
- 2015–2016: Phamacometrics bootcamp

2013–2015 **Research Assist.**, *Yale University*, Department of Astronomy, New Haven, CT.
- Exoplanet group

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

Open-source software

2015– **Stan: a probabilistic programming language**, *mc-stan.org* .
- 2024 **Organizer**, StanCon 2024, Oxford, UK
- 2023 **Organizer**, StanCon 2023, St Louis, MO
- 2022– **Elected member**, Stan Governing Body (two year term)
- 2016– **`C++` core developer**, `Stan-Math` automatic differentiation library
- 2015– **Co-creator**, Torsten: an extension of Stan for pharmacometrics modeling

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

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

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

[6] 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.

[7] 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] David Heurtel-Depeiges, Charles C Margossian, Ruben Ohana, and Bruno Régaldo-Saint Blancard. Listening to the noise: Blind Denoising with Gibbs Diffusion. *International Conference on Machine Learning*, PMLR (accepted), 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. *International Conference on Machine Learning*, PMLR (accepted), 2024.

[5] 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.

[6] 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.

[7] 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.

[8] 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.

[9] 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.

[10] 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.

[11] 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.

[12] 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.

[13] 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.

[14] 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".

Academic services

2020– **Reviewer**.

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

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

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.

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 **Developing a Bayesian workflow to model the Covid-19 outbreak**, 12^{th} 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.

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 May 2024